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92. Diagram Navigator

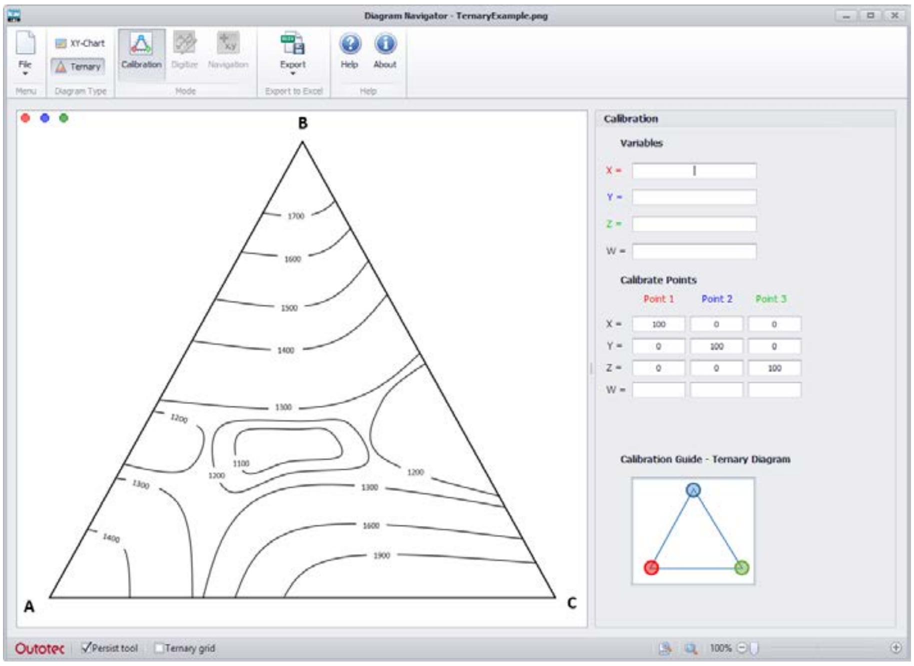
Diagram Navigator is a tool to simplify the viewing of ternary phase diagrams. It provides the user with a simple way to get ternary coordinates of any point within the diagram. It can be also used to calculate e.g. the liquidus temperature at a given point for liquidus ternary diagrams, if the user defines the isothermal lines.

92.1. Calibrating the diagram

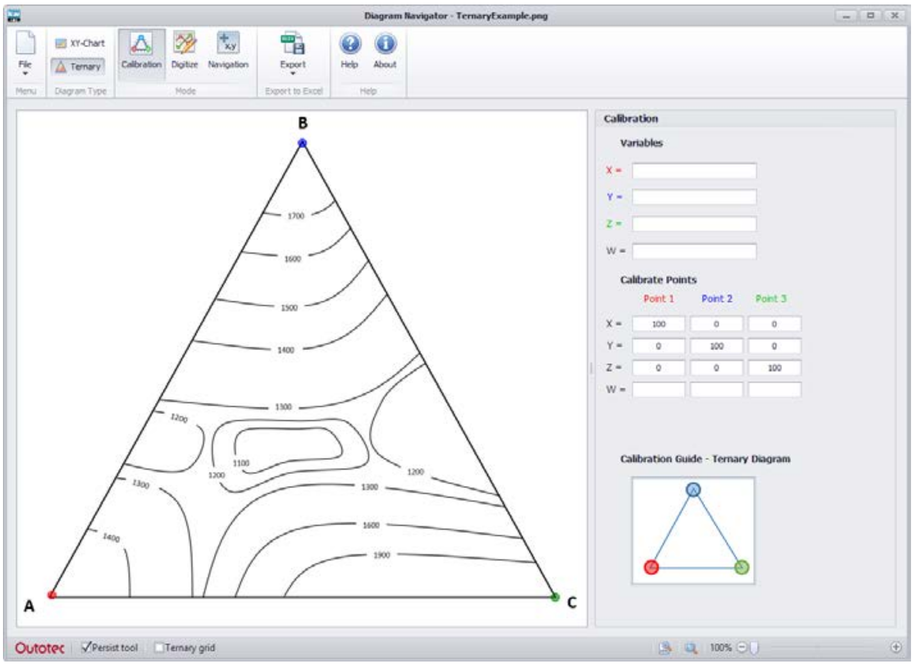
In order to navigate a ternary phase diagram, the user needs to define the parameters of the diagram during the calibration process.

In this example we will use an imaginary A-B-C liquidus diagram.

