

ParameterDDB Organizer

DDBSP - Dortmund Data Bank Software Package



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1. Introduction

The parameter data bank contains fitted parameters. Many of the stored parameters are

- a variety of pure component properties like saturated vapor pressures, densities, viscosities, thermal conductivities and more,
- g^E model interaction parameters for Wilson, NRTL, UNIQUAC, and others,
- equation of state mixing rule parameters,

but there are (or can be) a lot more different types of parameters.

Sources for the parameters in the DDB software package are

- PCPEquationFit: Pure component properties equation parameters,
- RecVal: g^E model interaction parameters (complex simultaneous fit to different data types),
- OPT/SOPT: g^E model interaction parameters (simple T independent fit),
- GenMixRulesParameters: equation of state mixing rule parameters.

2. Getting Started

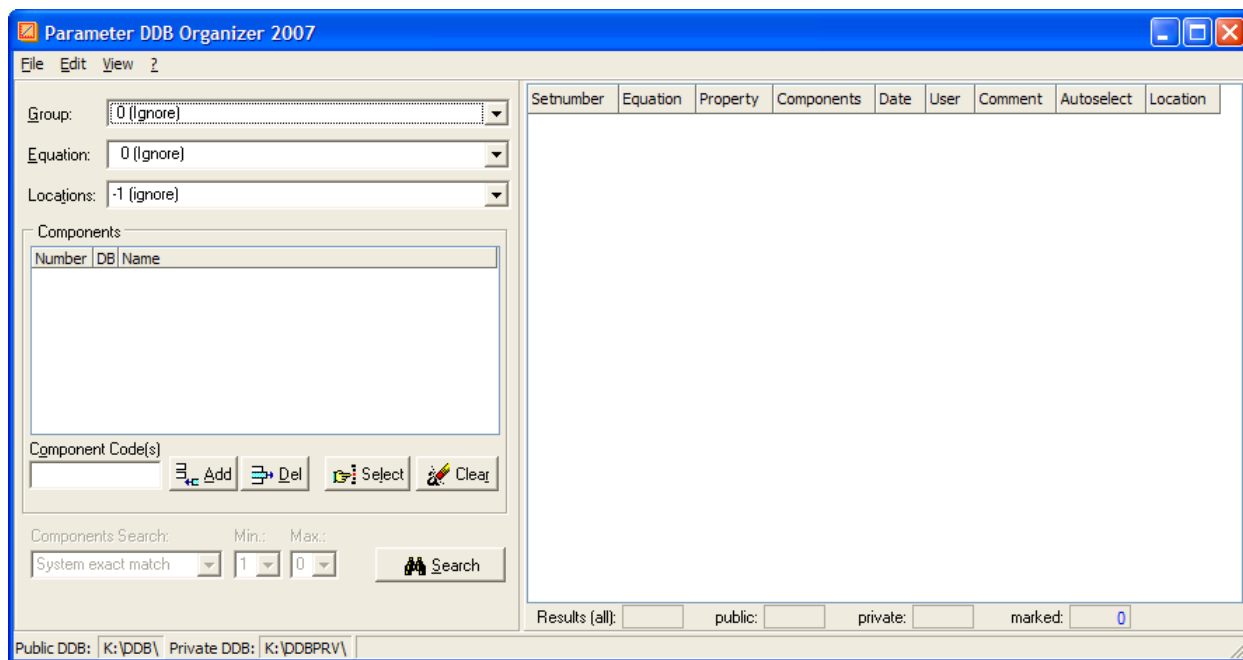


Figure 1: Opening Dialog

Searching

The Parameter DDB Organizer groups equations by their type.

These groups determine which equations are shown in the Equation combo box.

