

# Proper iso- $T_h$ curves in the $H_2O$ -NaCl system

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## Fluid System H<sub>2</sub>O–NaCl in Fluid Inclusions

what do we know?

what can we calculate?

what equations do we use?

what are the uncertainties?

do we still need to discuss about this?

do you need help?

# iso- $T_h$ lines

experimentally determined with synthetic fluid inclusions

*„lines of constant homogenization temperature are linear in temperature-pressure space and can be represented by the following:  $P = A_1 + A_2 \cdot T$ “*

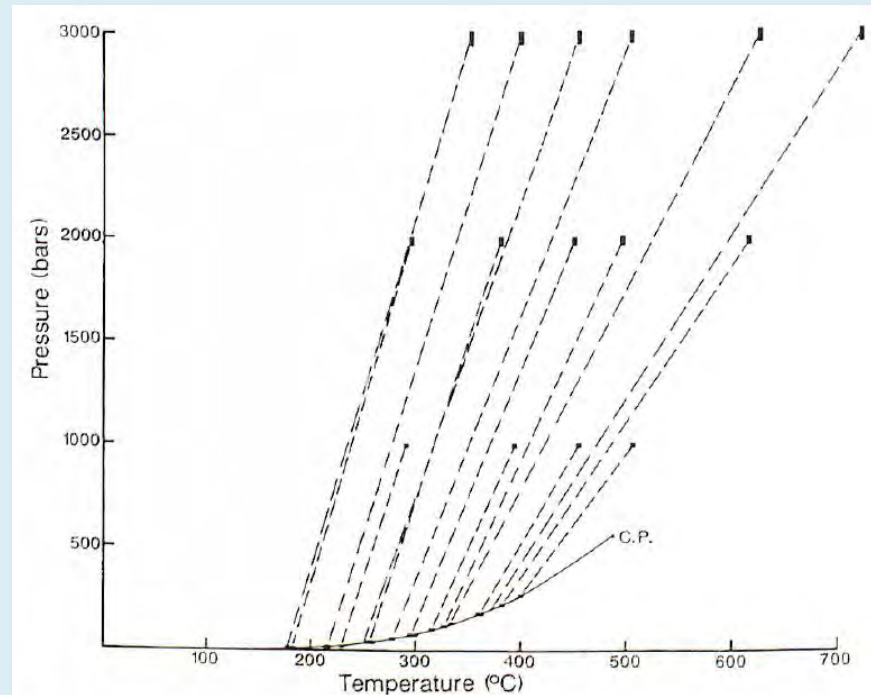
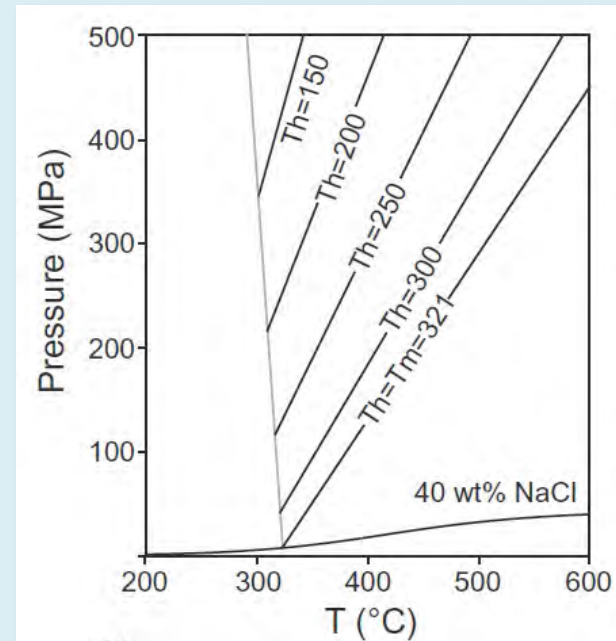
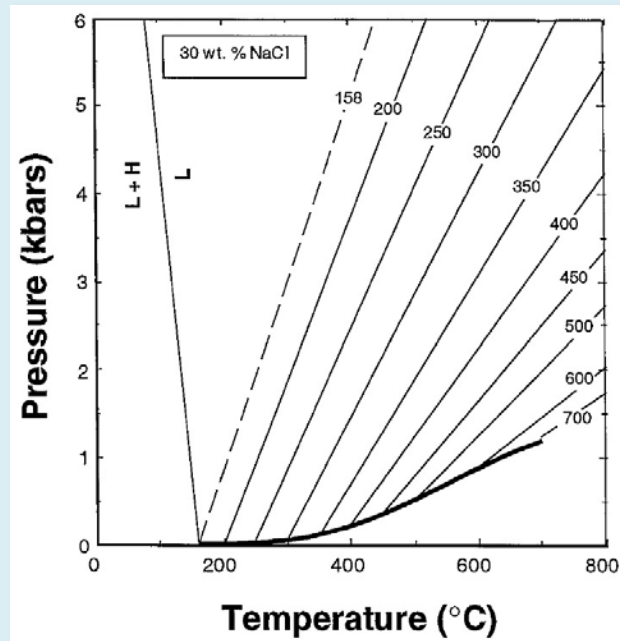


Fig. 3. Plot of temperature, pressure and homogenization temperature of experiments using a 2.0 molal NaCl-H<sub>2</sub>O solution. See text for details.

