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.
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%.
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 $\lambda_1$, $\lambda_2$, $\lambda_3 \geq 0$ 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 $\lambda$ 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:

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

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

$$ \lambda_3 = \lambda^* - \lambda_1 - \lambda_2. $$
### 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 $(x_j, y_j)_{j=1}^{m_{L_i}}$ 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 $i$, $i = \{1, \ldots, n\}$ to set $L_R$ if the following is true for $L_i \in L$:

\[
\left( P_N, (x_j, y_j) \right) \cap \left( (x_k, y_k), (x_{k+1}, y_{k+1}) \right) \in L_p = \emptyset, p \neq i,
\]

\[
p \in \{1, \ldots, n\},
\]

\[
k \in \{1, \ldots, m_{L_p} - 1\},
\]

\[
j \in \{1, \ldots, m_{L_i}\}.
\]

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

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

\[
\left( P_N, (x_j, y_j) \right) \cap \left( (x_k, y_k), (x_{k+1}, y_{k+1}) \right) \in L_p = \emptyset, p \neq i,
\]

\[
p \in \{1, \ldots, n\},
\]

\[
k \in \{1, \ldots, m_{L_p} - 1\}.
\]

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

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