Plotting

Documentation

DDBSP – Dortmund Data Bank Software Package

DDB

DDBST

Dortmund Data Bank
Software & Separation
Technology

Contents

1 Quick Overview

1.1 Chart Pages

The plot windows are arranged in pages. If there are several possible charts for the presented data, every chart is put on a separate page in the same plot window.
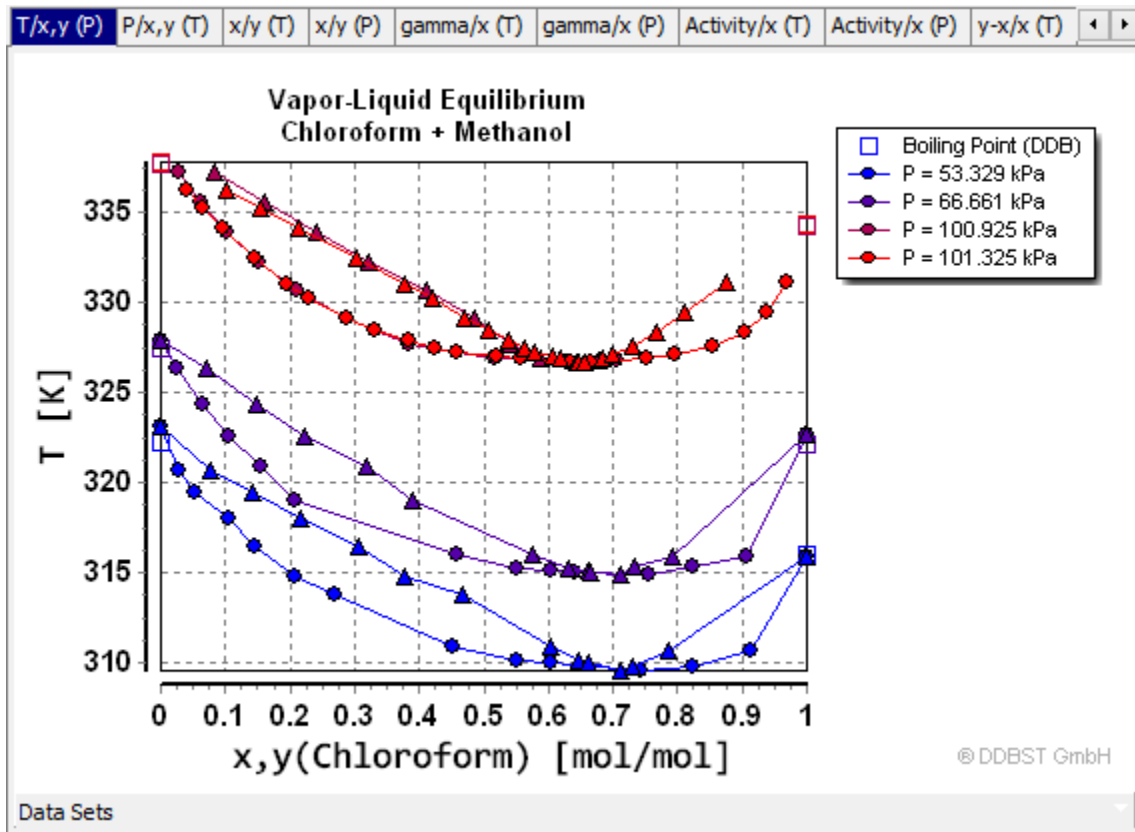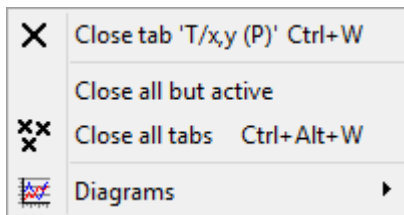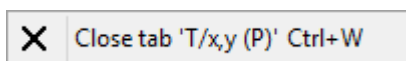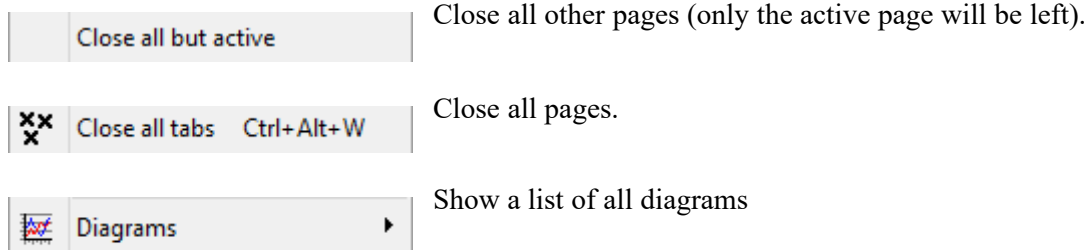

Figure 1: Main diagram window with tabs

The **page bar** has a context menu:

  Close the selected page. The tab's title is displayed in the context menu ('SLE-Triangle 3D' resp. 'P/y1/y2' in the screen copies).