Zhang & Frantz (1987)

# iso- $T_h$ lines

$$P = A_1(w) + A_2(w) \cdot T$$



*Bodnar & Vityk (1994)*

*Bodnar (1995)*

*Lecumberry-Sanchez et al. (2012)*

*Steele-MacInnes et al. (2012)*

do they really look like this?

is this consistent with thermodynamic models?

synthetic fluid inclusions

p-T-V-x modelling

iso- $T_h$  lines

isochores

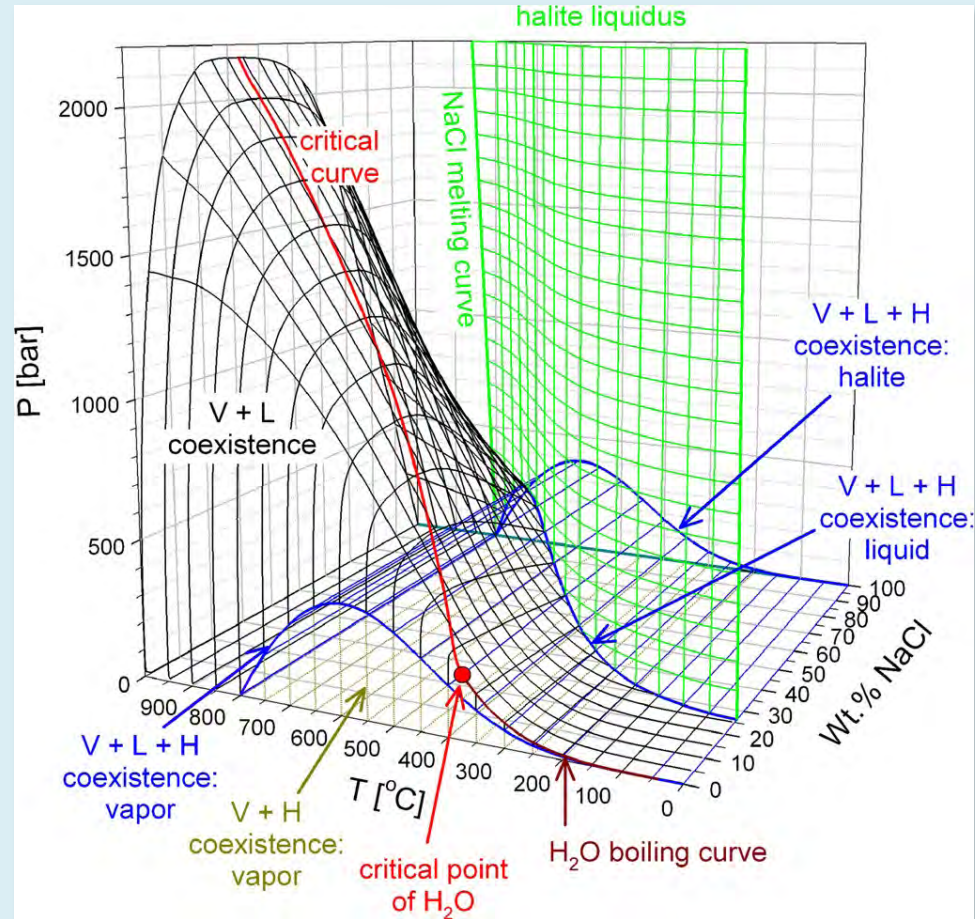


volumetric properties host crystal  
(quartz)

iso- $T_h$  lines

isochores

# p-T-V-x modelling

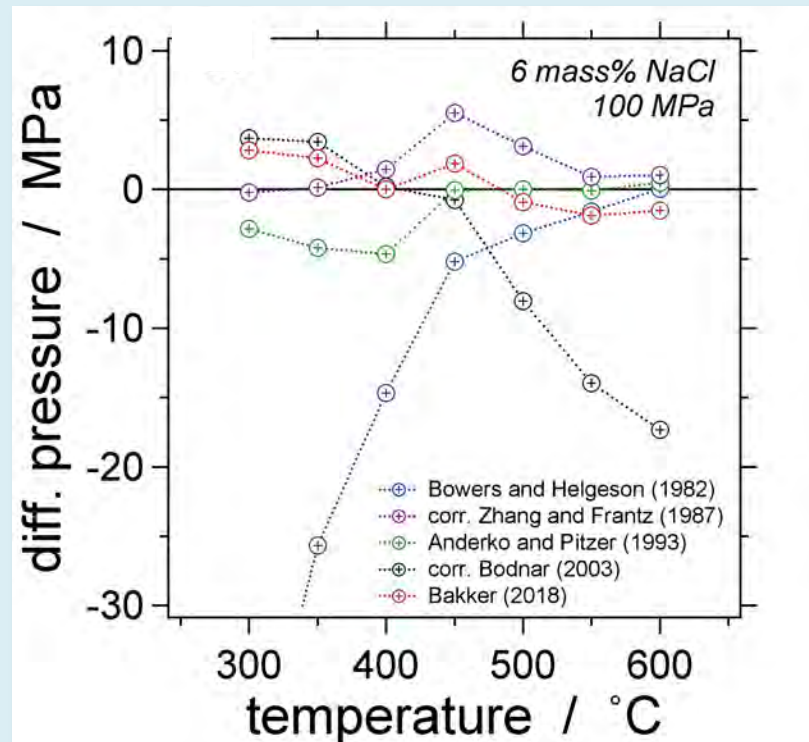


Driesner & Heinrich (2007)



example accuracy  
p-T-V-x data - model

*data Gehrig et al. (1983)*



p-T-V-x modelling

empirical modification of a  
unified Helmholtz energy  
function of pure H<sub>2</sub>O  
(Haar et al., 1984)



H<sub>2</sub>O-NaCl  
(Driesner & Heinrich, 2007)

Start

Fluid Inclusion Laboratory Leoben **FILL**

© R. J. Bakker, 2013  
modification 09/2017  
developed with XOJO Version 2017  
<http://fluids.unileoben.ac.at>

**AqSo-NaCl**  
Software Package Fluids, v.2  
Fluid system: H2O-NaCl

Ref.  
Bakker RJ (2018) AqSo\_NaCl: computer program to calculate p-T-V-x properties in the H2O-NaCl fluid system applied to fluid inclusion research and pore fluid modelling. Computers and Geosciences, vol. xx, p. xx-xx.

