Edit Pure Data

Editing / Modifying DDB Pure Component Data

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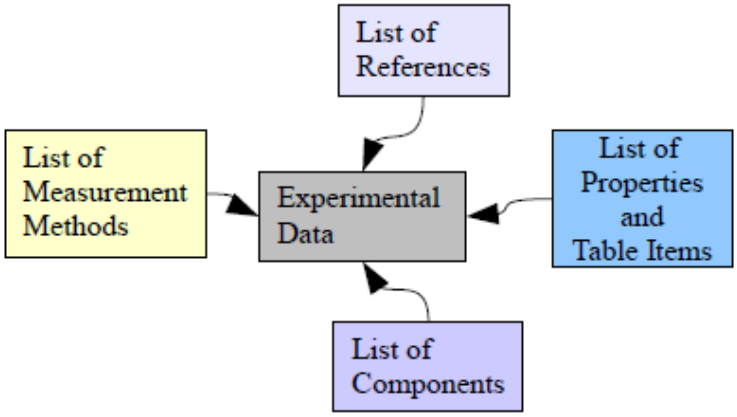
1 Introduction

This document is a tutorial for storing private pure component data in the Dortmund Databank (DDB).



The pure component properties database contains experimental data plus additional data like references, measurement methods, a component specification and some other related information.

Components, measurement methods and references are stored separately from the experimental data. It is necessary to update these external lists before (new) references, methods, or components can be selected.

Properties and table items are also defined outside this editor in a definition file.

Figure 1: Simplified data bank structure

EditPureData does not edit sets in the database directly. Instead it works on files which can be added to the database. This working mode allows keeping originals of the edited data whereas the database only contains recalculated and even somewhat “trimmed” data.

Editing data bank sets directly is possible though and will be explained at the end of this tutorial. This document is a stepwise introduction in the usage of this program. It starts with the necessary prerequisite for all DDB data sets. The main window looks as follows:

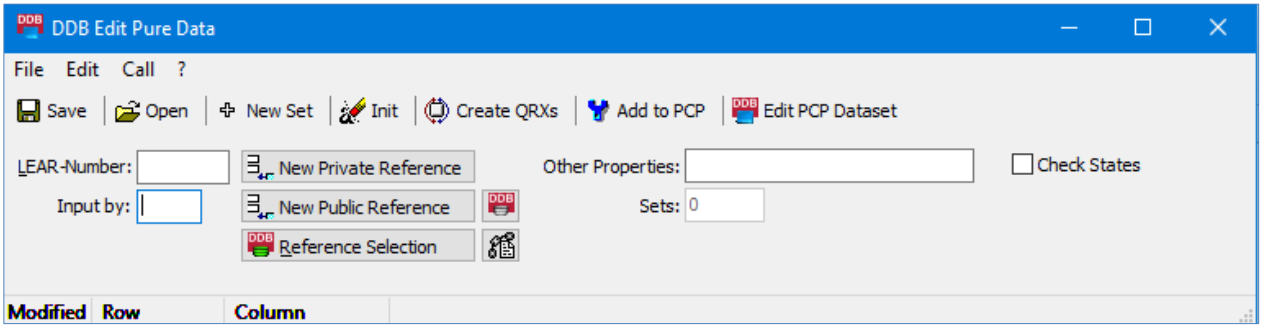


Figure 2: Main window

2 Defining the Reference

Every data set in the DDB is referenced. The reference is usually an article from a scientific journal but might also be a thesis or a report.

2.1 Adding a New Reference

For new private data sets it is recommended to create a new private reference.

A new reference can be inserted by selecting the button *"New Private Reference"*. A menu item in the "Edit" menu is also available. If no private literature databank is present, the program asks if it shall create a new one. After confirming with "Yes" the literature management program displays the edit dialog for a new reference (see below).

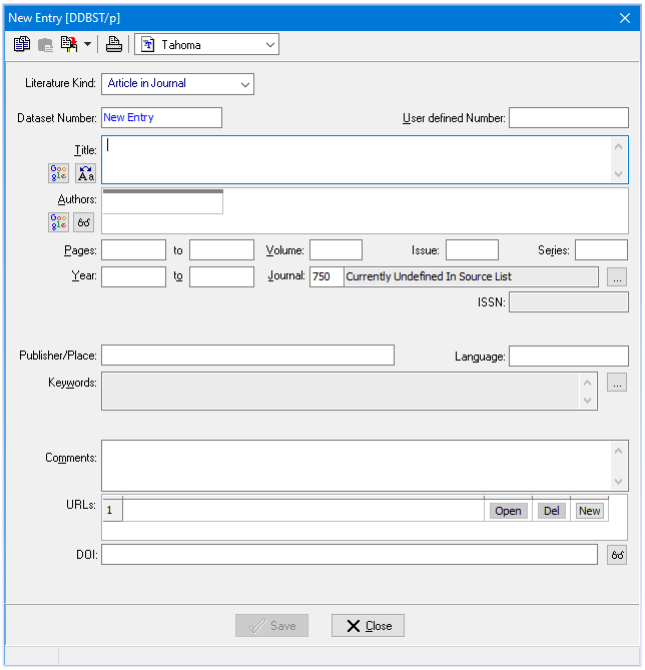


Figure 3: New reference editor

None of the entries are necessary to enter; even the completely empty sheet can be saved. But it is recommended to define at least authors.

A more detailed description of the literature management program DDB Literature is available.

2.2 Searching for References

If you don't want to create a new reference you have to search the available literature databank for the wanted article or report. After selecting the "*Reference Selection*" button a search query dialog is opened.