Close all but active	Close all other pages (only the active page will be left).
✗✗ Close all tabs Ctrl+Alt+W	Close all pages.
〽 Diagrams ▸	Show a list of all diagrams

When the last page is closed the main window is closed.

1.2 Moving Around the Chart

1 Display Data Point Details

When the mouse pointer is near a point a connection line to the point is drawn (like a **rubber band**). The maximum length of the rubber band can be customized in the global options (default: 75 points). When a point is focused some data information is displayed in the **information area** below the chart.
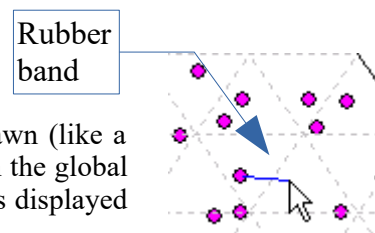
```
DDB-Number: VLE 5416 [Public DDB]
Ref.:[1796] Arm H., Bankay D., Helv.Chim.Acta, 51(6), 1243-1245, 1968

Components:
(1)     C12 Diethyl ether C4H10O
(2)     C110 Methanol CH4O

Constant: T = 298.15 K
```

The data information can change with every point, for example. if more than one system is displayed in the chart. The selected text can be copied using the context menu. When nothing is selected the whole text will be copied.

2 Status Bar

The **status bar** contains data point information. In the first fields the (untransformed) axis values of the current point are displayed. They are followed by all other data point information, at last the available constant value information is displayed.

The same information as shown in the status bar is also displayed as moving hint window following the mouse cursor.

This advantage of this hint window is that it all entries are visible. Entries in the status bar might become invisible when the window becomes smaller.

```
y(C12):        0.8245 mol/mol
y(C11):        0.1755 mol/mol
P:             35.837 kPa
x(C12):        0.2 mol/mol
x(C11):        0.8 mol/mol
K1:            4.1225
K2:            0.21937
SepFac:        18.792
y1-x1:         0.6245
Act.Coeff.1:   2.06382
Act.Coeff.2:   1.00135
T:             298.15 K
```

3 Show Data

The **data table** to a selected point can be displayed using the series context menu.

The data table will be displayed within the Dortmund Data Bank program.

4 Copying Data

Use *"Copy Series Data to Clipboard"* to copy the **series data** to the clipboard. A "series" is typically representing all points of a data set and has either the same color or the same symbols.
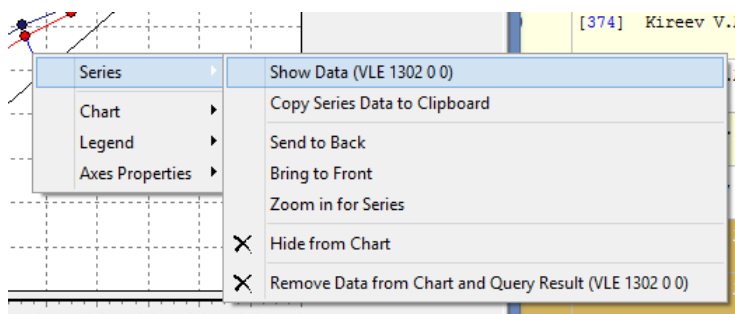

*Figure 2: Chart Context Menu: Series*

5 Changing Z-Order

To access series points which are hidden behind another series use *"Send to Back"* or "Bring to Front" to change the **Z-order** of the series. This changes the order in the legend, too.

6 Zoom in for Series

This function zooms in to show the connected series only. It is a short cut for the function in the following paragraph "Zoom" below.

7 Hide from Chart

This hides the connected series. If any series is hidden an additional entry "Unhide All Series" is shown in the context menu which makes all hidden series visible again.
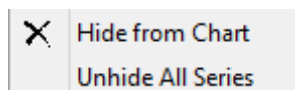
8 Remove Data from Chart and Query Result

This function removes the connected series from the diagram and also directly the marked set from the query result in the Dortmund Data Bank program.