Pure H2O properties from thermodynamic model Haar et al. (1984). Purely empirical equations are added to calculate fluid properties p-V-T-x of binary H2O-NaCl mixtures (Driesner and Heinrich, 2007; Driesner 2007). Equations are adapted for fluid inclusion analyses in addition to general pore fluid research.

Composition: 0 - 1 x(NaCl)  
Temperature: 0 - 1000 °C  
Pressure: 0 - 500 MPa  
Extrapolation possibilities to higher T and P

[references](#)

Select calculation procedure

<input type="radio"/> pure NaCl	<input type="radio"/> Halite Vapourus (SV)
<input type="radio"/> Critical Curve H2O-NaCl	<input type="radio"/> Bubble-Point and Dew-Point (LV)
<input type="radio"/> SLV Curve above 0.1 °C	<input type="radio"/> Molar Volume
<input type="radio"/> SLV Curve below 0.1 °C	<input type="radio"/> Isochore
<input type="radio"/> Halite Liquidus (SL)	<input type="radio"/> Microthermometry and Vol.%

[continue](#)



# Software: AqSo-NaCl

Bakker (2018) Computers and Geosciences, vol. 115, 122-133

## module: Isochore

Isochore construction H<sub>2</sub>O-NaCl fluid mixture

clear all

x(NaCl)0.01w(NaCl)3.172925%

Molar Volume40cm<sup>3</sup>/molDensity0.460482g/cm<sup>3</sup>

Corresponding homogenization conditions

hom. cond. Homogenization on the bubble-point curve in the liquid phase

Temperature406.1494°Celsius

Pressure29.59592MPa

Molar Volume40cm<sup>3</sup>/mol

Temp. Unit

☐ Kelvin

☒ °Celsius

SLV intersection\* isochore intersect SLV curve (ice or HH) below 0.1 °C


Temperaturexxx°Celsius

PressurexxxMPa

Volume fraction liquidxxxvol.%

T4xxx°Celsius

\* high molar volume isochores (low density) may have multiple intersections with the SLV curve, and are partly located in the vapour+solid field

Phase changes in fluid inclusion: 

limits molar volume

bubble point at 1 °C18.04962cm<sup>3</sup>/mol

critical point40.54156cm<sup>3</sup>/mol

SLV (vapour)----cm<sup>3</sup>/mol

----cm<sup>3</sup>/mol

1.755839e cm<sup>3</sup>/mol

dew point at 1200 °C109.7201cm<sup>3</sup>/mol

4474.084cm<sup>3</sup>/mol

Homogenization conditions in vapour phase cannot be calculated between these two

Isochore correction

Expansivity and compressibility of quartz (Hosieni et al., 1984) can be included to correct the fluid density along an isochore

☒ No

☐ Yes, starting point hom. cond.

☐ Yes, starting point SLV inter.

Temperature limits of isochore

isochores can be constructed in both one-phase field (homogeneous) and two-phase field (heterogeneous) on either side of the homogenization temperature

