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

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Lecture – 38
Computer Software for Fluid Inclusion Data (Contd.)

Welcome to today's lecture. We will continue our discussion on the Software for Fluid Inclusion Data and we already saw and also demonstrated one of the one type of software, that was were shown to you just as an example that what logic could possibly be applied in developing is computer software which will cater to the need of the fluid inclusionist who generates data on all types of inclusions that he is observed in the samples.

And we know the know all the possible types of inclusions, and the input parameters, the possible input parameters as of now a state of the art, that what are the input parameters, micro thermometry parameters that acquired and these data need to be put in one package and could be processed so that, it will cater to the need of the fluid inclusionist in terms of the presentation of the data.

The calculation of the volumetric property like density, isochore and plotting of the data in the form of histograms for the input data like a temperature of homogenization, the calculated parameter like salinity and density and also can plot the isochore on A P T space, and also the isochore if there are pairs of coeval inclusions of different compositions, their intersection of the isochors by using the equation of state which is available.

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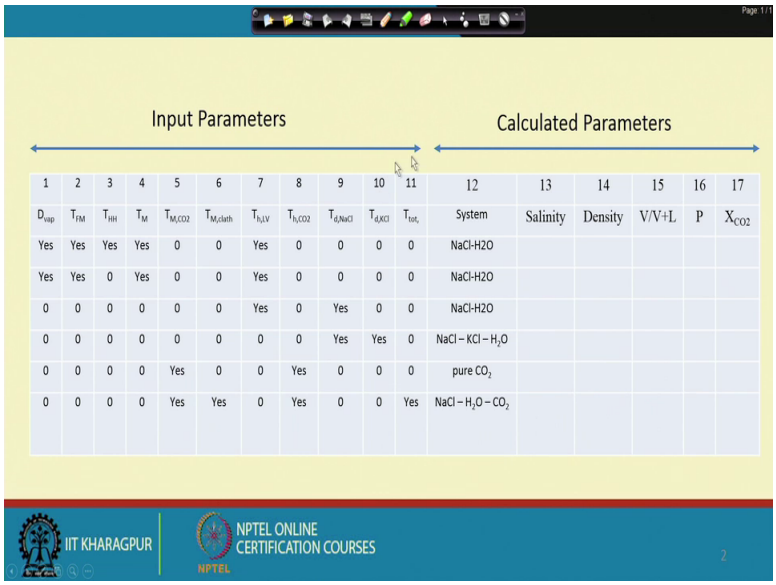

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
D_{vap}	T_{FM}	T_{HH}	T_M	$T_{M,CO2}$	$T_{M,clath}$	$T_{h,LV}$	$T_{h,CO2}$	$T_{d,NaCl}$	$T_{d,KCl}$	$T_{tot,}$	System	Salinity	Density	V/V+L	P	X_{CO2}
Yes	Yes	Yes	Yes	0	0	Yes	0	0	0	0	NaCl-H2O					
Yes	Yes	0	Yes	0	0	Yes	0	0	0	0	NaCl-H2O					
0	0	0	0	0	0	Yes	0	Yes	0	0	NaCl-H2O					
0	0	0	0	0	0	0	0	Yes	Yes	0	NaCl – KCl – H_2O					
0	0	0	0	Yes	0	0	Yes	0	0	0	pure CO_2					
0	0	0	0	Yes	Yes	0	Yes	0	0	Yes	NaCl – H_2O – CO_2					

And in that process, we just I will just like to recapitulate here that the logic which was actually applied here, and this is just given for an example and it could be further developed. For example, see here the this table in this table there are some 11 parameters which are shown, which are the possible input parameters like the vapor bubble diameter at room temperature, the temperature of first melting; that means, referring to the eutectic temperature in a binary or a ternary as the case may be.

The temperature hydro halite melting as it is often observable in a ternary system like NaCl CaCl H 2 O where the hydro halite melting is significant and from which ratio of sodium is to calcium can be found out; and the temperature of melting of ice. So, this parameter and then, for a carbonic pure carbonic inclusion the temperature of melting of carbon dioxide, if it is an aqueous carbonic inclusion, the temperature melting of glass weight, and then the temperature of liquid vapor homogenization for the aqueous inclusion, the temperature of homogenization of the carbonic inclusion, temperature of dissolution of daughter crystal like sodium chloride, daughter crystal of potassium chloride and in case of an aqueous carbonic inclusion, the temperature of total homogenization.