9 Zoom

The mouse can be used to **zoom** into an area by holding down the left mouse button and mark the rectangle to be zoomed beginning in the *top left corner* of the area. To **scroll** the chart contents hold down the right mouse button and move in the desired axis directions. To **undo zoom** or scroll either the "Undo Zoom/Scroll" button ( )
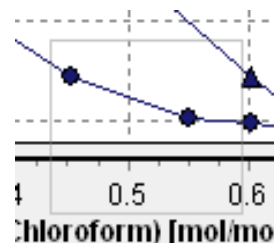
can be used or by marking an area with the left mouse button pressed beginning in the *top right corner* of the area.
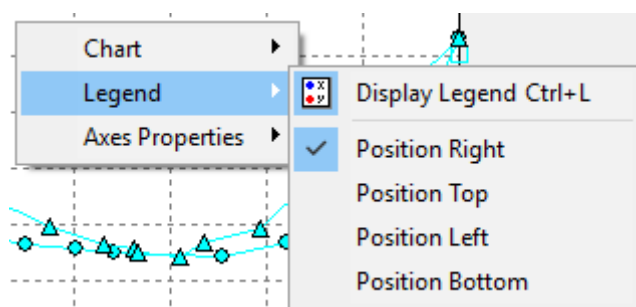

Figure 3: Zoom In

1.3 The Legend

Figure 4: Chart Context Menu: Legend

The **legend** can be turned on/off using the button or the corresponding entry in the legend part of the chart context menu. The legend position can be left from, right from, above or below the chart.

If not all legend entries can be displayed at once the legend contents can be scrolled using the mouse wheel or by holding down the left mouse button an move up- or down within the legend. The possible scrolling directions are reflected by the mouse pointer shape.

In most charts the **pointer shape** reflects the phase information. A circle is used for the liquid phase. If there's more than one liquid phase the different phases are distinguished by using left and right triangle. The vapor

phase is represented by a triangle and the solid phase by a rectangle.

1.4 Data Set List

The list of data sets is available through a pop-up window ("Data Sets") below the diagram. If opened, this
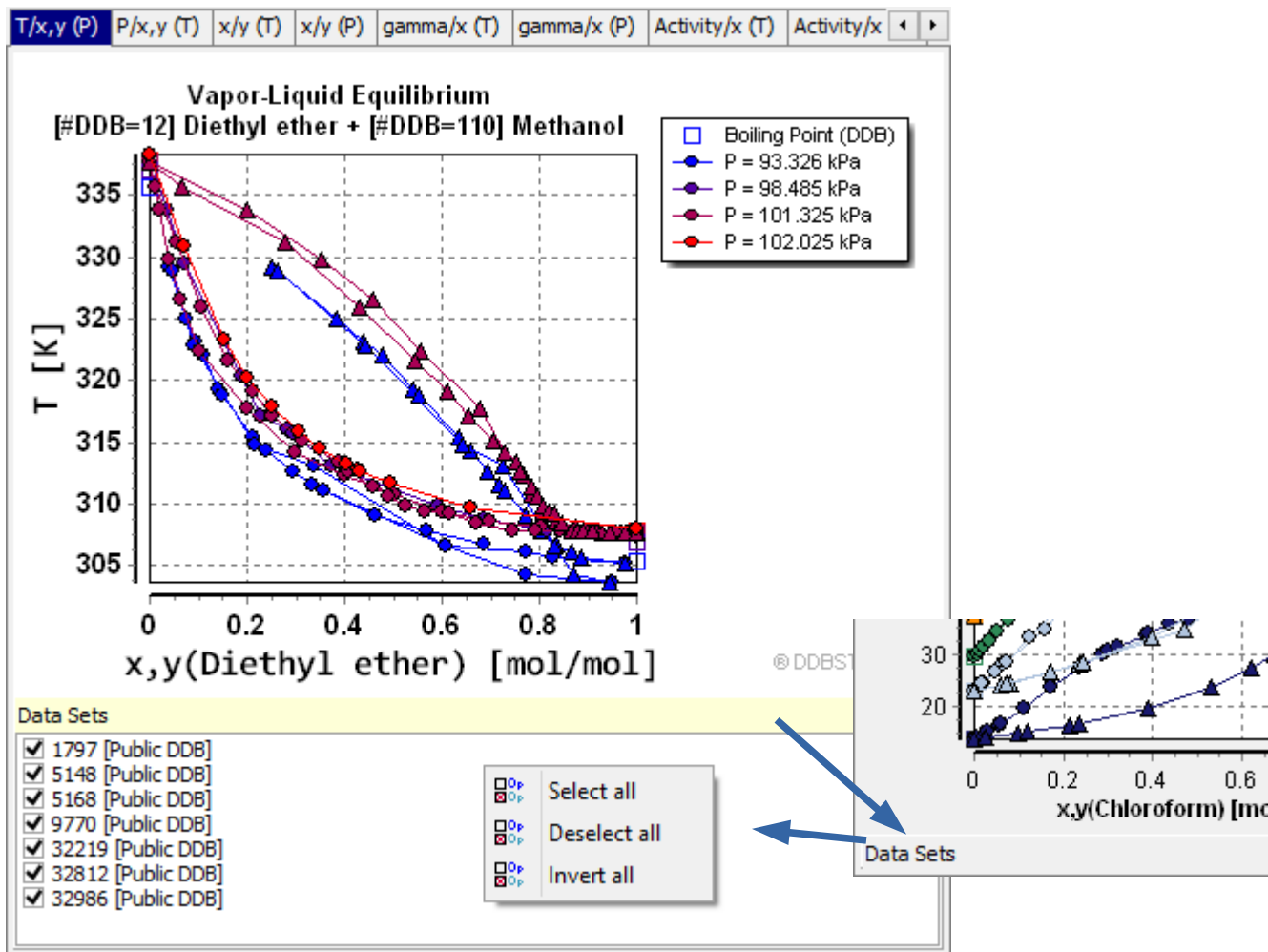
control shows the list of data sets. This allows to show or hide single data sets from the chart. The control has a pop-up menu that allows selecting, deselecting, and inverting all check boxes. The title line is shown in light yellow if opened and can be close by clicking on this yellow title line.