lower temperature410°C

upper temperature610°C

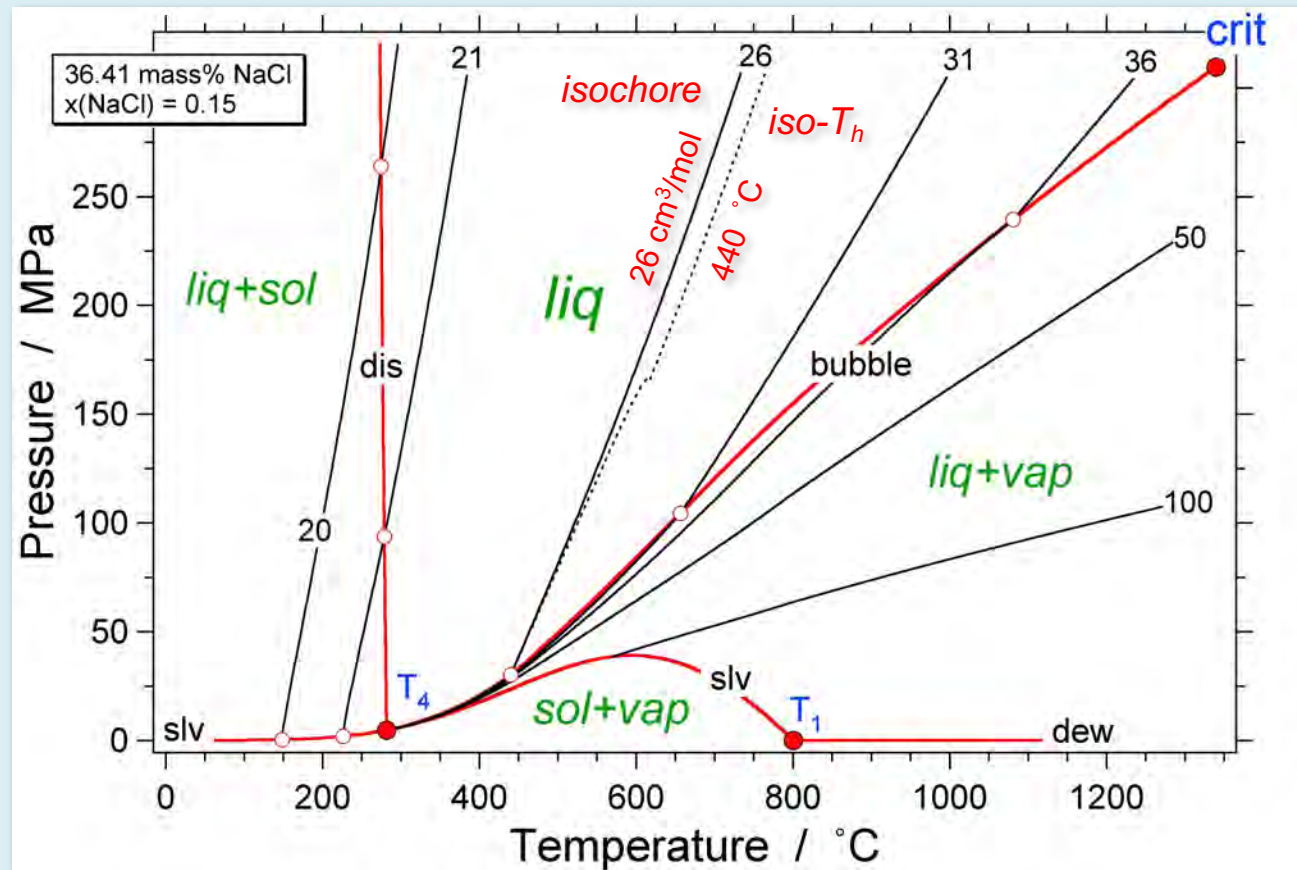
size temperature interval10degree

calculate isochore

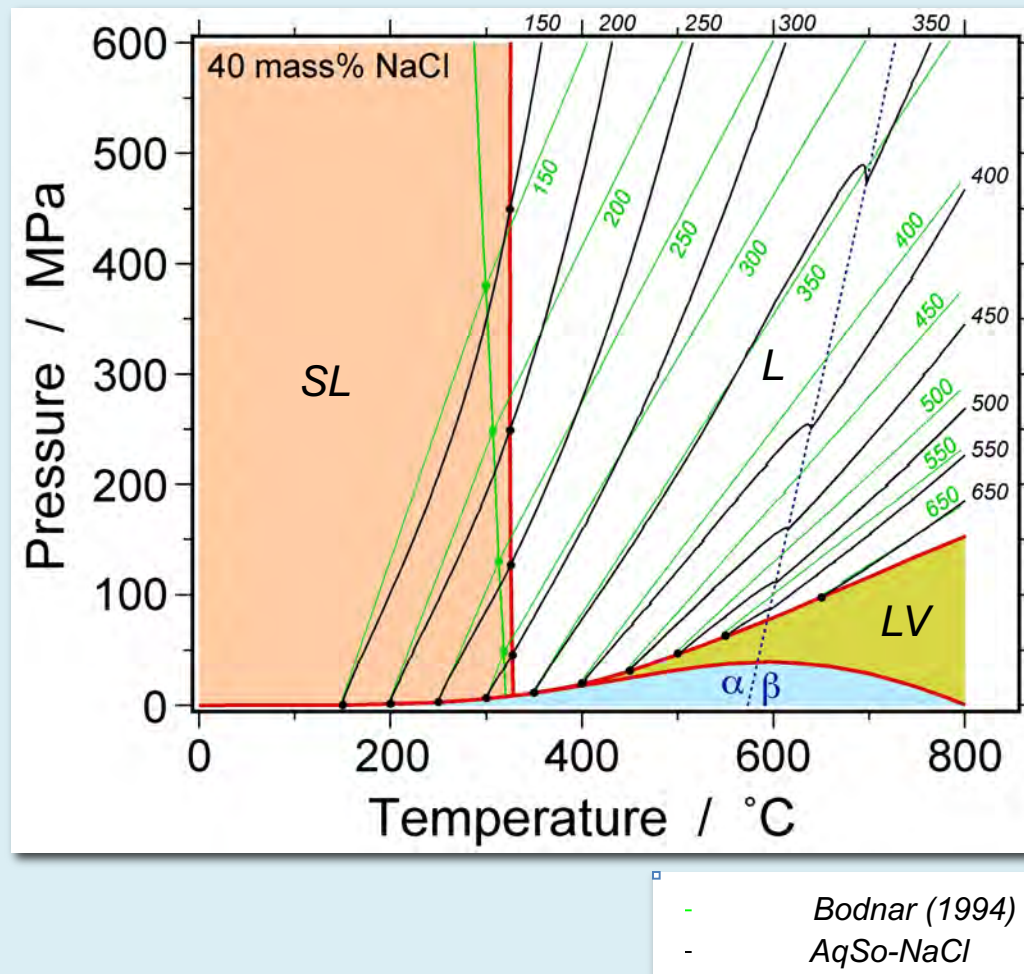
export data is available in: 40.txt

Temperature (°C)	Pressure (MPa)
410	31.15349
420	35.25484
430	39.42758
440	43.66064
450	47.9445
460	52.27092
470	56.63277
480	61.02391
490	65.43898
500	69.87334
510	74.32298