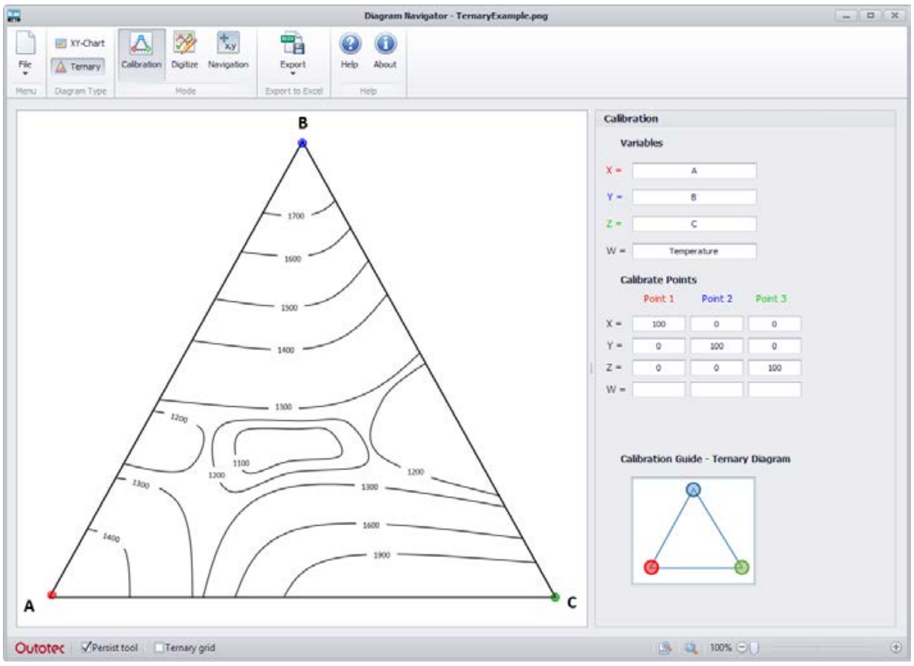
1. Open the diagram image using “File > New Phase Diagram > Ternary Diagram". The image is opened in the Calibration mode.



2. The idea of the calibration process is to place calibration markers (red/blue/green dots) at the vertices of the diagram triangle. This can be done simply by dragging the markers.



3. Next, we need to set labels for the vertices. Enter the names (A, B, C) in the corresponding text boxes. Enter the name of the parameter shown on the diagram (if any), in our case – “Temperature”.

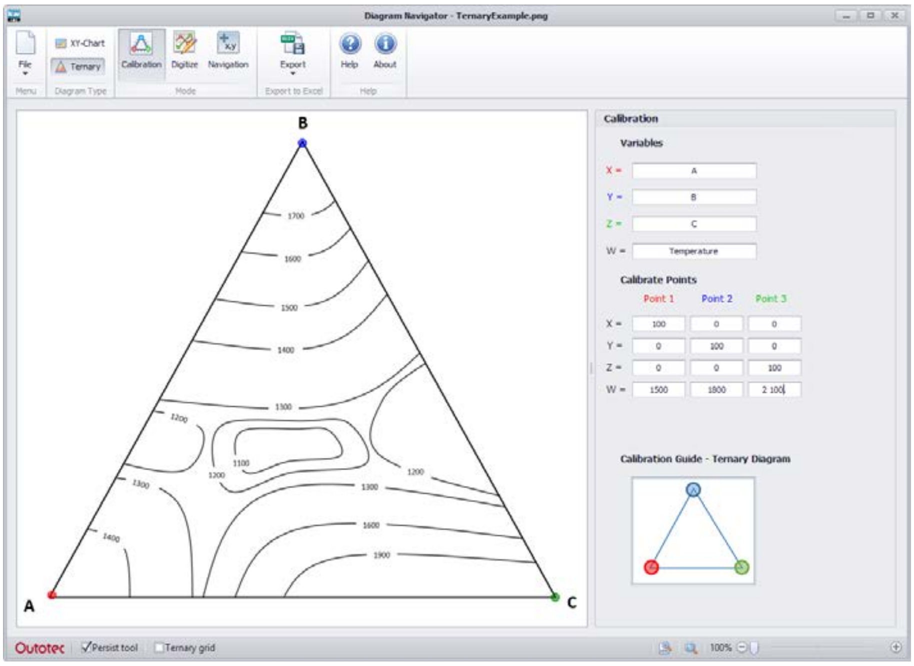


4. Next, we need to set minimum and maximum values for the axes. In this case, the mass fraction of the constituents is assumed in the range of 0-100%, so we do not need to change the values. Otherwise, enter the values into the “Calibrate Points” text boxes.