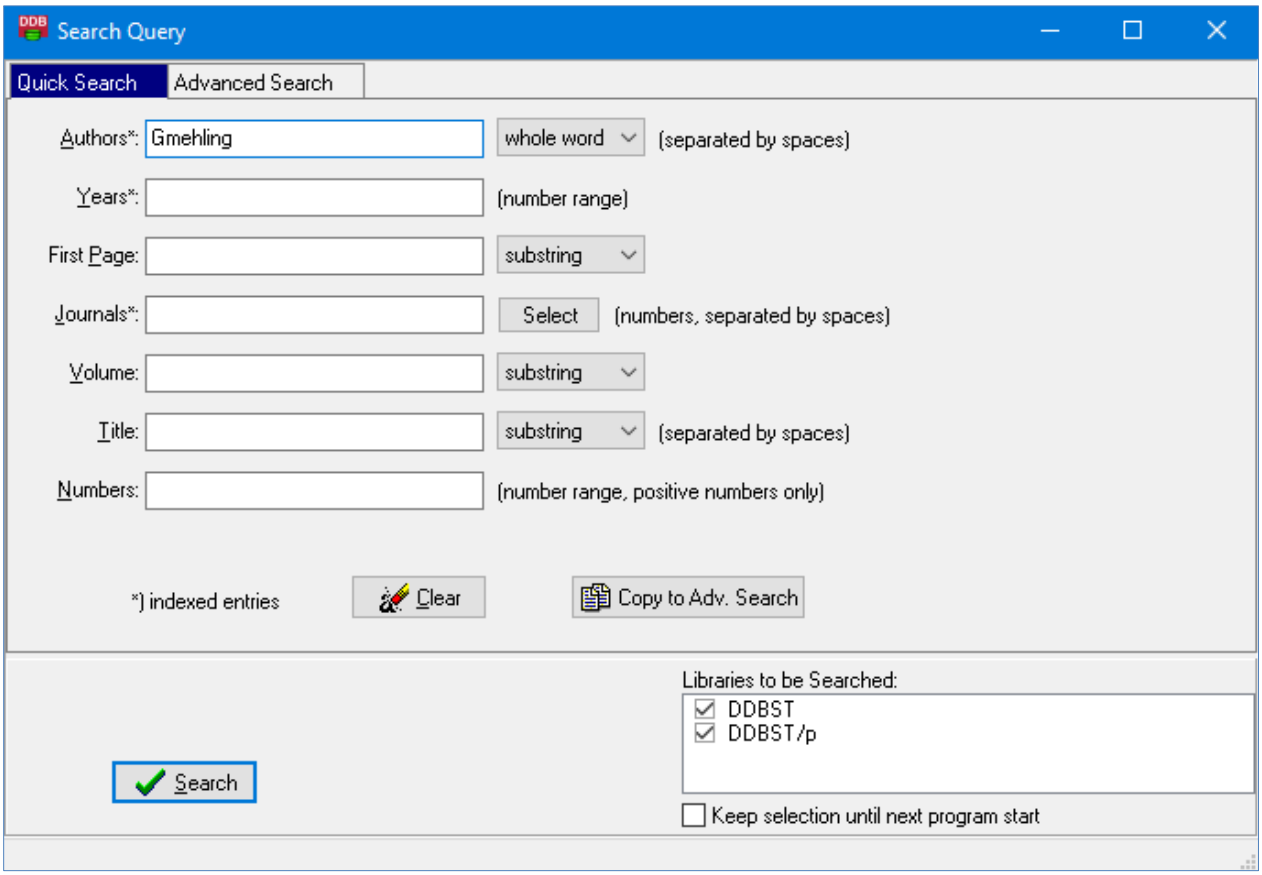


Figure 4: Reference search – search query.

The result for the given example is

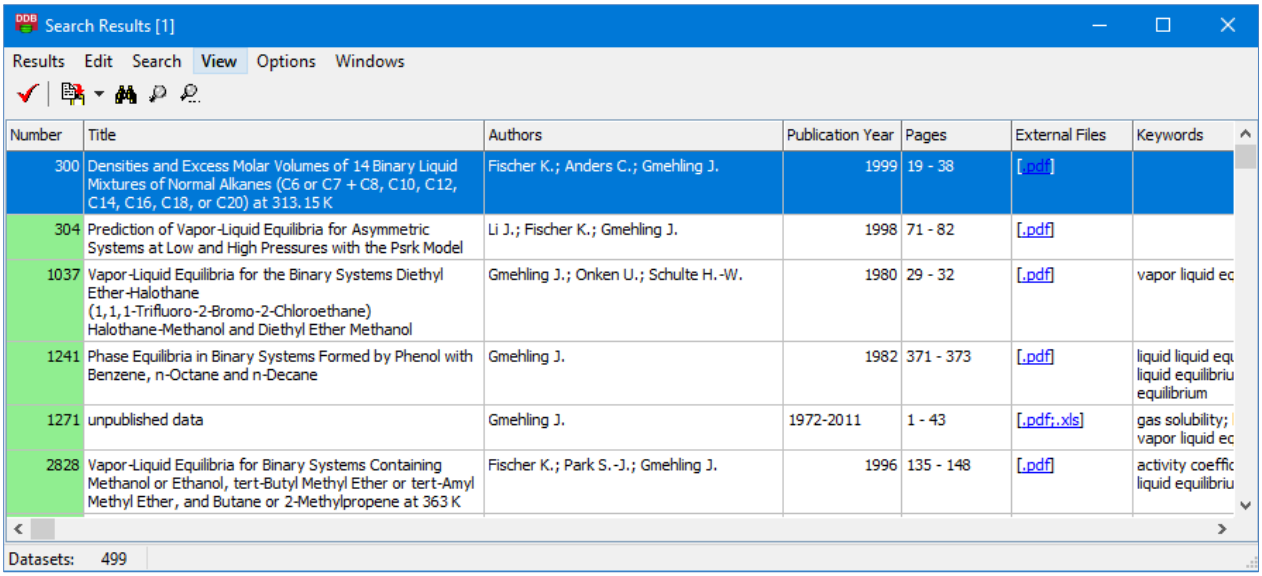


Figure 5: Reference search – search results.