## Software: AqSo-NaCl



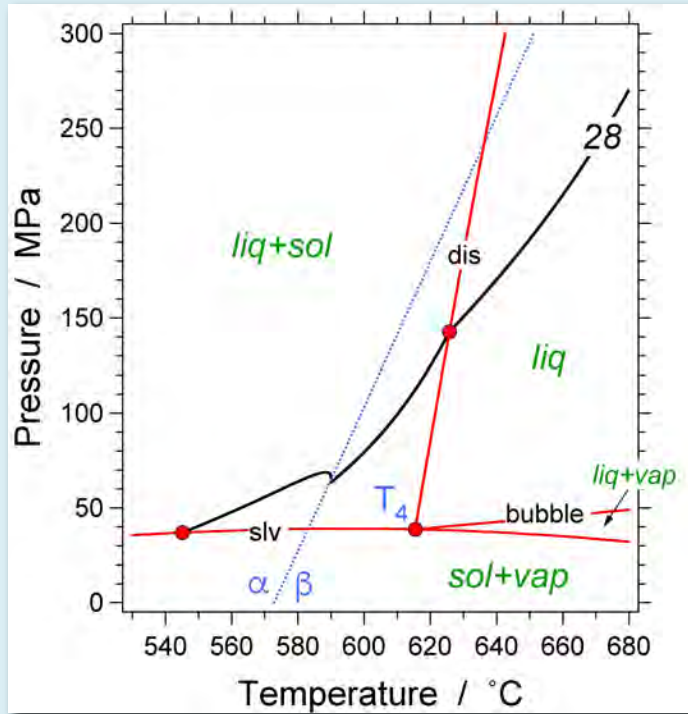
## comparison iso- $T_h$ curves



# Software: AqSo-NaCl

iso- $T_h$  line

625.8 °C



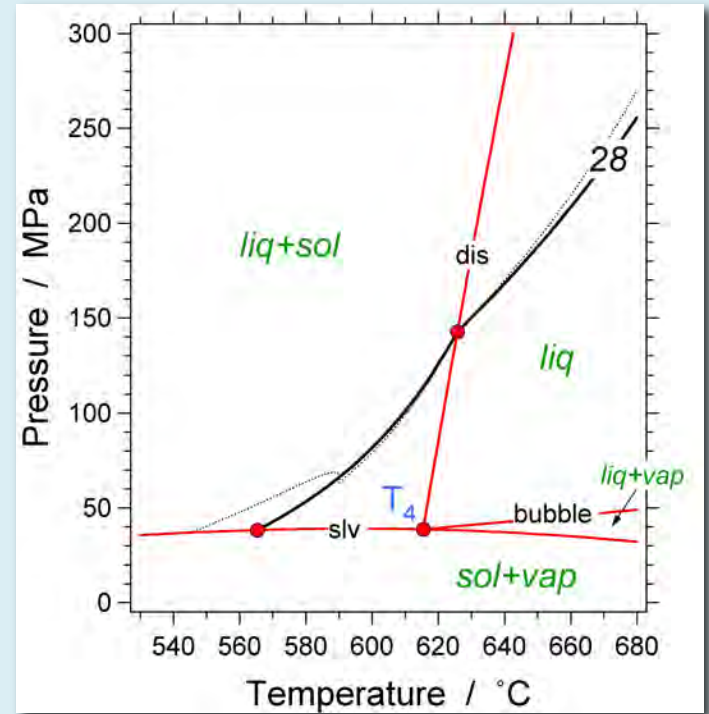
$$T_m (\text{SLV} \rightarrow \text{SL}) = 545.2 \text{ } ^\circ\text{C}$$

$$T_h (\text{SL} \rightarrow \text{L}) = 625.8 \text{ } ^\circ\text{C}$$

$x(\text{NaCl}) = 0.5$

isochore

28 cm<sup>3</sup>/mol



$$T_m (\text{SLV} \rightarrow \text{SL}) = 565.4 \text{ } ^\circ\text{C}$$

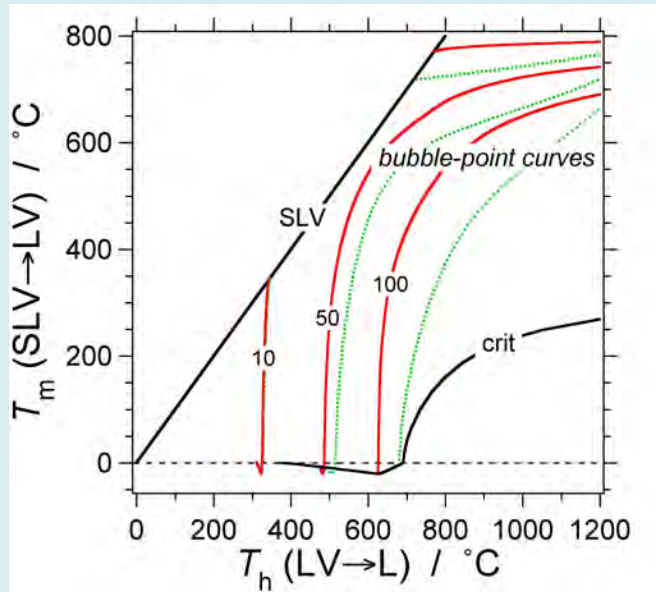
$$T_h (\text{SL} \rightarrow \text{L}) = 625.8 \text{ } ^\circ\text{C}$$



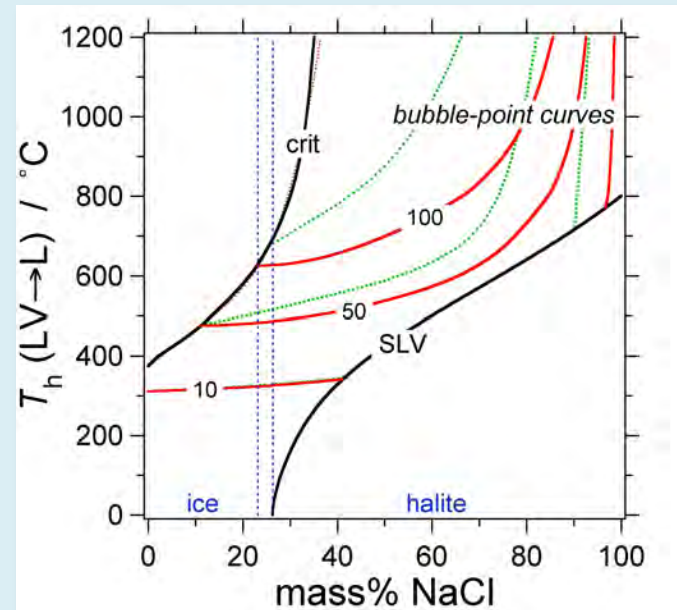
## Software: AqSo-NaCl

starting point of isochore / iso- $T_h$  curve

bubble-point curves



isobars



- HOKIEFLINCS\_H2O-NACL  
- AqSo-NaCl

# Software: AqSo-NaCl

## example text file of an isochore

Isochore and sub-isochore not corrected for modifications in quartz volume (Fig. 5a)