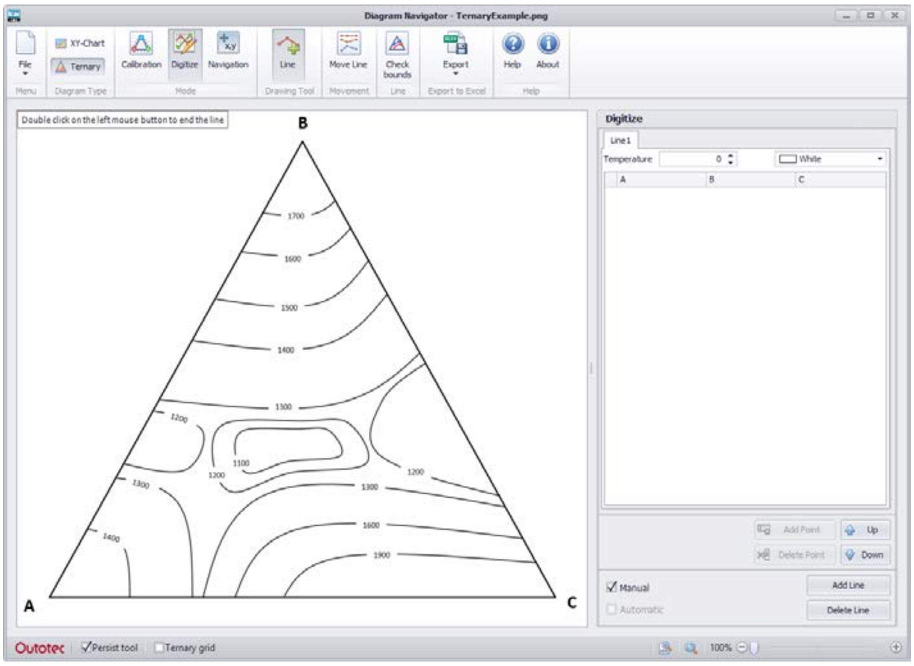
92.2. Digitizing the diagram

In order for the navigator to calculate the liquidus temperature, we need to digitize the diagram lines by creating polylines on top of them.

1. First, we need to set the liquidus temperature in the vertices of the triangle. In our example, we need to enter the melting points of pure A, B, and C in section W of Calibrate Points in the Calibration mode. In this example, we use the following W-values for the vertices: A=1500, B=1800 and C=2100.