1.5 Customizing the Chart

10 Chart Title

The **chart title** can be changed by a single click on it.
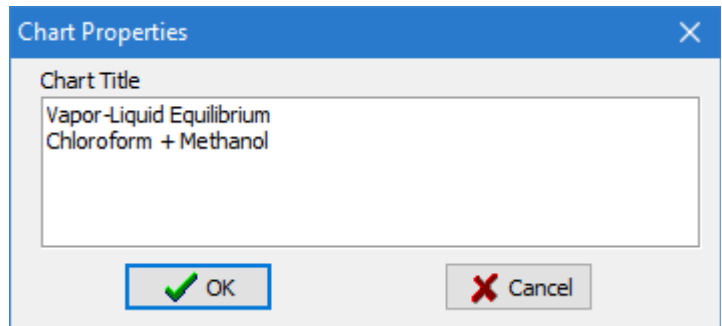

Figure 5: Edit Chart Title

11 Axis Properties

The **axis properties dialog** can be accessed by double-click on the desired axis or by using the axis context menu (right-click on the diagram).

The axis properties dialog allows to change the axis title, axis title
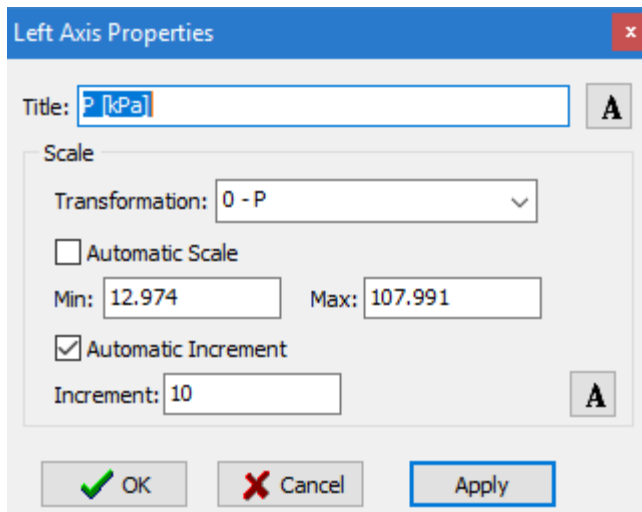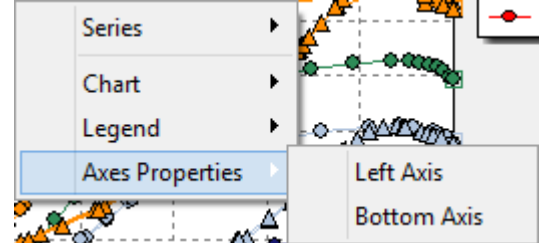
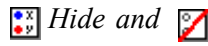*Figure 6: Chart Context Menu: Axes Properties*

Figure 7: Axes Properties

font (upper **A**) and the font of the axis labels (lower **A**). In several cases the axis can be transformed for example to get a representation like log(P) vs. 1000/T. Furthermore the minimum and maximum axis value can be set manually. The axis increment can be set manually or automatically.

The buttons and allow switching quickly between the *log(y) vs 1000/x scale* and *normal scale* representation.

12 Other Tool Bar Options

The *Make Chart Area Quadratic* button is useful for reports which often contains quadratic charts. This function adjusts the height of the diagram and leaves the width untouched.