H<sub>2</sub>O-NaCl fluids (liquid vapour and solid)

reference: Bakker RJ (2018) Computers and Geosciences

AqSo\_NaCl: computer program to calculate p-T-V-x properties in the H<sub>2</sub>O-NaCl system applied to fluid inclusion research and pore fluid calculation

Molar Volume = 28 cm<sup>3</sup>/mol

Density = 1.365321 g/cm<sup>3</sup>

x(NaCl) = 0.5

Homogenization conditions: 625.8161 Celsius and 142.6436 MPa

SLV intersection conditions: 565.3914 Celsius and 38.27447 MPa

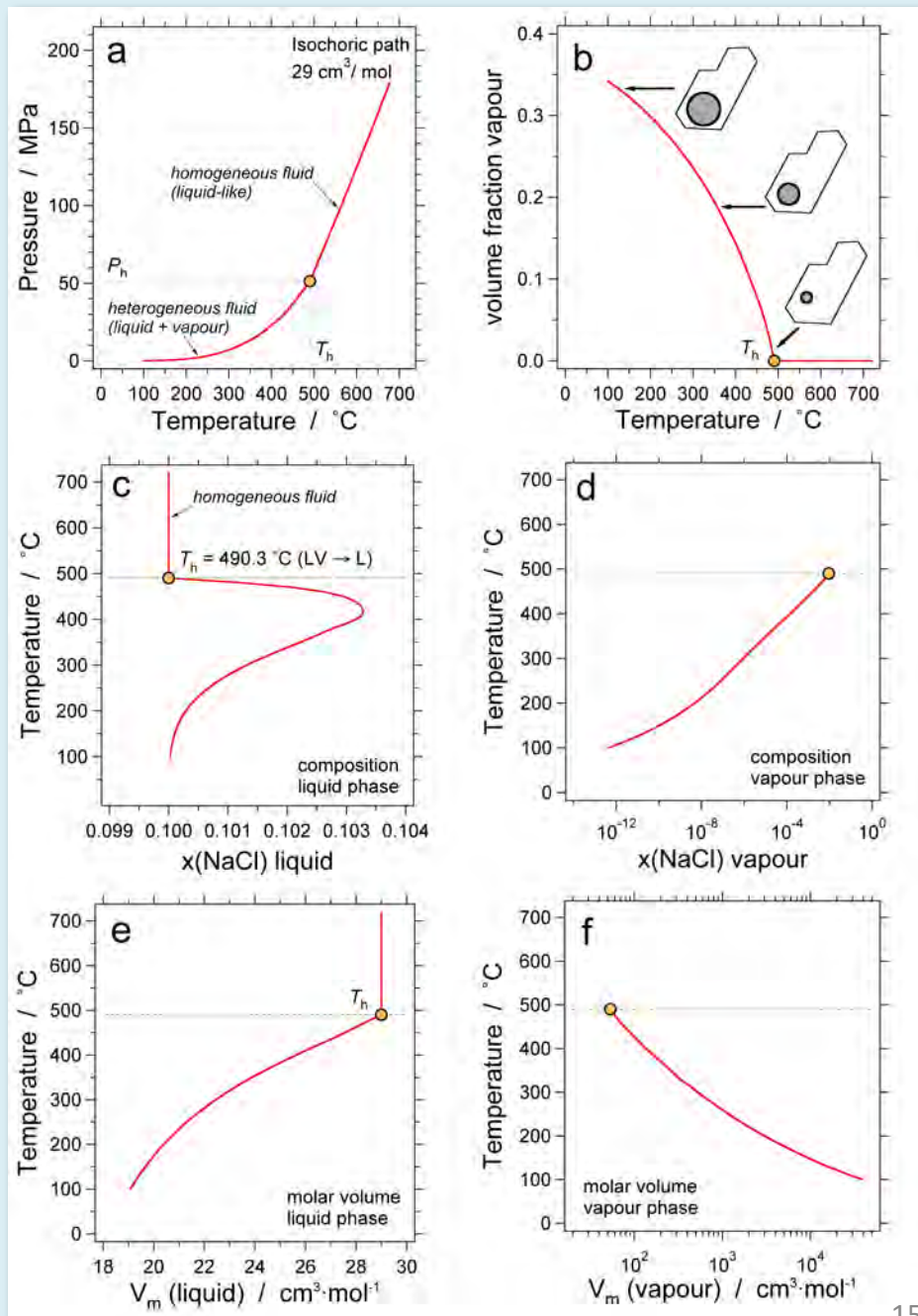
Definition quartz phase: 0 = alpha; 1 = beta