Now, we could see here what has been a missed in on this particular table, sometimes or it is mandatory to have the mode of homogenization of a pure carbonic inclusion whether it is to liquid of vapor, which will be deciding factor and calculation of the density and

the parameters to be used which was given to you in the previous discussion. And also, it also apply to a liquid homogenization in case of aqueous biphase inclusions, there also the mode of homogenization of vapor or liquid need to be specified.

So, this is just an example to show that how this logic could work and I just said that the user the fluid inclusionist did not have to know or did not have to furnish the word system, the inclusion fluid should belong to and also the what equation of state that is to be chosen and the fluid inclusion is still not be asked for any other parameter then, what is actually coming from the micro thermometric experiments.

For example, any visual estimation of volume or molality or any other kind of parameters are not going to be used as any input parameter for calculation of the volumetric property.

Is an example, as has been given here suppose the field under the vapor bubble diameter is enter, the temperature of first melting is also furnished temperature of hydro halite temperature of melting of ice and the temperature of liquid vapor homogenization also is given. So, by virtue of the input parameter has been given in this four, five fields, if the system automatically decides that it has to be an NaCl H 2 O system because we know that whatever may be the composition of the brain in terms of presence of any other cat ionic species, the salinity will be expressed in terms of NaCl weight percent equivalent and the volumetric property will be calculated based on whatever equation of states are available in the NaCl, H 2 O system.

So, here the thing is that there could possibly a lot of equations of state that might have been proposed in literature over a period of time. And the one which will possibly having the maximum range of applicability in terms of temperature and salinity and also would have been based on a much larger set of data that equation of state, which would be applicable and is possibly the one, which will be have the best applicability, so that will be automatically that equation of state parameters will be used to calculate the volumetric property of the fluid inclusion. This is to say that this is pretty dynamic.

So, if there are constant work is going on for refinement of the P P T, it is relationships in such kind of fluid mixtures and whenever there is a proposition of an equation of state which is more which is more accurate or better or better reproduces the experimental data or are based on more stronger few radical background like as I discus the for a

aqueous electrolyte, if the volumetric property could be retreat from basic thermodynamic relationships and then, the formulations could possibly we tried and then if the experimental observations are very accurately reproduced, then that could possibly furnish that could be possibly the available as the best or most applicable or most in a most applicable this equation of state to be used.

Similarly, if someone if the field in the vapor diameter vapor bubble and the temperature of first melting temperature of melting of last ice and depending on whether the temperature of hydro halite is available or not, still it is be NaCl H 2 O system and then there is a situation in which the temperature of liquid vapor homogenization value is given and just the temperature of the dissolution of the sodium chloride daughter crystal is given. So, that also is automatically belonging to the NaCl H 2 O system. And just for example, it is also given that if the data a for dissolution of sodium chloride and the dissolution of potassium chloride both are entered, then it automatically goes to the NaCl KCl H 2 O system.

You could possibly recall that in such kind of inclusions, we did not have to do any freezing study to see there any melting of ice or melting of any of the hydrated salt. It is a the salinity and density are all determined from the dissolution of the daughter crystal the two or three cases, where the T D could be less than T H liquid vapor homogenization or the T D is more than the liquid vapor homogenization that only decides the but then, the system remains the same for example, if it is only T D NaCl and T H L V and in this case also the T H L V has to be given.

So, if it is temperature of dissolution of Na Cl and K C L then from this standard phase relations that were shown, so it automatically goes to the Na Cl K Cl at water system. And then, it if the if we have a equation of state available where as I have said that there could be possibly more number of such input parameters; for example, like if we have an equation of state available where the sodium by other cationic species.

For example sodium by potassium or sodium by calcium or for that matter any other ratio which is determined from either this phase relations in the freezing point freezing studies or available from micro analytical data, they could also be entered in as input parameter.

And then, in any case the system automatically is decided as to what a system it could belong to and the best available equation of state will be used for calculation of the volumetric property. And for example, you have a pure carbonic inclusion where temperature melting of carbon dioxide and the temperature of homogenization the carbon dioxide with some more is specified, then it goes to pure carbonic system.

And then, if a temperature of melting of carbon dioxide, temperature of melting of the clathrate, temperature of partial homogenization of the carbonic phase and the temperature of total homogenization of the inclusion, then it goes to the NaCl H 2 O C O 2 system and so, these are this is just as an example, any person any enthusiast who writes or a develops his own program, writes his own code can always come up with some logic in this particular line or could better logic for a used or writing of a code to do the work or to analyze the data that is generated by micro thermometric experiments.