Hide and *show the legend*. The first icons is shown if the legend is visible and hides the legend, the second is shown when the legend is hidden and shows the legend (see also the paragraph "The Legend").
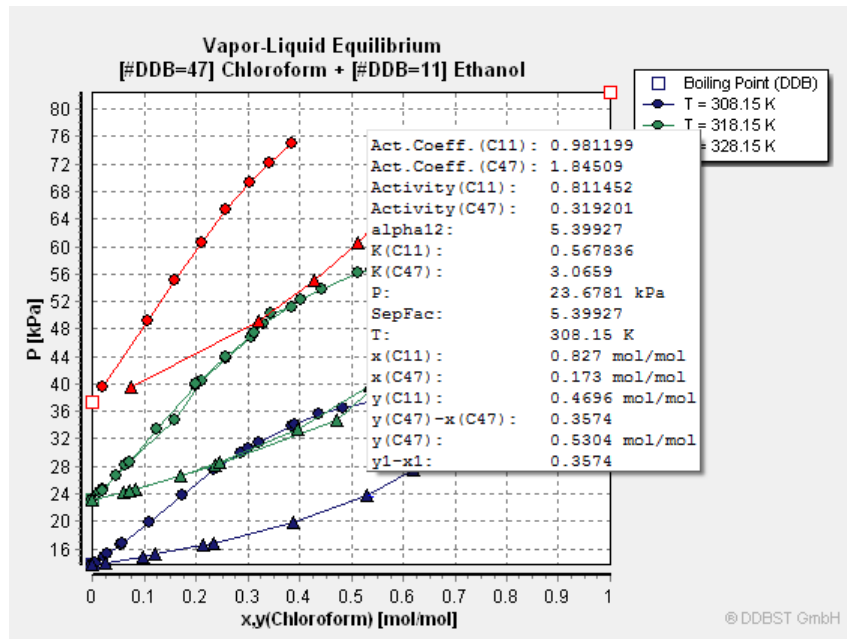

Figure 8: Point Specific Data in a Floating Window

Hide or show a floating window with point specific data.

Hide or show dotted grid in the diagrams.

Hide or show context information box with further data point and data series information.

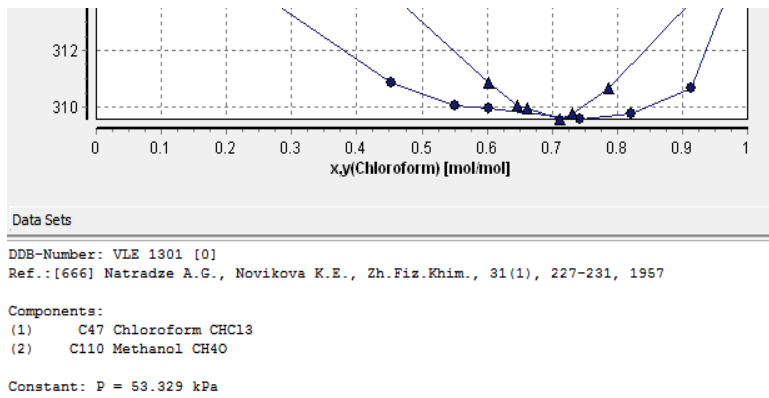The *Chart Editor* is a powerful integrated tool which allows to change nearly all settings in the chart. This

```
DDB-Number: VLE 1301 [0]
Ref.:[666] Natradze A.G., Novikova K.E., Zh.Fiz.Khim., 31(1), 227-231, 1957

Components:
(1)     C47 Chloroform CHC13
(2)     C110 Methanol CH4O

Constant: P = 53.329 kPa
```

Figure 9: Context Information Box

editor allows to change almost every details including hiding lines and points, changing every color, modify markers, etc.
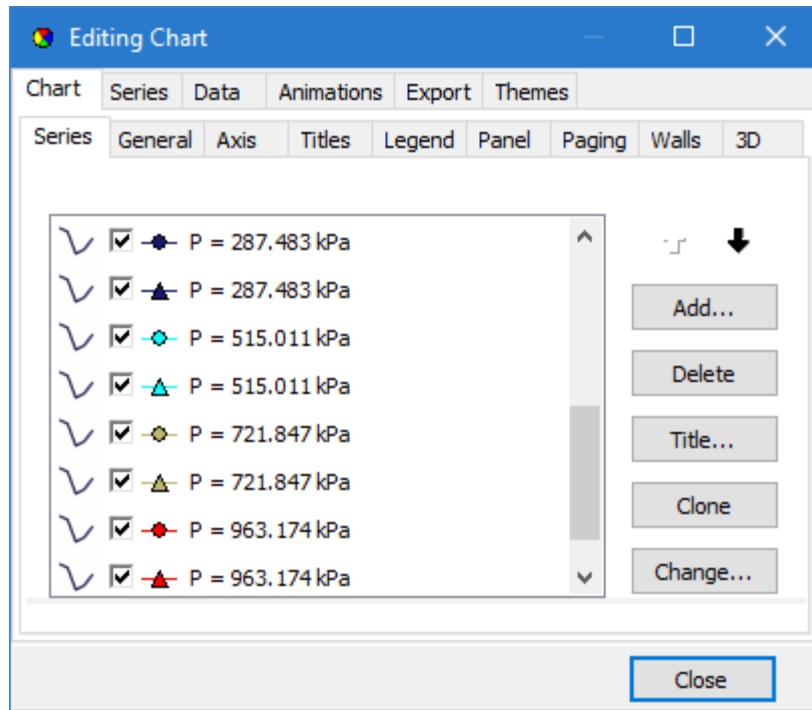

Figure 10: Chart Editor

Set Chart Size: This dialog allows to set the size of the diagram in pixels. This feature is especially useful when the size of the diagram is important like they are in publications.