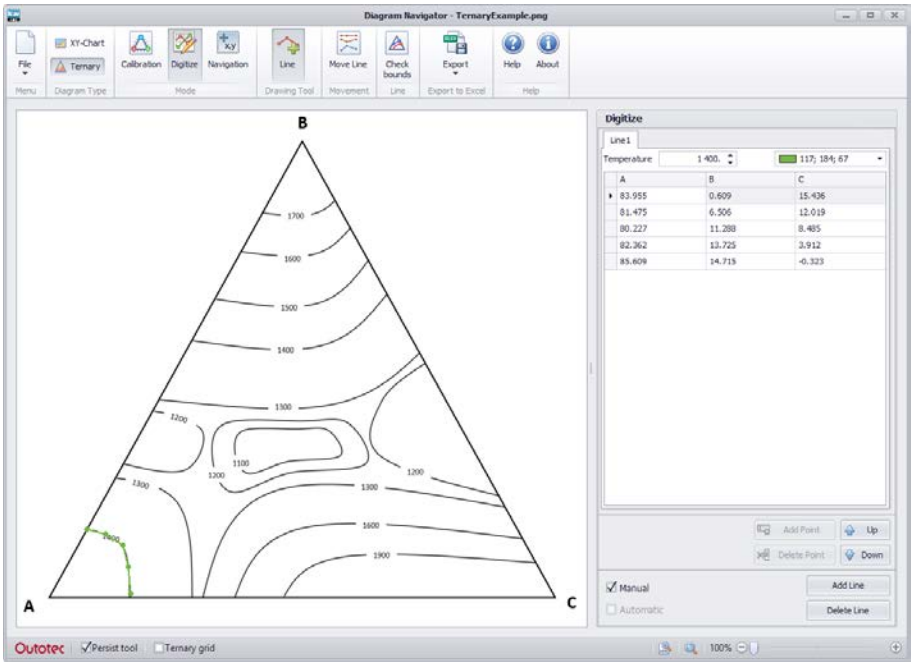


2. Select the “Digitize” mode. This mode allows the creation of the polylines.

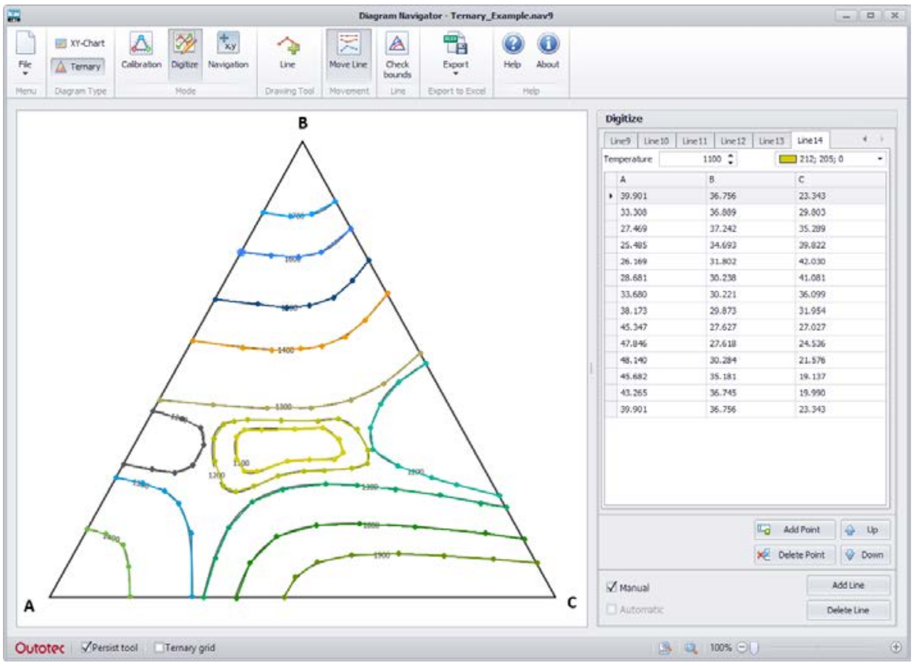


3. Draw the first polyline (use “Line” mode; start drawing by left-click and finish the polyline with a double-click).

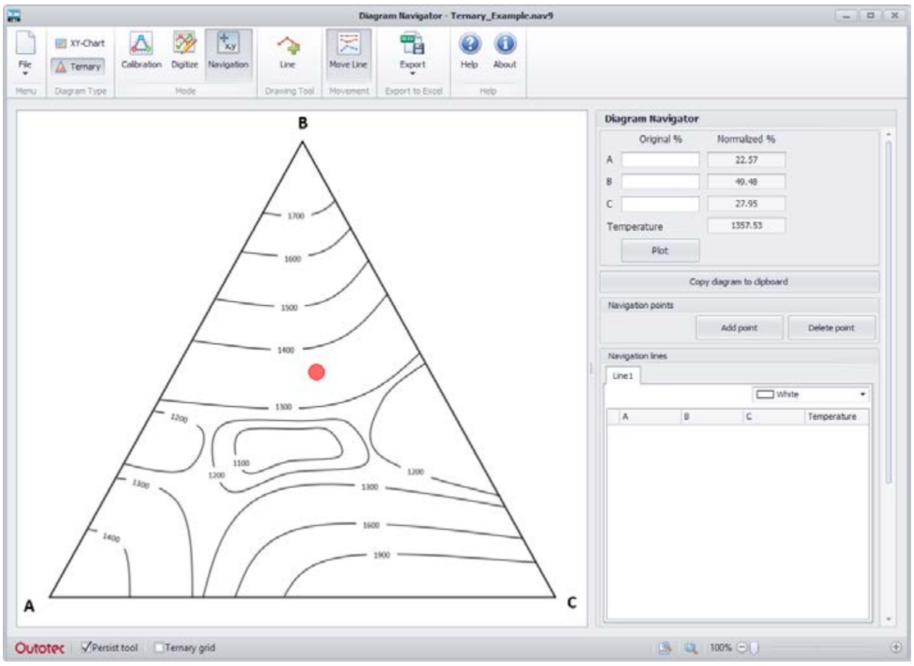
4. Set the line temperature



5. Repeat the process for the other lines in the diagram. You do not need to set lines for the triangle boundary, as they are calculated automatically.



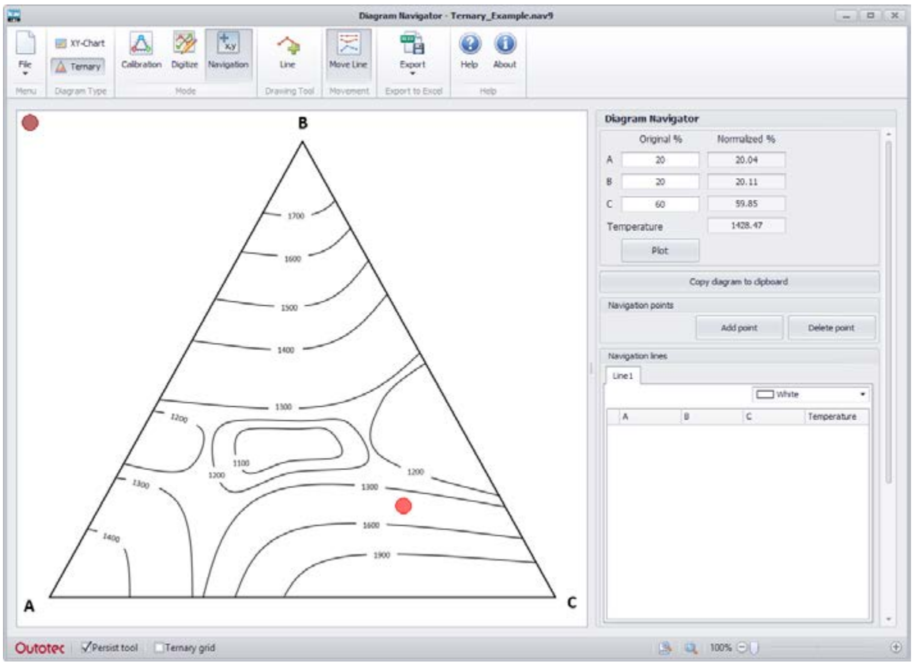
6. Once all the lines have been added, the Navigation mode can be used to calculate the liquidus temperature at the given point.