So, now here these columns like this column from 12 to 17 or it could to go to any other value are the calculator parameter. So, once this values are entered in the respective fields, the and the calculations is carried out by clicking up the mouse or appropriate button, then the column number 12 to 17 are automatically filled up depending on what system it belongs to. The system, the salinity if it happens to be a aqueous inclusion or the aqueous component of the aqueous carbonic fluid the density total density of the inclusion at temperature of homogenization, the vapor plus liquid ratio if someone think that it is an important parameter.

It can be included or not depending on what exactly V 1. In case of the aqueous carbonic inclusion where we can estimate the minimum pressure of entrapment that also we can calculate and the mole fraction of C O 2 as we saw from diagrams phase diagrams in the NaCl H 2 O CO 2 system.

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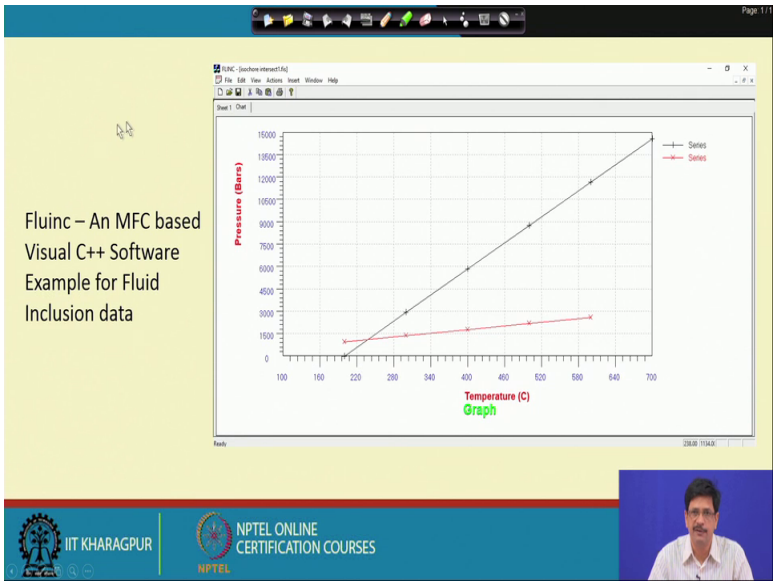

So, this software packages like the one which was discussed before. So these are essentially and as we know that whatever code we are writing and with a because this is a very fast growing and very very fast going field, so the programming languages in the features available to us to write the software package, to develop a package it all depends on what is available at that particular point of time.

So, this is a, so the example that I am showing here as it is given from the you could see here that the program is isolate as a generated 2 isochors; this isochore is of an aqueous biphase inclusion and this isochore is a pure carbonic inclusion, and there the coexisting two inclusions when their isochors are constructed and we could see an intersection of the two and also the intersection value the pressure temperature value corresponding to the intersection is also displayed on this particular screen.

So, this is essentially a package which was developed on visual C plus plus I mean, the visual C plus plus program a language, and was compiled and executed on visual platform. And previously like the packages of Fluinc curve that we are discussing, they were when they were developed they need a lot more of efforts to develop such kind of graphical user interface when there is when this object oriented programming was not there.

So, with the advent of the object oriented programming language and the development of this Microsoft foundation class libraries, then the development of graphical user interface

packages become very easy and handy, and one could with the available wizards, one could always design his one software package in the graphical environment whether it is to the single window or a multiple window, the editable box is the static fields, the editable box says the menu, the dropdowns and all these are very simple looking features, but based on the extensively available libraries of the Microsoft foundation class.

So, this is one example. So, as I just said that we need to cater to the need of a fluid inclusionist. In present, giving all sorts of types of output that is required; here is an example that isochore and the isochore intersection is a plotted and such kind of features should also or such kind of software packages if it has the utility that if I have more than one such pairs of coexisting or coeval inclusions, all the data could be plotted on one single graph and that is also been implemented.

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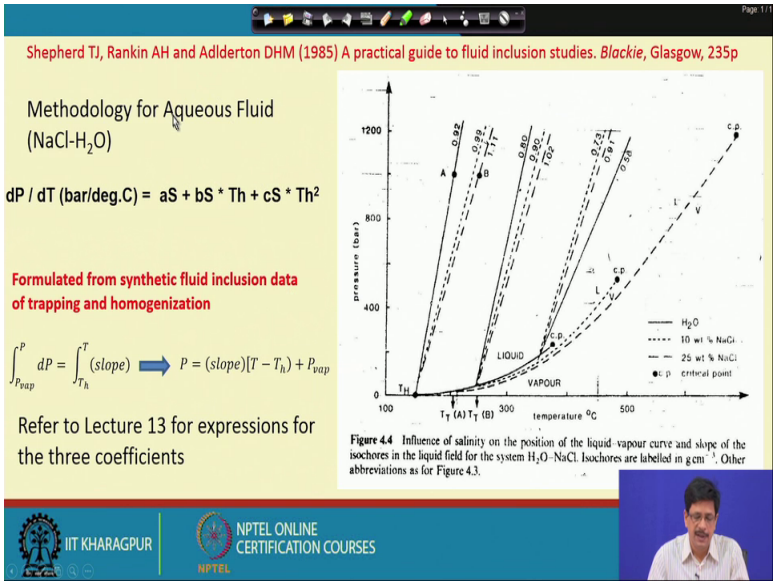