Show List of Systems: If a diagram contains data from multiple mixtures (=systems) this function allows selecting the data for a single system and browse through the diagrams for all single mixtures.
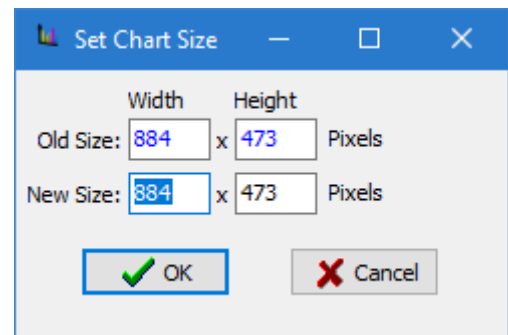

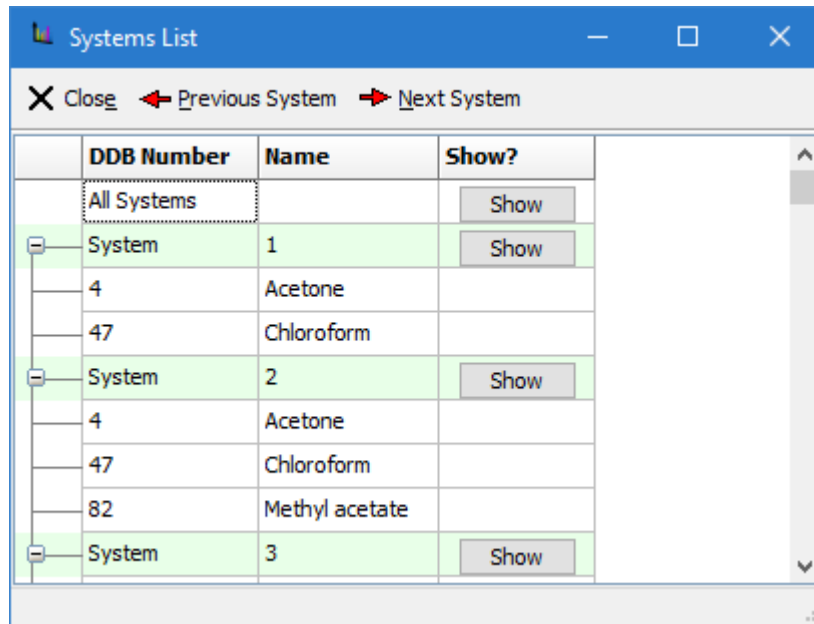*Figure 11: Setting diagram size manually*

Figure 12: List of Systems

1.6 Customizing 3D-Charts

The 3-dimensional chart has some additional features represented by the tool buttons which are only visible when a 3D-chart is active.

When the **3D Normal Mode** is activated the mouse can be used to zoom and scroll the chart like in the 2D mode.

When the **3D Rotate Mode** is activated the mouse can be used to rotate the chart in all directions. When the chart is in "orthogonal mode" at the beginning of the rotation the orthogonal mode is automatically turned off.

When the **3D Move Mode** is activated the mouse can be used to move the chart around in the plot area.

When the **3D Zoom Mode** is activated the mouse can be used to change the size of the chart. When the global option "Zoom Text" is set the size of the axis labels changes with the size of the chart.

When the **3D Depth Mode** is activated the mouse can be used to change size of the depth axis.

The **Toggle Orthogonal** button can be used to switch to the orthogonal chart and back. The size of the depth axis and the zoom scale is set for the orthogonal chart separately.

To switch between 2D and 3D the **Toggle 3D Mode** button can be used.

2 Save and Copy

The ⊟▾ button can be used to save the chart as enhanced meta file (EMF), bitmap (BMP), D2P (a DDB internal file format), PNG, or TEE (the chart's own format). The save option is partially also available in the chart context menu.
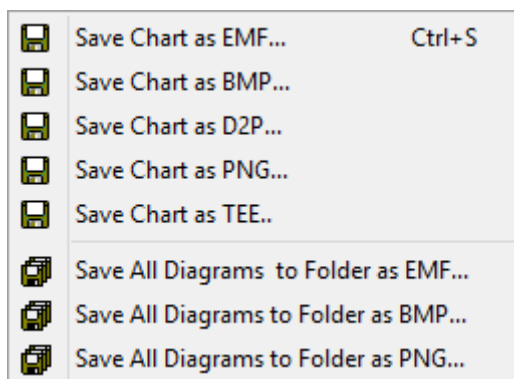
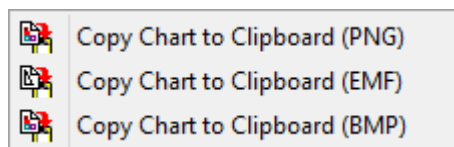The "Save All Diagrams" function allow storing all diagrams in the current windows to a specified folder. The plot program automatically generates file names describing the content.