Select  to select the reference.

3 Adding Datasets to the Current Reference

EditPureData works reference-centered. All datasets from a single reference can be edited together.

For appending data sets to the current reference select the *New Set* button:

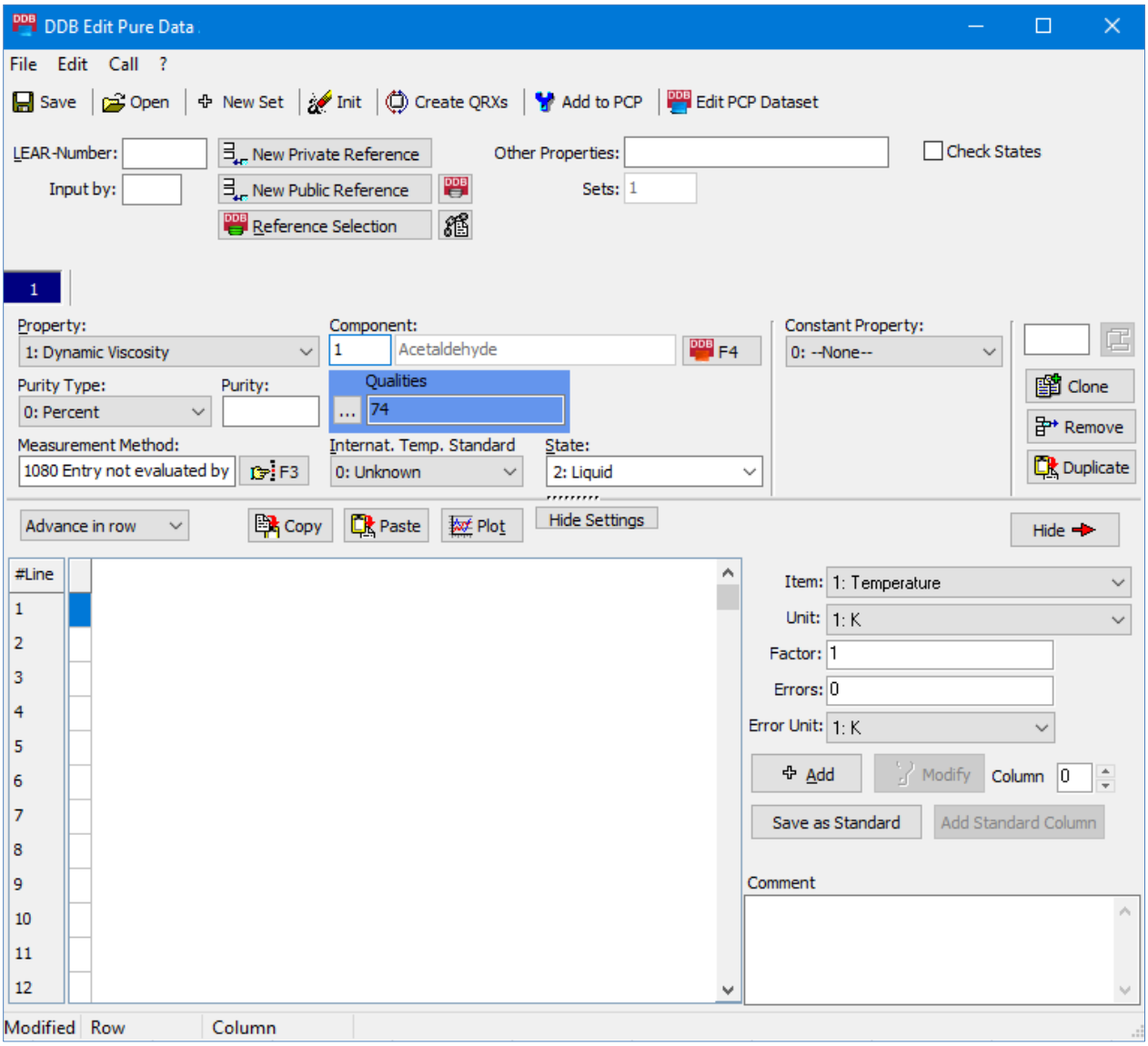


Figure 6: Adding data sets

The buttons *Clone*, *Remove* and *Duplicate* allow duplicating the current with data filled set, removing or duplicating the current set. It is also possible to move the current data set to another position (see button and input box above the *Clone*-button).

4 Adding Necessary Specifications for Single Sets

Necessary specification are

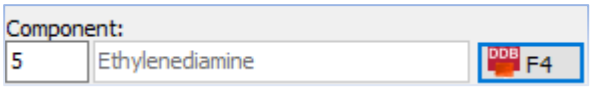
- Component
- Property
- Table entries
- Units of table entries

Additional specifications are

- Purity of the component
- Quality of the measurement or data
- Used internal temperature standard
- State ('Unknown' is possible)
- Measurement method
- A constant value, its unit and value
- Errors for table items with their units

4.1 Component Selection

The key F4 or selecting the *F4* button starts the program DDB Components. After a search you can double-click on a search result line and then the selected component is shown now in the edit field besides the search button.



4.2 Property Selection

DDB Edit Pure Data provides a list of available and editable properties. The list of properties is controlled by a definition file named PURSEL.DEF in the public DDB folder. It is intentionally not described here since it **must** not be modified by users. If there is an urgent demand for further properties please contact DDBST.

4.3 Specifying Table Entries and Their Units

The table entries and units dialog is a docked dialog at the right side of the data grid.