Temp.	Pres.	liquid phase			vapour phase			solid phase		Q
		x(NaCl) fraction	V <sub>m</sub> cm <sup>3</sup> /mol	vol. frac	x(NaCl) fraction	V <sub>m</sub> cm <sup>3</sup> /mol	vol. frac	V <sub>m</sub> cm <sup>3</sup> /mol	vol. frac	
Celsius	MPa									
540	36.54117	0.3699956	27.20788	0.7653775	0.000273	136.9526	0.0184467	29.02132	0.2161757	0
550	37.33353	0.3851384	27.43269	0.7929678	0.0002791	137.5364	0.0115547	29.07018	0.1954775	0
560	37.98522	0.4008956	27.66455	0.8231862	0.0002818	138.7253	0.0041897	29.1197	0.1726241	0
570	42.64961	0.4167751	27.80645	0.851376	0	0	0	29.16284	0.148624	0
580	53.30524	0.4323557	27.83819	0.875743	0	0	0	29.19604	0.124257	0
590	66.04527	0.4479672	27.87244	0.9016171	0	0	0	29.22574	0.0983829	0
600	81.62444	0.463392	27.90844	0.9287319	0	0	0	29.25052	0.0712681	1
610	101.0265	0.4783337	27.94503	0.9565855	0	0	0	29.26852	0.0434145	1
620	125.4994	0.4924037	27.98059	0.9843521	0	0	0	29.27736	0.0156479	1
630	149.9007	0.5	28	1	0	0	0	0	0	1
640	167.9995	0.5	28	1	0	0	0	0	0	1
650	187.3453	0.5	28	1	0	0	0	0	0	1
660	208.1905	0.5	28	1	0	0	0	0	0	1
670	230.8211	0.5	28	1	0	0	0	0	0	1
680	255.5576	0.5	28	1	0	0	0	0	0	1



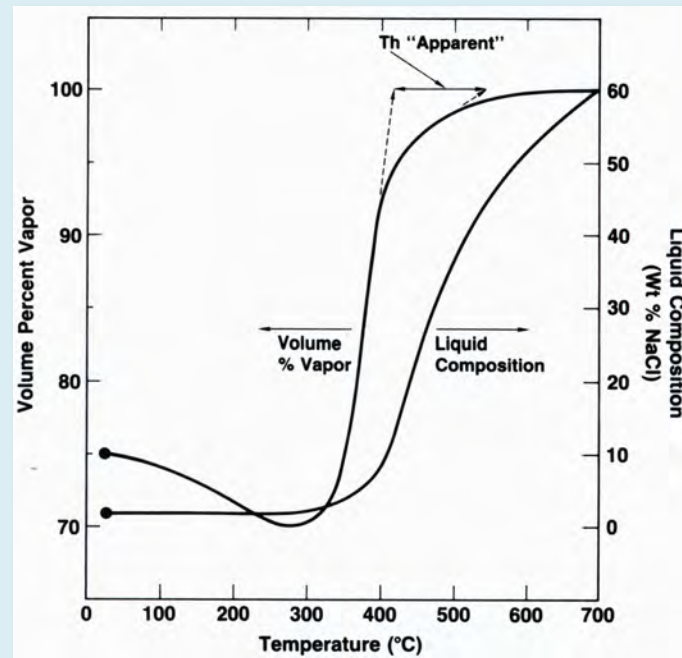
# Software: AqSo-NaCl

properties fluid inclusions along  
isochore or iso- $T_h$  line



what about  
homogenization to the vapour phase

impossible to detect?

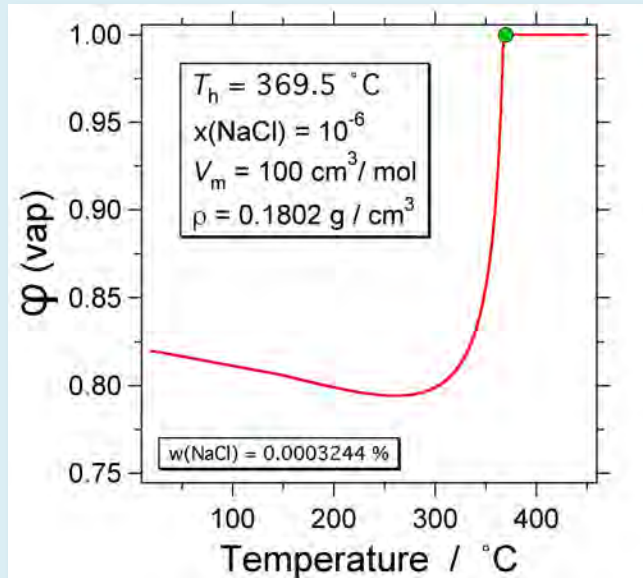
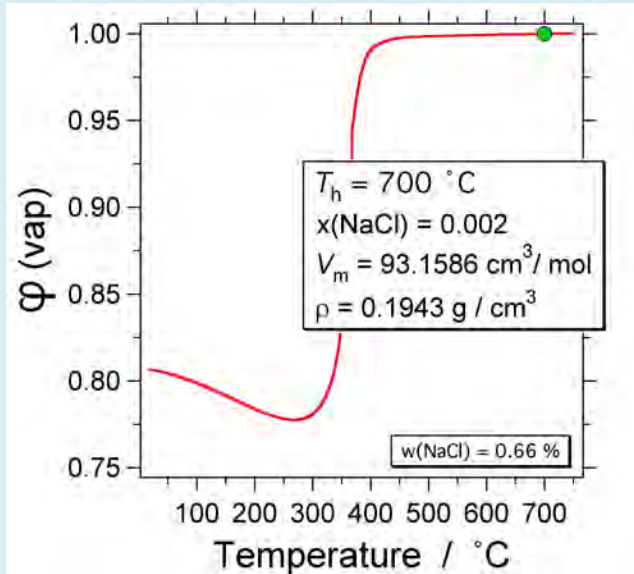