The ![icon] button can be used to copy the chart content to the clipboard as EMF (enhanced Metafile), as BMP (Bitmap), or as PNG (Portable Network Graphics).

D2P files are a DDB internal format that is described in the separate document "Plot Input Files for Ternary and Binary Plots.pdf".

3 Global Plot Options

The global plot options dialog can invoked by a tool button. The plot options change all diagram for all properties and data types.
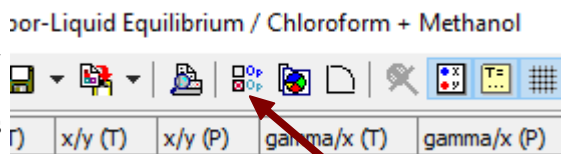
1. **Zoom Text (3D only)** – This concerns axis descriptions.

2. **Restrict Rubber Band Length** – This limits the length of the connection of the mouse cursor to the closest data point. If the mouse moves further away the line is hidden.

3. **Display Full Data Point Info in Status Bar** – If checked all available data are displayed and if unchecked only the data used in the diagram is shown

4. **Show Status Info as Hint** – The information shown in the status bar is also shown in a hint window. The option "Display Full Data Point Info in Status Bar" also affects this option.

5. **Use Window Color for Info Area Background** – If this option is checked the information area use the normal Windows background color for windows; if unchecked the color for button is used.

6. **Zoom Outside Default Boundary** – If this option is checked some fixed boundaries, especially the boundaries 0.0 and 1.0 for mole fractions, can be ignored for zooming and panning.

7. **Round Constant Temperatures to x Decimal Places for Grouping** – This option is meant for isothermal data sets and groups data sets at slightly different temperatures control by this setting.

8. **Use Component Names (Axes)** – This option switches between the display of full component names or the display of the DDB number only.
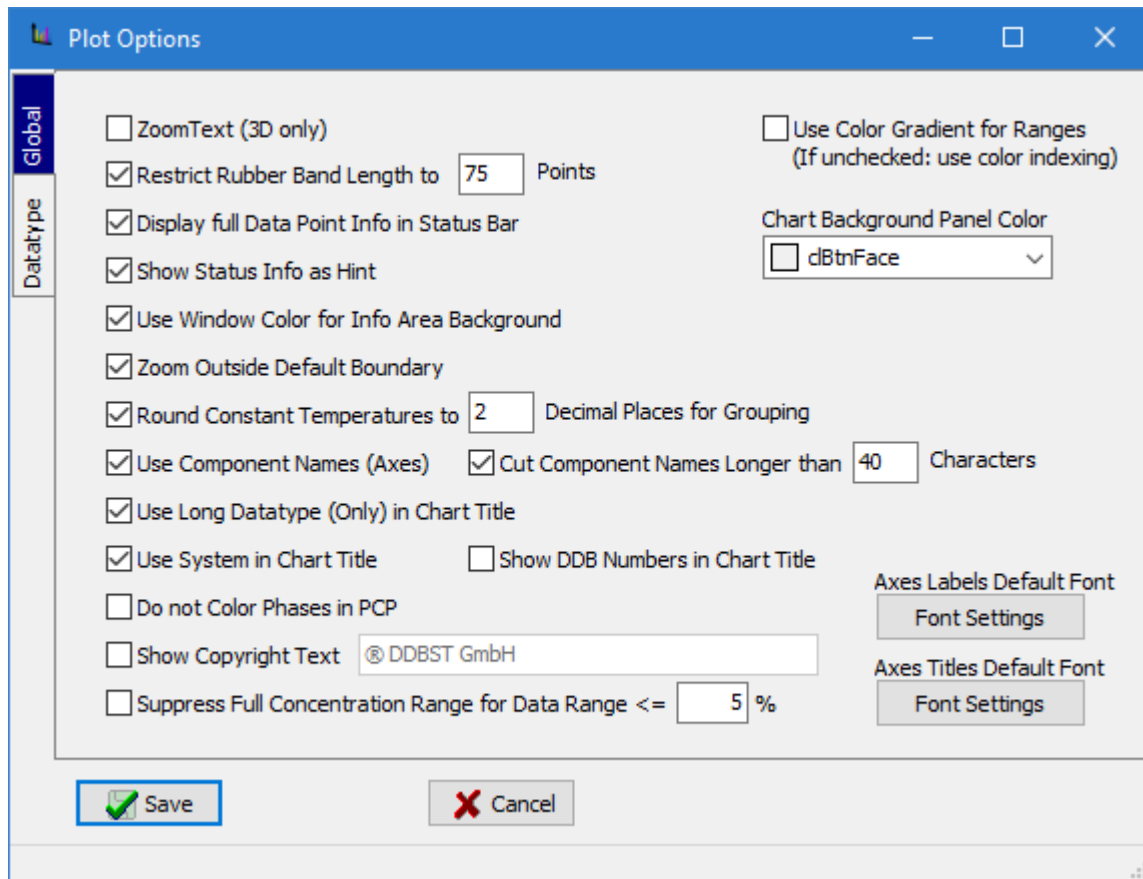
Figure 13: Global Plot Options