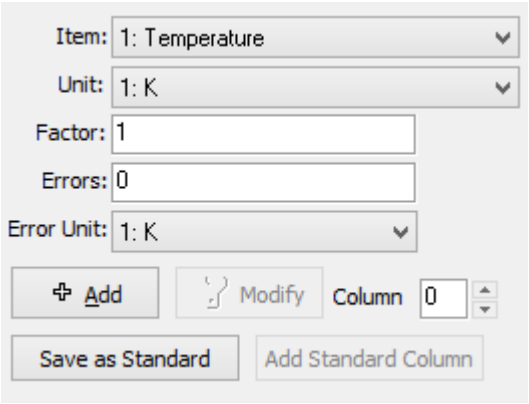


Figure 7: Table entry specifications

This dialog allows defining a single column in the data table. The table item can be either selected from the drop-down menu or from a pop-up-menu. The pop-up menu is somewhat more concise since it displays the complete list of table items at a glance.

The unit drop-down menu only contains the units for the currently selected table item.

The factor might be a numerical value but can also be one from this list opened by a pop-up menu:

LOG: logarithm to the basis 10
LN: natural logarithm
E10: power of 10
EXP: power of e
EINS: divided by 1 over value
TAUX: divided by 1000 over value

Additionally, it is possible to add an error for the entire column. It is also possible to specify a different unit which is only valid for the error (necessary for percent errors).

The button *Add* adds a new column to the table and the button *Modify* would change the specified column. The *Modify* button is only enabled if a column in the main edit window gas been selected. The "Column" spin-edit 

displays the selected column. EditPureData allows currently only up to six columns. If constant errors are used the column count decreases by the number of constant errors.

The *Save as Standard* button allows defining a single table item to be set as a standard which then can be added by a single mouse click of the *Add Standard Column* button. This is useful for editing multiple data sets in a row with the same independent data type like temperature or pressure.

4.4 Purity of the Component

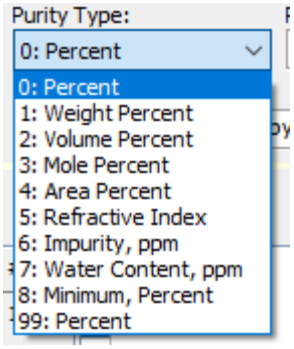


Figure 8: Purity

Both values 0 and 99 refer to an unspecified percentage.

4.5 Measurement Qualities and Source

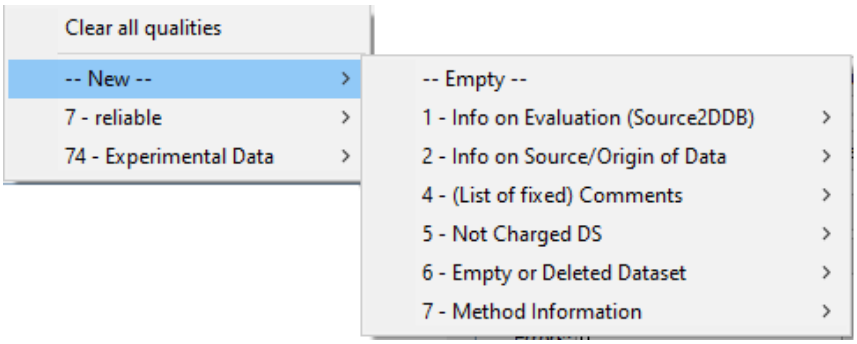


Figure 9: Qualities

Qualities: The dataset can be labelled by different Quality marks from seven categories.

4.6 International Temperature Standard

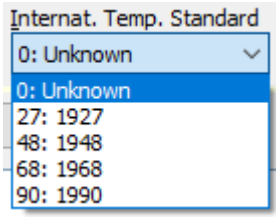


Figure 10: Temperature Standard

Five possible entries are possible like shown.

The ITS defines the (linearized) relationship between resistance and temperature in Platinum resistance thermometers.

4.7 State

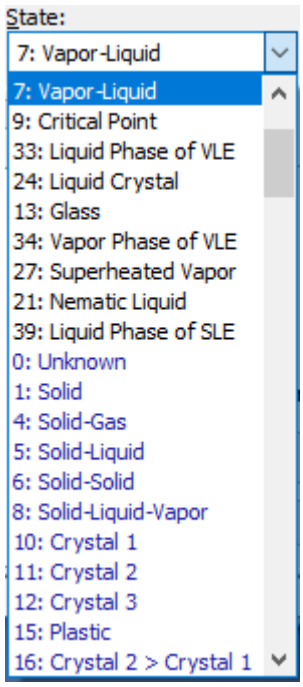


Figure 11: States Drop Down Menu

This menu is showing the complete list of possible states. The drop-down menu needs some scrolling to see all possible states. A right click on the menu opens a complete overview over all possible states.

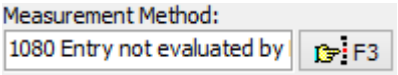
DDB Edit Pure Data has an internal list which states are suitable for a given property. These states are sorted to the front of the list. The selection of other state description is still possible, though.

Possible Pitfalls:

DDB Edit Pure Data allows selecting the state “Unknown” but since this entry is sometimes essential for a correct property identification it is very recommended to select the correct state.

Another possible pitfall is the consistency between the selected property and the state. Please be aware that some properties need special states. For example, the states “vapor-liquid” or “solid-vapor” have to be used for heats of vaporization. Other states are incorrect. DDB Edit Pure Data is unfortunately currently not able to check these possible problems.

4.8 Measurement Method



The list of methods for the pure component properties data bank is extremely long since it more a collection of random strings imported from many sources than a man-made validated list of methods.