92.3. Navigating the diagram

Once the diagram has been calibrated, the “Navigation” mode can be used to calculate ternary coordinates for a point within the diagram.

Move the red marker on the diagram, and the right panel will show the ternary coordinates of the marker. There is also a reverse operation. A red marker can be plotted on the diagram on the basis of the normalized variable values.



92.3.1. Saving calibrated diagrams

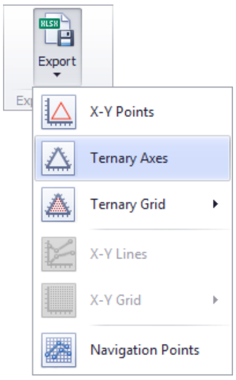
The calibrated diagram can be saved using **Save As**. This saves the diagram image along with an XML file that contains the calibration and digitizing settings. When the image file is open, Navigator searches for the XML file and loads settings from the file if it is found.

92.3.2. Printing the diagrams

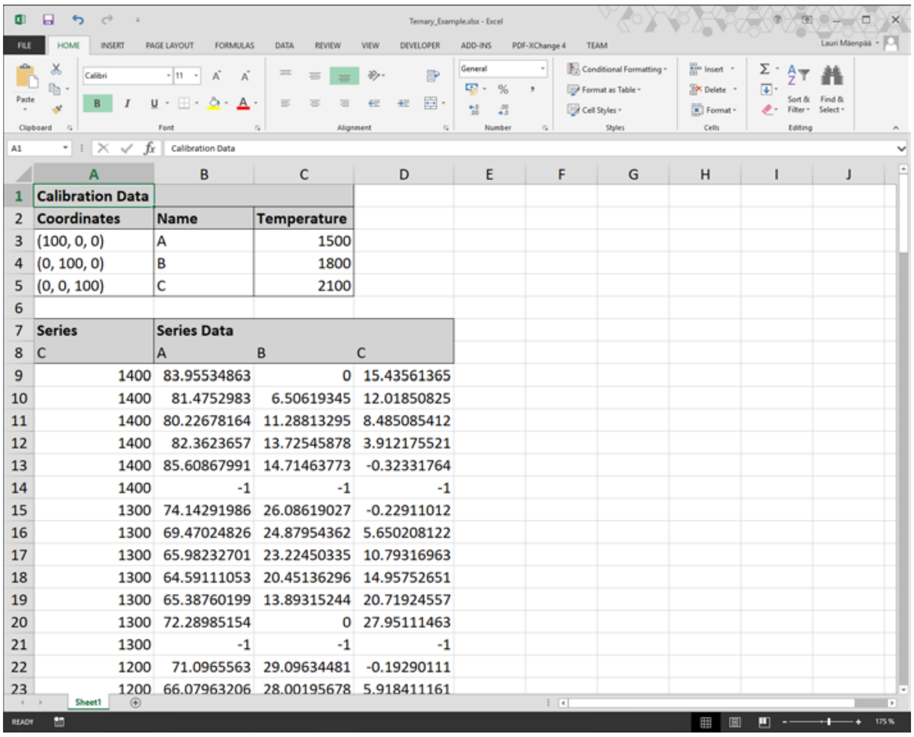
The calibrated diagram can be printed using the “Print” button. If the print is called from the Navigation tab, a table with navigation information is also printed.

92.3.3. Navigating with Add-In function in Excel

Digitized ternary diagrams can be navigated also in Excel by using NavTernary( ) function. The function requires that the data is first exported to Excel in the correct format. To do this, select “Excel Export > Ternary Axes” for the digitized diagram.



The export procedure lists information about the corner points and about the digitized lines.