Figure 4.4 Influence of salinity on the position of the liquid–vapour curve and slope of the isochores in the liquid field for the system H_2O–NaCl. Isochores are labelled in g cm^{-3}. Other abbreviations as for Figure 4.3.

Well, just to give you an idea that what exactly, so, anyway, so we are writing this or this anyone can write a program on a graphical user interface mode and can implement the equation of states available in different fluid system, and then can generate such kind of information some such kind of plots without any problem.

Now, the actually what I will just like to give a little bit of idea as to what exactly have been implemented in a software package, which I just was demonstrating. Before that, I would just like to point out one thing that in the all the previous discussions in the

lectures, there has been reference extensively given to all the references where actually on the research papers, that were published over the last more than four decade period, four decades of period.

And although all of them are taken from the work of different authors published during this period of time; and there are actually the, as far as fluid inclusions studies are concerned there is not much of text books available, but the one which is a very widely referred a text book and wide and the very popular text book, which is by Shepherd Rankin and Adlderton. The title of the book is practical guide to fluid inclusion studies and this book actually gives all sorts of practical tips along with the fundamentals, the principles of fluid inclusion studies and which is essentially referred to by any fluid any person who begin who is a beginner in fluid inclusion studies.

And so, here as I said that we will see that in case of aqueous fluid, aqueous biphase or aqueous polyphase, when it comes to an aqueous fluid, we need to determine the density. The density is calculated on the basis of temperature of homogenization and the salinity, the salinity been determined from the depression in freezing point or the temperature of dissolution of the daughter crystals.

So, once a salinity and density determined given the I could using the formulation, whichever again we think to be the most appropriate one basing on a large set of experimental data and through rigorous analysis like the one I showed before.

So, and then the isochore the disc curve from the slope of the isochore which is also the equation for which is given. Referring to just recapitulate, we saw this kind of an equation for the slope of the isochore where it is a function of the temperature of homogenization as a S plus b S into T h plus c S into T h square.

To you may please note that these kind of equations this were derived or formulated based on the synthetic fluid inclusion experiments, where the temperature and pressure of trapping is known and those inclusions temperature of homogenizations are also known.

So, essentially based on two points on A P T space, the line is drawn with the basic assumption that the fluid has followed a constant density isochore and from that these equations are formulated. And from that which we know that any pressure at any point of

any and anywhere on the P T space, we can calculate the pressure by integrating this equation as we showed as we did before.

Now, the purpose of showing this particular diagram here is that this is the, this is the taken from the book of Shepherd Rankin and Adlderton, you could see this is the figure in chapter 4 where the basic principles of micro thermometry has been explained and you could see that the here the solid lines represent the pure water and the dotted line, dash line are representing 10 and 25 weight percent NaCl.

As we know from these kind of equation, if we put the value of salinity, then this equation clearly tells us that keeping a temperature of homogenization is fixed, then the density or the slope of this isochore is going to increase with increasing NaCl content, but here we see which is absolute, which is exactly the opposite. For example, a 0.92 grams per c isochore has a steeper as a slow, then which is 0.99 of the 1 which is 1.11 which should have been the reverse case.

And also interestingly, on these three set of isochors if one which is having the most gentle slope 0.5, 0.58 which is corresponding to pure water and the one which is 0.91 has a steepest slow which is which in agreement to this particular equation has been shown and 0.73 again which is density is less is following is steeper isochore.

So, here it looks like is if the there has been some kind of a reversal. So, when we this exactly is not very clear as to how this isochors are constructed, but not actually going by which one will be more accurate, which one is not.

So, this kind of things if will always create a little bit of difference here but then, if we apply the available equation of the available formulation on the slope of the isochore and what we can calculate from here we could see from this particular table, let us say that these are different temperatures, this table has been generated by using the formulation which has been shown here for calculation of the slope.