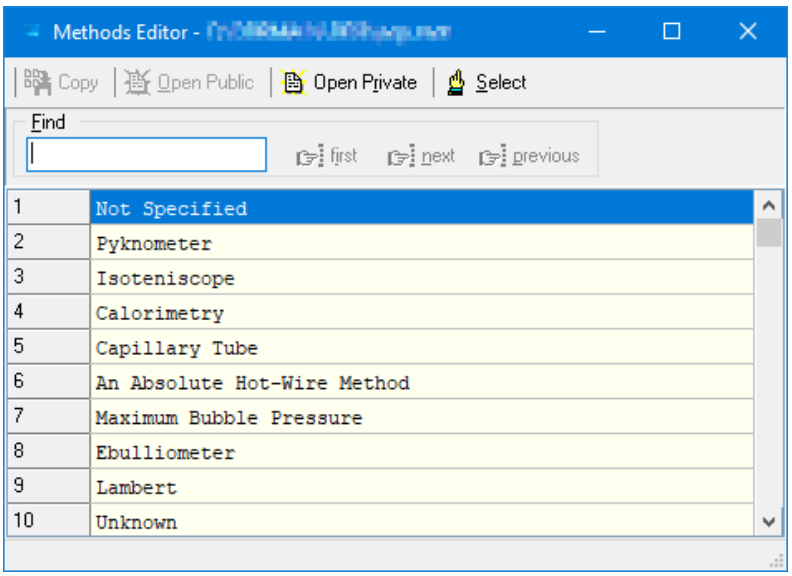


Figure 12: Measurement methods

A method can be selected by the *Select* button or by double-clicking the line.

Open Private resp. *Open Public* allows to switch a public and a private method's list.

4.9 Constant Property, Value and Unit

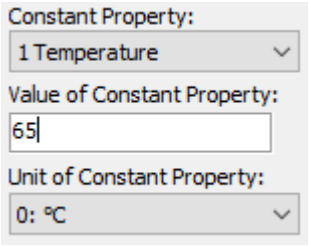


Figure 13: Constant

It is possible to define exactly zero or one constant value for a dataset.

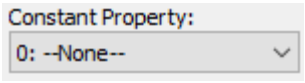


Figure 14: No constant

4.10 Data Input

Data input can be started after all columns have been defined. The specified table entries are displayed in the top rows of the columns together with their units, factors, and column errors.

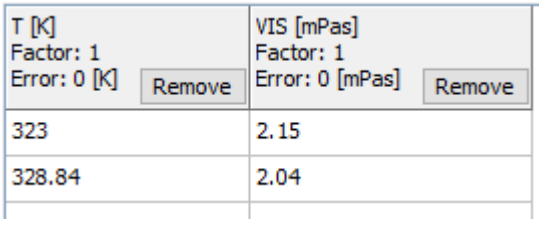


Figure 15: Example input

In this example we have two columns – a temperature and a viscosity column.

The options “Advance in Row” and “Advance in Column” change the behavior of the return/enter key for the “auto-advance mode” of the grid. After typing a value and hitting the enter/return key the cursor jumps to the next cell either in the next row (“Advance in Row”) or the next column (“Advance in Column”).

The button *Plot* allows displaying a quick plot of the currently edited data set. If there are already data sets available in the pure component properties data bank these data are plotted together with the new set.

The new data points are red squares, the PCP data points are black stars.

The diagram can be copied (as metafile) and printed. The *Show DDB Sets* button starts the Dortmund Data Bank program and displays the data sets already available in the DDB.

The "Scales" allows switching between the display of "x vs. y" and "1000/x vs. log y".

The "Polynomial Fit Deviations" can be used to take a quick look if the experimental data points are lined up properly – which is obviously a suitable criterion only for some properties.

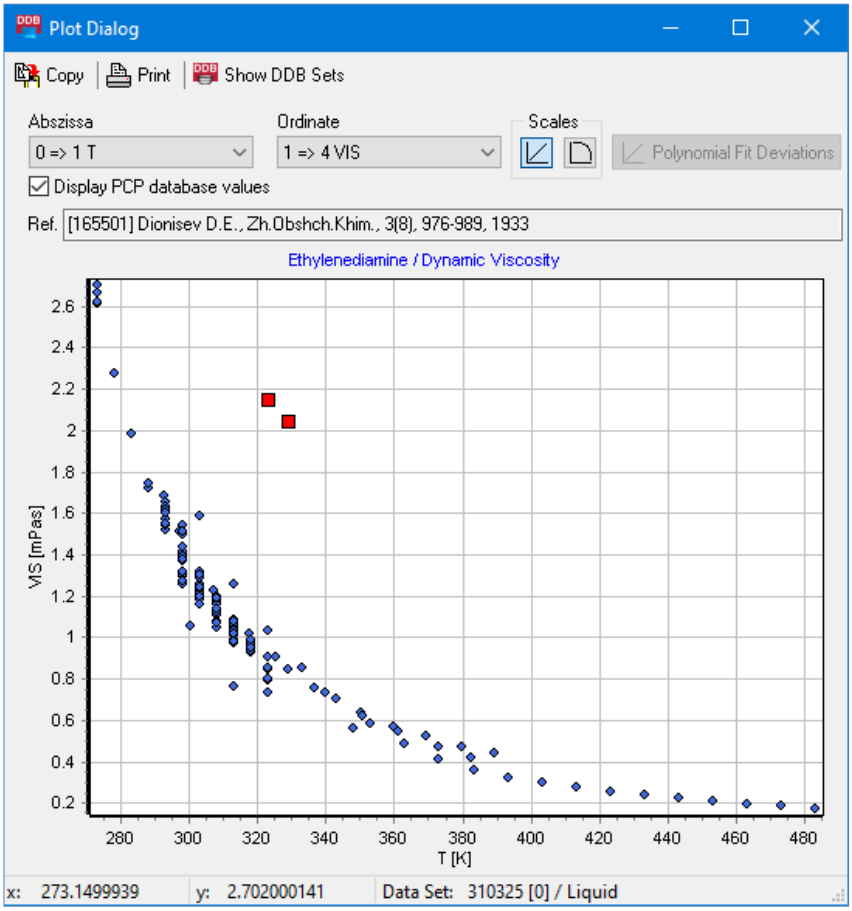


Figure 16: Plot

The buttons *Copy* and *Paste* allow to copy and paste the data grid to and from the Windows clipboard – for modifying data outside DDB Edit Pure Data e. g. in a spread-sheet.