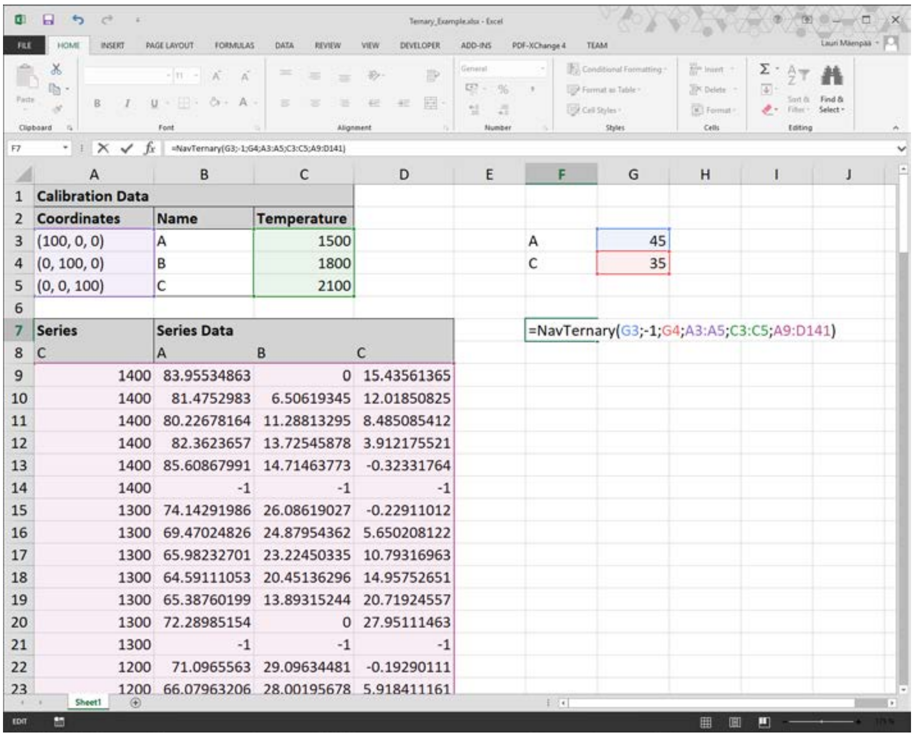


	A	B	C	D
1	Calibration Data			
2	Coordinates	Name	Temperature	
3	(100, 0, 0)	A	1500	
4	(0, 100, 0)	B	1800	
5	(0, 0, 100)	C	2100	
6				
7	Series	Series Data		
8	C	A	B	C
9	1400	83.95534863	0	15.43561365
10	1400	81.4752983	6.50619345	12.01850825
11	1400	80.22678164	11.28813295	8.485085412
12	1400	82.3623657	13.72545878	3.912175521
13	1400	85.60867991	14.71463773	-0.32331764
14	1400	-1	-1	-1
15	1300	74.14291986	26.08619027	-0.22911012
16	1300	69.47024826	24.87954362	5.650208122
17	1300	65.98232701	23.22450335	10.79316963
18	1300	64.59111053	20.45136296	14.95752651
19	1300	65.38760199	13.89315244	20.71924557
20	1300	72.28985154	0	27.95111463
21	1300	-1	-1	-1
22	1200	71.0965563	29.09634481	-0.19290111
23	1200	66.07963206	28.00195678	5.918411161

For the function to return the calculated liquidus temperature, the following parameters need to be used:

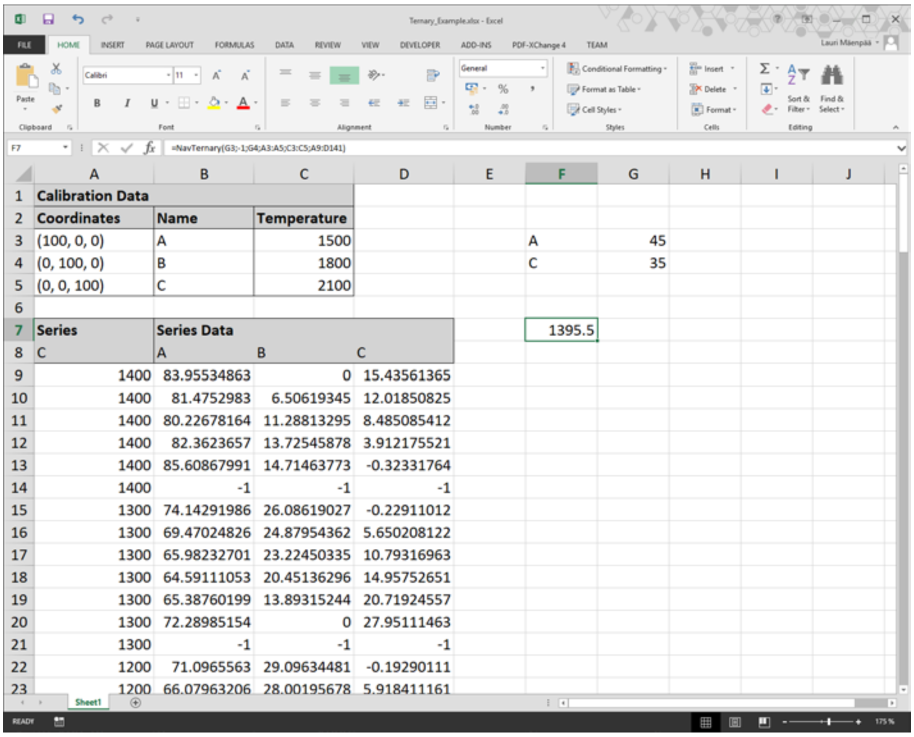
- 2 coordinate values (the 3rd coordinate is passed as -1)
- Vertex coordinates
- Vertex W-values
- Digitized lines