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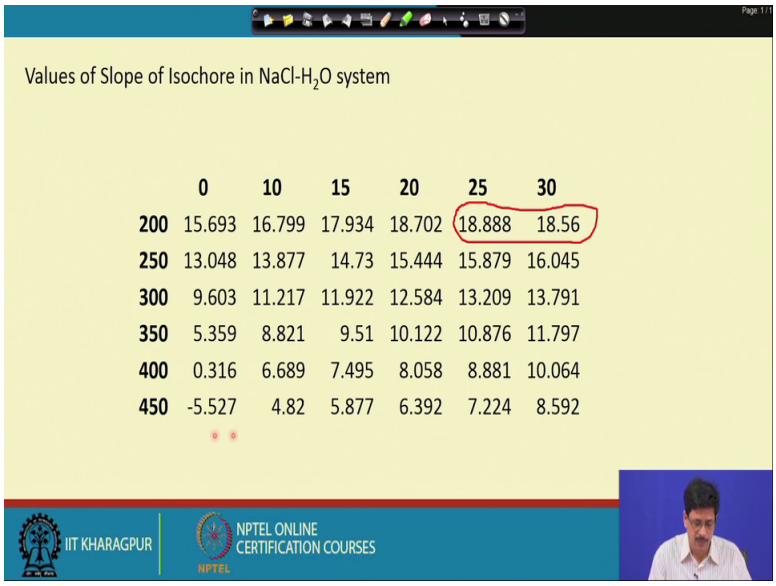

So, you take the temperature from 200 to 450 and NaCl content from 0 to 30 weight percent and we see is all the values with an increasing value; that means, as the a weight percent NaCl increases from any particular temperature, then the value of the slope of the isochore goes on increasing with a little bit of a deviation here decreasing from 18.88 to 18.5.

Otherwise, in entire value the set of value that is presented here, we could see that the value of the slope of the isochore is increasing and only situation is where it is a pure water the value corresponding to 450 is showing kind of an anomalous value.

And as the of a, so if this is the equations the proposer of this equations they say that the range of applicability would be the temperature up to 800 degree Celsius or the critical temperature whichever is lower and if it is a pure water, then the critical temperature is 374 degree Celsius and we see that it is a 400 calculation than at 450 degrees Celsius.

So, it is expected that this value could possibly would be not in agreement what the on basis of for the formulation have been made. So, this just for the reference, but then we definitely go by the formulations which are the later ones.

And a based on much larger data set and is widely been used with a much greater range in a salinity and temperature and, so tentatively, we can say that possibly there might

have been some problem in calculation of the isochors where the higher salinity fluid is being shown as an isochore it is slope which is less than that of a lower density one.

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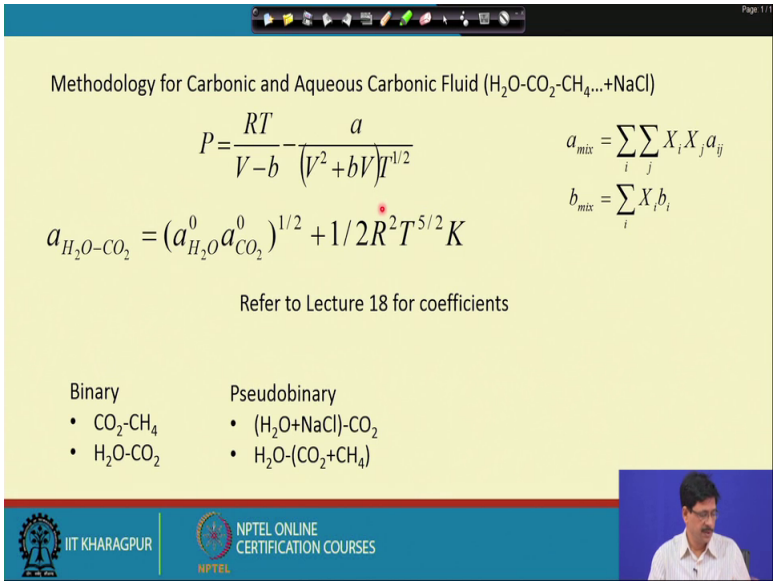

So quickly to just to see that what is the formulation that we are using for aqueous carbonic system and that is that is the situation in case of the aqueous fluid whether it is a water NaCl and because we are expressing the salinity as weight percent NaCl equivalent whether our fluid is water plus NaCl CaCl 2 water plus NaCl KCl.

And, the slope that you are calculating is still expressing it is weight percent NaCl equivalent and do you would wait for more refined formulation to come where the salt containing other electrolyte species there, the equation of better equations to be available for calculation of the slope of the isochors.

So, till that time we will be using this and anyone who is trying to present is data present the micro thermometric data has to use this type of equation what is available now. So, we will continue discussing on this topic from the in the next class.

Thank you.