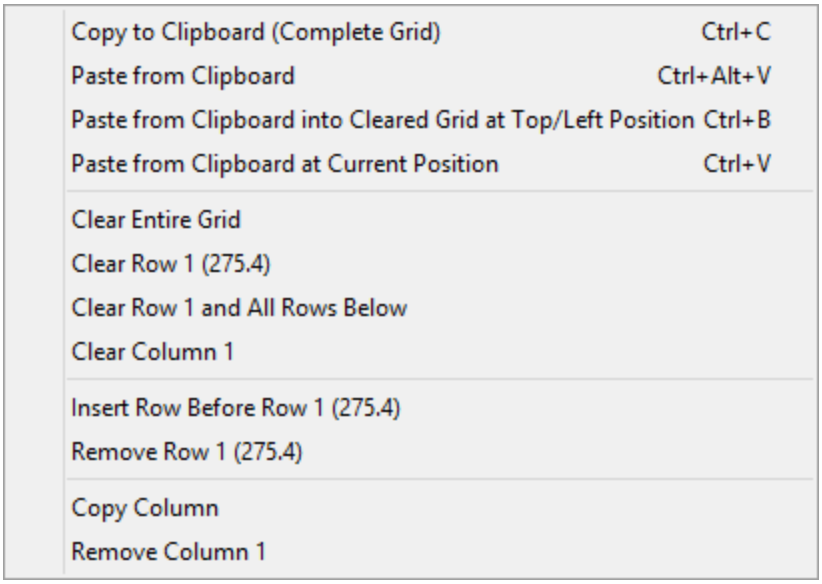


Figure 17: Data grid context menu

The data grid has a context (pop-up) menu with some additional functions.

The functions do not change the column specifications, they only manipulate the grid content.

5 Saving Data to File

After selecting the *Save* button a standard Windows save dialog is used to determine a filename.

The filename extension must be ".ol".

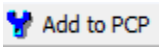
DDB Edit Pure Data has not stored any data in the database yet. The stored file contains the originally typed data and is a common text file where the single entries are identified with tags.

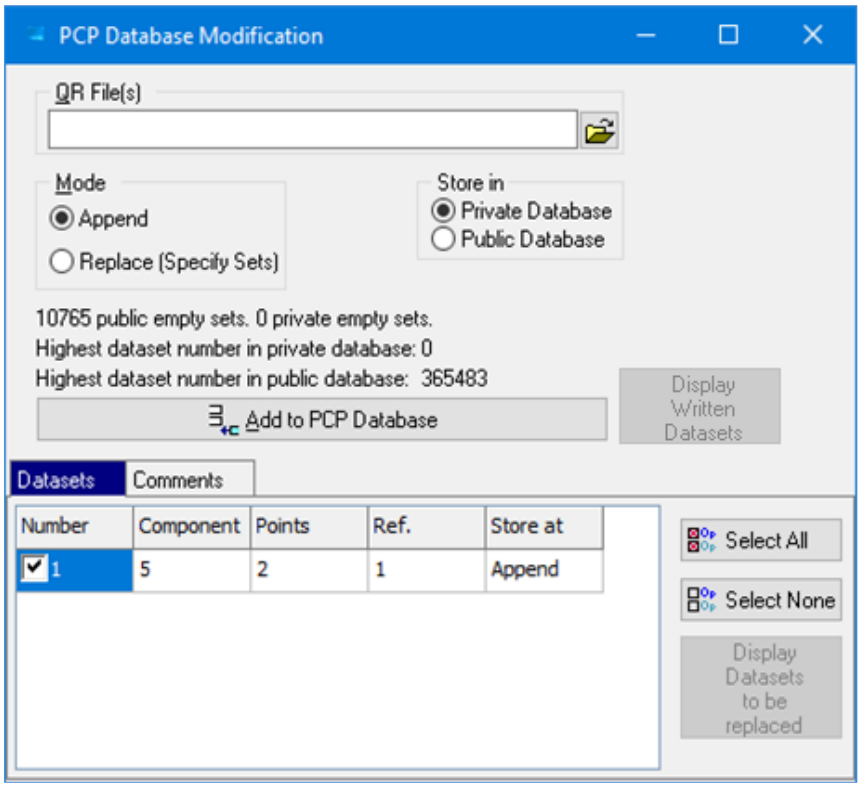
It is recommended to store and archive these files for future maintenance. Only these files can be reloaded.

In the background DDB Edit Pure Data automatically stores another files with the same name but different extension.

The "QRX" files contain recalculated data and will be used to append the data to the pure component properties database.

6 Adding Data Sets to the Private Databank





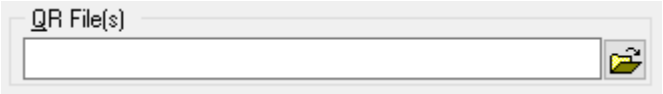
This dialog might need some seconds to be responsive because the program searches initially for deleted sets.

The list of deleted sets is necessary because DDB Edit Pure Data offers an option to overwrite previously removed data sets.

Figure 18: Adding data sets to the data bank.

The following steps are necessary to add datasets to the pure component properties databank.

First Step: Select "QRX" or "QR" files



The program uses a standard Windows open dialog. After the data sets have been loaded the program displays the number of data sets found ("`File contains 15 data set(s)`") in the "Comments" page and the complete list of sets in the "Datasets" page.

Second Step: Select update mode.
It is possible to append new data, overwrite existent datasets or overwrite already deleted datasets

1. Append: All datasets found in the file will be appended at the end of the databank. It is possible to select only some of the loaded data sets by setting or removing the check marks in the "Data sets" page (see Figure 28 Dataset List - Append Mode).
2. Replace (Specify Sets): The datasets will replace existent datasets. The user has to specify the dataset number (see Figure 29 Data Set List - Replace Mode).