For example, we can calculate the liquidus temperature for the point A=45% and C=35%.



Formula bar (F7): =NavTernary(G3;-1;G4;A3:A5;C3:C5;A9:D141)

	A	B	C	D	E	F	G
1	Calibration Data						
2	Coordinates	Name	Temperature				
3	(100, 0, 0)	A	1500			A	45
4	(0, 100, 0)	B	1800			C	35
5	(0, 0, 100)	C	2100				
6							
7	Series	Series Data				=NavTernary(G3;-1;G4;A3:A5;C3:C5;A9:D141)	
8	C	A	B	C			
9	1400	83.95534863	0	15.43561365			
10	1400	81.4752983	6.50619345	12.01850825			
11	1400	80.22678164	11.28813295	8.485085412			
12	1400	82.3623657	13.72545878	3.912175521			
13	1400	85.60867991	14.71463773	-0.32331764			
14	1400	-1	-1	-1			
15	1300	74.14291986	26.08619027	-0.22911012			
16	1300	69.47024826	24.87954362	5.650208122			
17	1300	65.98232701	23.22450335	10.79316963			
18	1300	64.59111053	20.45136296	14.95752651			
19	1300	65.38760199	13.89315244	20.71924557			
20	1300	72.28985154	0	27.95111463			
21	1300	-1	-1	-1			
22	1200	71.0965563	29.09634481	-0.19290111			
23	1200	66.07963206	28.00195678	5.918411161			



Formula bar (F7): =NavTernary(G3;-1;G4;A3:A5;C3:C5;A9:D141)

	A	B	C	D	E	F	G
1	Calibration Data						
2	Coordinates	Name	Temperature				
3	(100, 0, 0)	A	1500			A	45
4	(0, 100, 0)	B	1800			C	35
5	(0, 0, 100)	C	2100				
6							
7	Series	Series Data				1395.5	
8	C	A	B	C			
9	1400	83.95534863	0	15.43561365			
10	1400	81.4752983	6.50619345	12.01850825			
11	1400	80.22678164	11.28813295	8.485085412			
12	1400	82.3623657	13.72545878	3.912175521			
13	1400	85.60867991	14.71463773	-0.32331764			
14	1400	-1	-1	-1			
15	1300	74.14291986	26.08619027	-0.22911012			
16	1300	69.47024826	24.87954362	5.650208122			
17	1300	65.98232701	23.22450335	10.79316963			
18	1300	64.59111053	20.45136296	14.95752651			
19	1300	65.38760199	13.89315244	20.71924557			
20	1300	72.28985154	0	27.95111463			
21	1300	-1	-1	-1			
22	1200	71.0965563	29.09634481	-0.19290111			
23	1200	66.07963206	28.00195678	5.918411161			

92.4. Theory

92.4.1. Conversion between barycentric and Cartesian coordinates

In order to work with ternary diagram images we need to perform conversions between coordinates.

Ternary coordinates are a special kind of barycentric coordinates with only 3 vertices.
In order to define the conversion between ternary and Cartesian coordinates, we need to define

a. the Cartesian coordinates of the vertices
b. the maximum value of the ternary coordinates

We can calculate the barycentric coordinates with the location of the point.
Conversely, if the barycentric coordinates are known, we can calculate the location of the point.

Define P_1 , P_2 , P_3 as vertices of the triangle, where $P_i = (x_i, y_i)$.
Any point P on the triangle can be obtained from barycentric coordinates λ_1 , λ_2 , $\lambda_1 \geq 0$ such that $\lambda_1 + \lambda_2 + \lambda_3 = \lambda^*$ to Cartesian coordinates (x, y) :

$$P = \frac{\lambda_1 P_1 + \lambda_2 P_2 + \lambda_3 P_3}{\lambda^*}.$$

Substitute $\lambda_3 = \lambda^* - \lambda_1 - \lambda_2$ to find the reverse transformation, from Cartesian coordinates to barycentric coordinates:

$$P = \frac{\lambda_1 P_1 + \lambda_2 P_2 + (\lambda^* - \lambda_1 - \lambda_2) P_3}{\lambda^*}.$$