*Bodnar et al. (1985)*

*Sterner (1992)*

no - yes

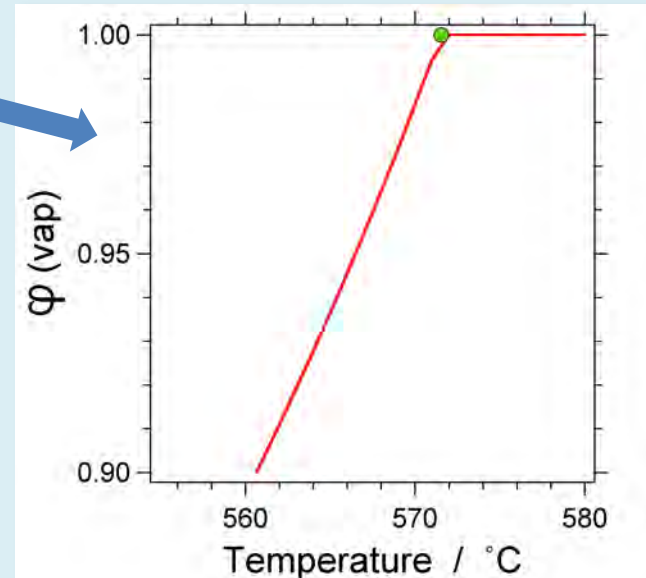
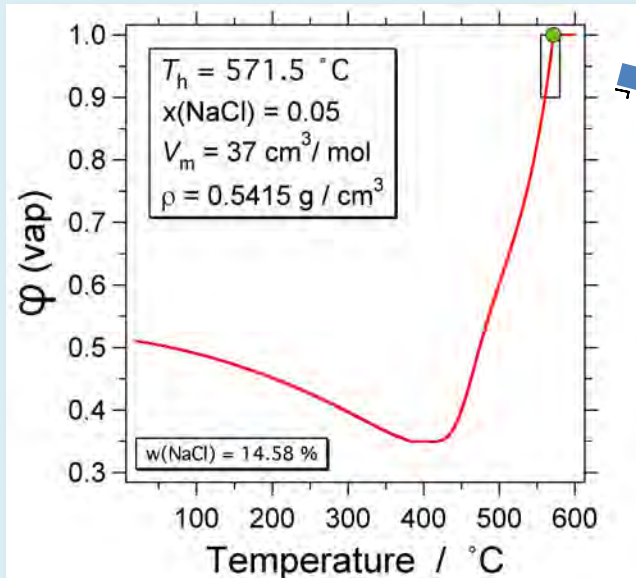
you cannot make a general statement



*all lines are calculated with AqSo-NaCl*

*(without taken into account the morphology of inclusions)*

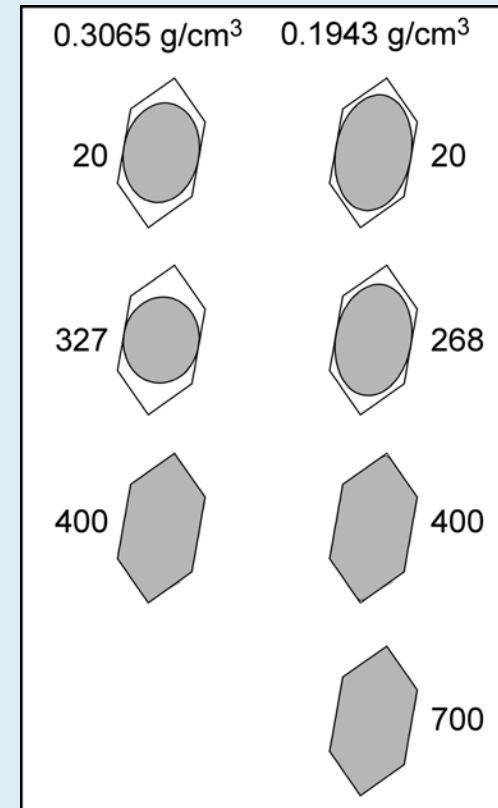
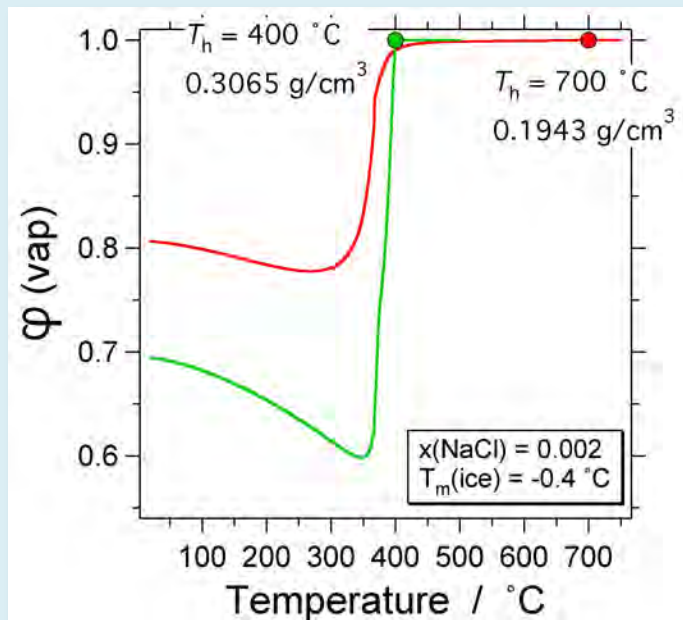
## apparent homogenization



*all lines are calculated with AqSo-NaCl*

underestimation of  $\pm 10^\circ$  results in a 1% density difference

can I tell the difference?



# conclusions

software AqSo-NaCl produces proper iso- $T_h$  curves that  
are significantly different from correlation-equations  
*(combining thermodynamic modelling of fluid with quartz properties)*

accuracy of this model is superior to correlation-equations

fluid inclusions properties can be modelled in the entire p-T-V-x space  
because vapour, liquid, and solid phases are involved  
*(modelling is not restricted to hom. liquid field)*