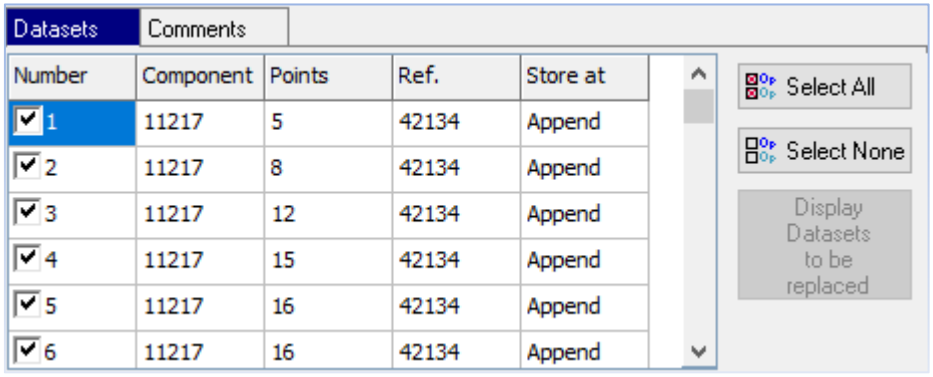


Figure 20: Data set list – append mode

Third Step: "Input by" specification.

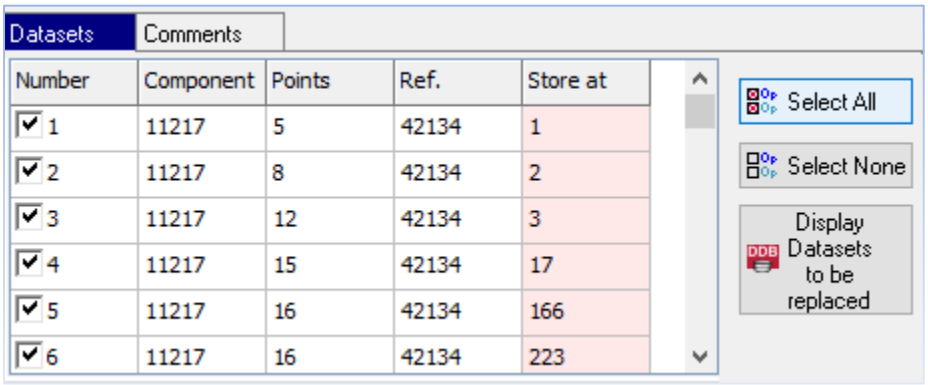


Figure 19: Data set list – replace mode

Every dataset has a two-character signature for the specifying the editor of the data sets.

The button *Display Data Sets to be replaced* starts the database retrieval program and displays the data sets selected for replacement.

Fourth Step: Select database

It is possible to store data in the public database (from DDBST) and a customer's database (private). Adding data sets to or replacing data sets in the public database is not recommended since future delivery would overwrite these changes.

Fifth Step: Add data sets

A last question has to be answered:

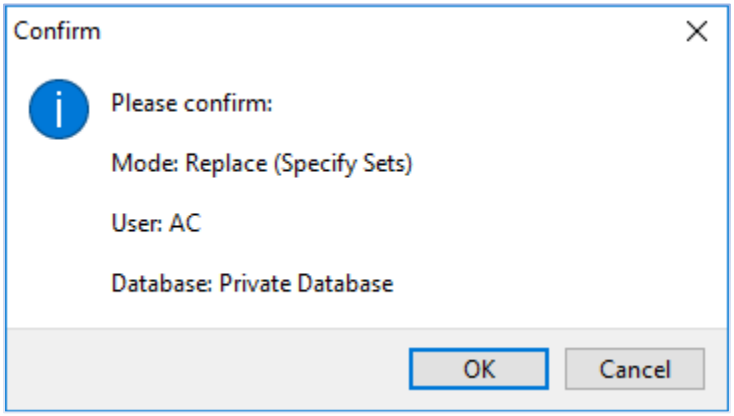


Figure 21: Confirm write access

After the data sets have been added DDB Edit Pure Data displays a protocol which shows the old data set count and some details of the new data sets like the reference and component number, the property code and the data set number.

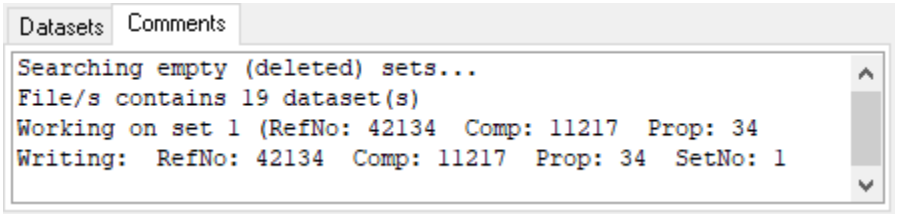


Figure 22: Update log

After this step the datasets are stored in the pure component properties database.

7 Modifying Datasets in the Database

If the original “ol” is not available or for a quick repair it is possible to modify data sets in the data bank directly. You have to know the data set number which can be obtained in the database retrieval program.

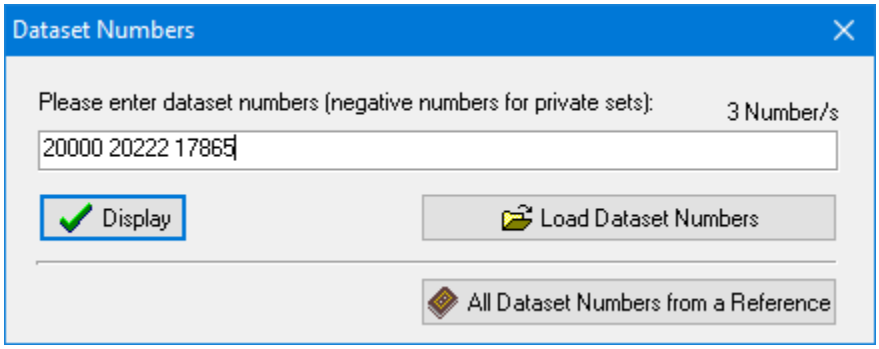


Figure 23: Edit window

The program opens a separate edit window for every data set entered in this dialog.