Rearranging, this is

$$\lambda_1 (P_1 - P_3) + \lambda_2 (P_2 - P_3) + \lambda^* (P_3 - P) = 0.$$

This linear transformation may be written more succinctly as:

$$T\lambda = \lambda^* (P_3 - P),$$

where λ is the vector of barycentric coordinates and T is a matrix given by

$$T = \begin{pmatrix} x_1 - x_3 & x_2 - x_3 \\ y_1 - y_3 & y_2 - y_3 \end{pmatrix}.$$

Now the matrix T is invertible, since $P_1 - P_3$ and $P_2 - P_3$ are linearly independent (if this were not the case, then P_1 , P_2 , and P_3 would be collinear and would not form a triangle).

Thus, we can rearrange the above equation to get

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = T^{-1} \lambda^* (P - P_3).$$

Explicit formulas for the barycentric coordinates of point P in terms of the Cartesian coordinates are:

$$\lambda_1 = \lambda^* \frac{(y_2 - y_3)(x - x_3) + (x_3 - x_2)(y - y_3)}{(y_2 - y_3)(x_1 - x_3) + (x_3 - x_2)(y_1 - y_3)},$$

$$\lambda_2 = \lambda^* \frac{(y_3 - y_1)(x - x_3) + (x_1 - x_3)(y - y_3)}{(y_2 - y_3)(x_1 - x_3) + (x_3 - x_2)(y_1 - y_3)},$$

$$\lambda_3 = \lambda^* - \lambda_1 - \lambda_2.$$

92.4.2. Liquidus temperature calculation

In order to calculate the liquidus temperature in Diagram Navigator, one should approximate the isothermal lines by defining polylines with constant temperatures and define temperatures in the vertices. Then, the following approach is used.

Suppose that the coordinates of navigation point P_N and set of isothermal polylines L are defined.

Set L is a set of ordered pairs of variables $(T_i, L_i)_{i=1}^{n}$, where T_i is the temperature of the line with the number i and L_i is an ordered set of points $\left(x_j, y_j\right)_{j=1}^{m_{L_i}}$ of the line with the Number i . The vertices of the triangle can be considered isothermal polylines consisting of one point.

We need to calculate liquidus temperature T_L at point P_N .

Let us define L_R - set of lines that the navigation point is located between.

The first step is to determine the location of the point relative to the lines.

First rule:

Add the number i , $i = \{1, \dots, n\}$ to set L_R if the following is true for $L_i \in L$:

$$\left(P_N, \left(x_j, y_j\right)\right) \cap \left(\left(x_k, y_k\right), \left(x_{k+1}, y_{k+1}\right)\right) \in L_p = \emptyset, p \neq i,$$
$$p = \{1, \dots, n\},$$
$$k = \left\{1, \dots, m_{L_p} - 1\right\},$$
$$j = \left\{1, \dots, m_{L_i}\right\}.$$

Let us define T_R as a set of temperatures corresponding to set L_R .

If the number of different temperatures in set T_R is not equal to two, then the set of lines is defined by the second rule instead.

Second rule:

Add the number i , $i = \{1, \dots, n\}$ to set L_R if the following is true for $L_i \in L$:

at least one j , $j = \left\{1, \dots, m_{L_i}\right\}$ exists such that

$$\left(P_N, \left(x_j, y_j\right)\right) \cap \left(\left(x_k, y_k\right), \left(x_{k+1}, y_{k+1}\right)\right) \in L_p = \emptyset, p \neq i,$$
$$p = \{1, \dots, n\},$$
$$k = \left\{1, \dots, m_{L_p} - 1\right\}.$$

If the second rule is applied, we need to redefine set T_R .

If the number of different temperatures in set T_R is more than two, then we need to check the lines from L_R for an intersection between them.

Some of the lines may be vertices of the triangle. If a vertex belongs to set L_R , we need to check for an intersection between the line segments.

The first line segment consists of the vertex and points of lines in L_R .

The second line segment is a line segment of the lines in L .

If an intersection exists, then remove this vertex.

Some of the lines from L_R can be located between other lines from L_R . These lines should be removed from set L_R .

The second step is the calculation of the distance between the point and the line.
If the number of different temperatures in T_R equals one, then T_L is assigned a value of any element of T_R .

Or we can calculate the distance between point P_N and every line in set L_R .

Among the obtained set of distances we choose two lines with the smallest distance. Let

t_1, t_2 - temperatures that correspond to selected lines,
D_{t_1}, D_{t_2} - distances between point P_N and selected lines,
Then the liquidus temperature can be calculated as

$$T_L = t_2 + \frac{D_{t_2}(t_1 - t_2)}{D_{t_1} + D_{t_2}}.$$