9. **Cut Component Names Longer than x Characters** – Place in diagram is scarce and this option switches between the display of long names and a shortened form.

10. **Use Long Datatype (Only) in Chart Title** – This option switches between the long display of a data type (e. g. Vapor-Liquid Equilibrium) and the short corresponding abbreviation (e.g. VLE)

11. **Use System in Chart Title** – Either the component names of the current system are shown or not

12. **Show DDB Numbers in Chart Title** – If this option is set the component names are preceded by their DDB number in square brackets. This option is also affected by the "Use System in Chart Title" setting.

13. **Do Not Color Phases in PCP** – Normally the plot program uses different colors for the different phase (vapor, liquid, etc.) for pure component properties (PCP). Unchecking this option will result in a single color for a single property ignoring the different phases.

14. **Show Copyright Text** – This setting allows adding a text in the right-bottom of the diagrams.

15. **Suppress Full Concentration Range for Data Range <= x %** – Some data types, e. g. solubilities only cover a small concentration range, may be below 1 % of one component in another. This option switches between the display of the full concentration range, e. g 0.0 to 1.0 mol/mol for mole fraction and the zoomed-in display.

16. **Use Color Gradient for Ranges** – This option affects the color of series over a temperature or pressure range. If this option is checked the color moves from blue for small values to red for high values. If not checked the color is arbitrarily selected from a predefined list of colors.

17. **Chart Background Panel Color** – The background color of the chart can be selected here.

18. **Axes Labels Default Font** – The font for the labels of the left, bottom, and depth axes and its size and color can be changed here.

19. **Axes Titles Default Font** – The font for the titles of the left, bottom, and depth axes and its size and color can be changed here.
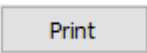
4 Printing

To avoid undesired results printing is only available using the button to open the **print preview dialog**.

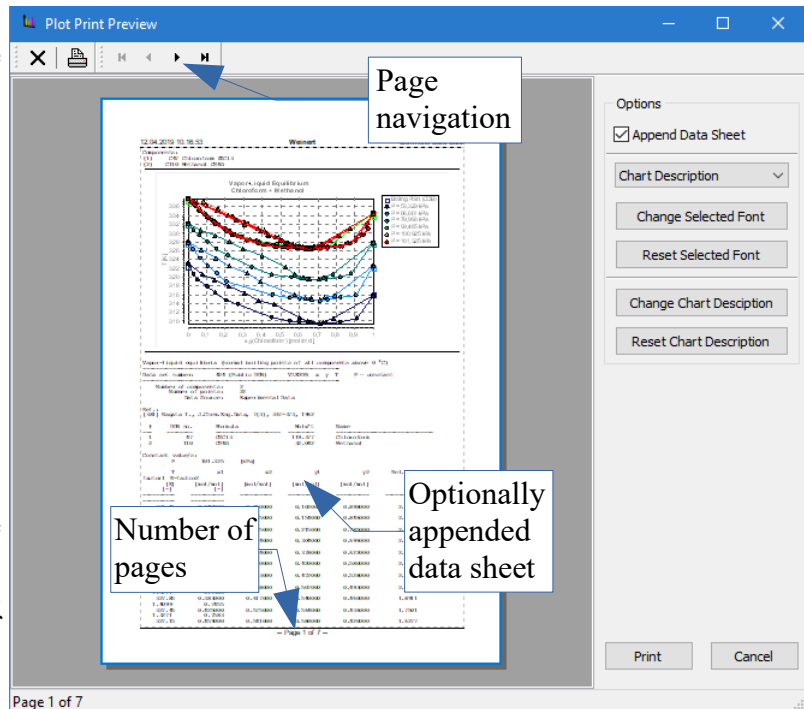The preview allows to set the fonts for

1. chart descriptions
2. data descriptions
3. header and footer

Additionally the chart description can be modified.

The "Append Data Sheet" option allows to append the data sets as text below the diagram and on following pages.

The [Print] button calls the standard Windows print dialog where a printer, the print area, and the number of copies can be selected.

The preview dialog support zooming the print area by left-clicking ( ) on the page.

Figure 14: Print Preview