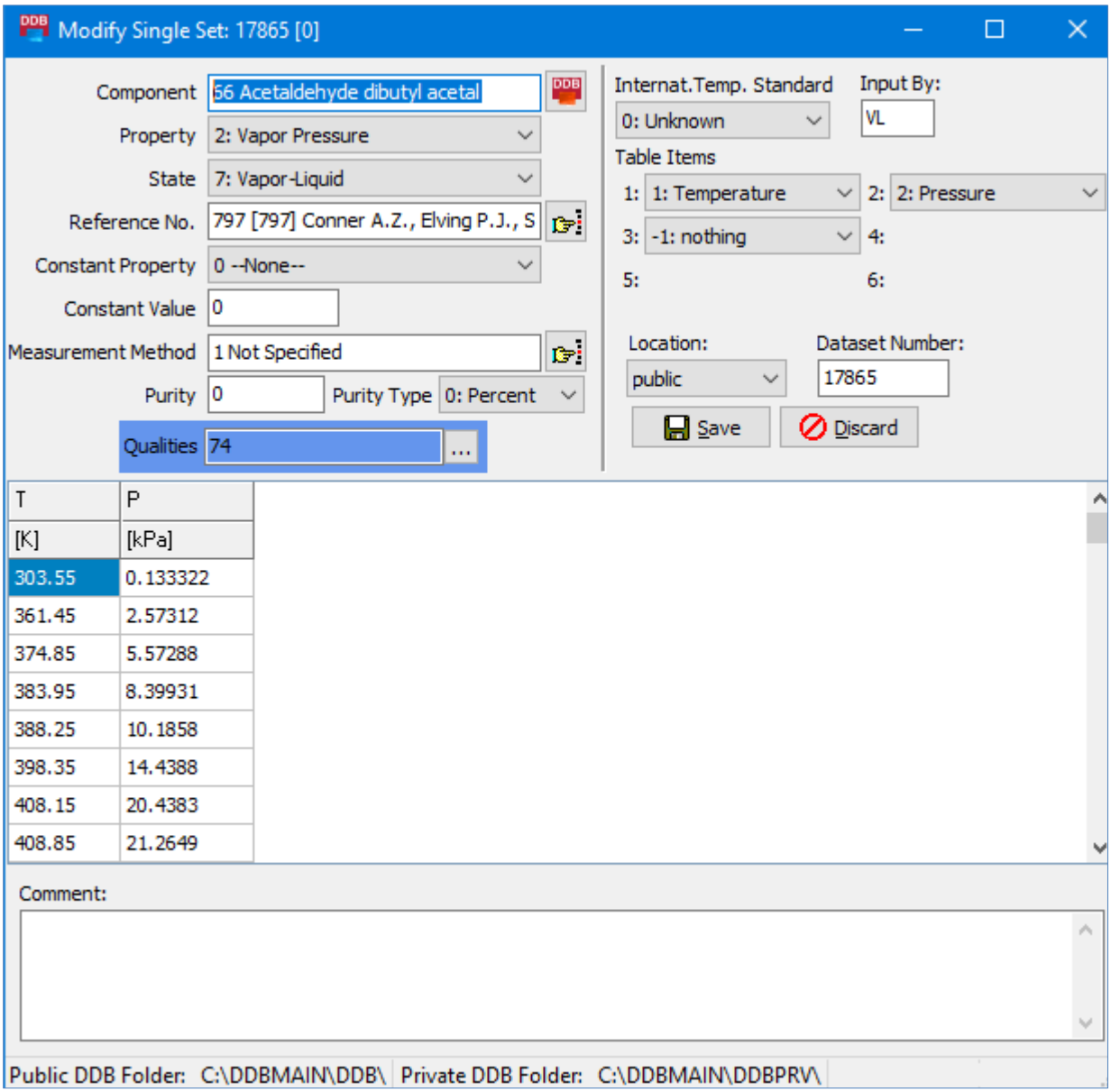


Figure 24: Direct database editor

The main difference is that the databank contains recalculated data sets with standard units and some few other restrictions. The editor does not allow to change units and the data set cannot be loaded from file or stored to disk.

Most other properties can be changed like it has been done in the normal file-oriented editor. Additional feature can be found in the context menu of the data grid.

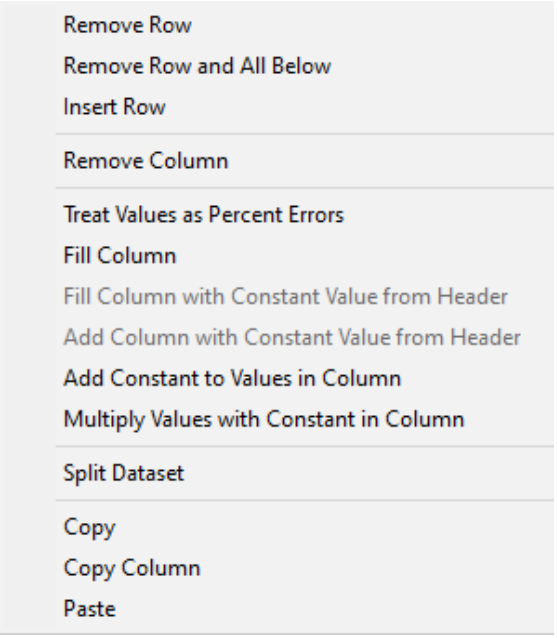


Figure 25: Data grid context menu

Several functions have been introduced due to common errors in the database.

The three buttons perform the following actions:

Save the modified data sets in the database.

Discard any modification