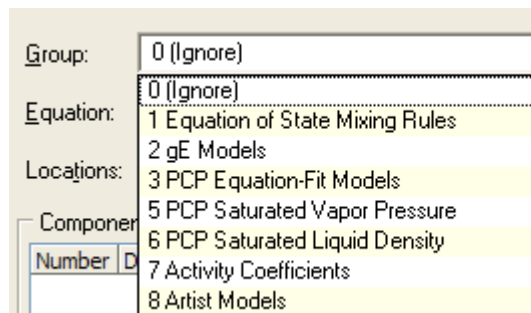


Figure 2: Group Selection

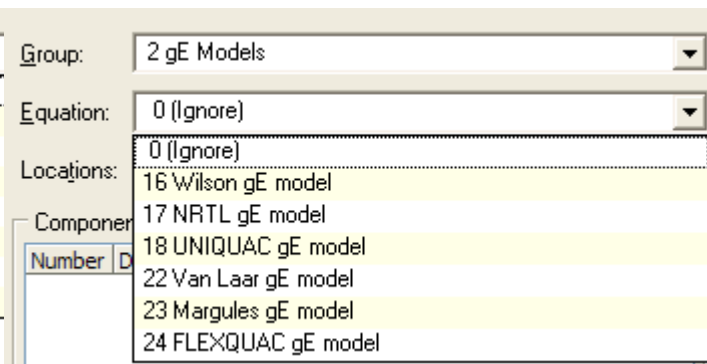


Figure 3: List of Equations (Group gE Models)

Locations are

- public (DDBST delivered parameters)
- private (custom parameters)

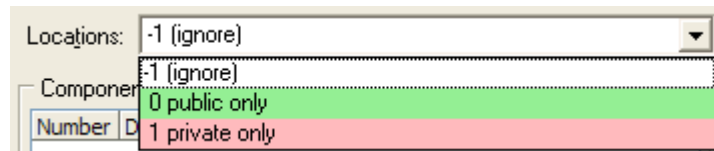


Figure 4: Locations

By using these configuration a search will result in displaying either all parameter sets from the parameter data bank or all all parameters set from a location or all parameter sets for an equation.

This search can be restricted to specific components or systems.

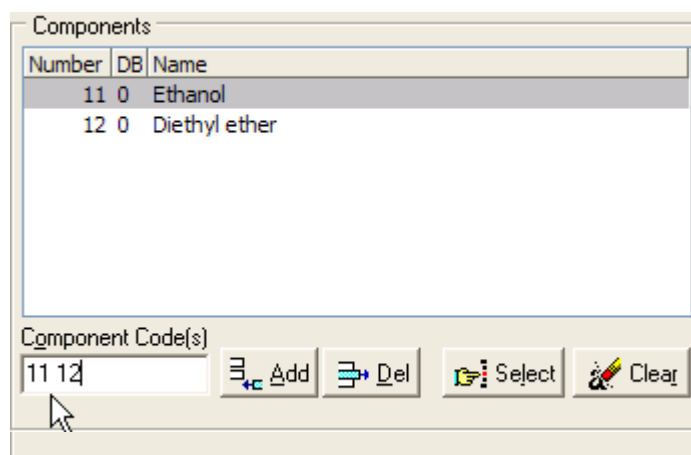
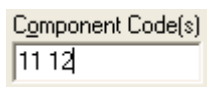



Figure 5: Component/System Specification


If the DDB component codes are known they can be typed directly in the “Component Code(s)” edit field.




The  button will read and display the component basic information.

The  button remove a single selected component. A single line in the component list can also be deleted

by double-clicking the line.

The  Select button calls the standard component selection dialog which allows to search the DDB component list by many different criteria.

The  Clear button removes all components.

The search for components can be performed in four different ways:

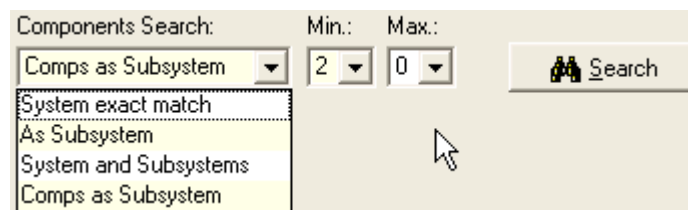


Figure 6: Component Search Options

- *Exact Match*: The list of components must exactly match.
- *As Subsystem*: The list of components must all be present in the parameter set but other components are also allowed.
- *System and Subsystems*: For unary parameter sets any single component specified in the search list will match. For binary parameter sets any binary system that can be build from the component list will match.
- *Comps as Subsystems*: Every parameter set is found where a single component of the defined components are available.

Search Result

The search result grid contains the following columns:

| Setnumber | Equation | Property | Components | Date | User | Comment | Autoselect | Location |
|-----------|----------------------------|------------------------------------|------------|------------|---------|---------------------|------------|----------|
| 11 | Wagner Equation (2-5-Form) | PCP - Saturated Vapor Pressures | 11 | 1996-05-15 | Cordes | | undef. | public |
| 22 | Wagner Equation (2-5-Form) | PCP - Saturated Vapor Pressures | 22 | 1996-05-15 | Cordes | | yes | public |
| 668 | Antoine Equation | PCP - Saturated Vapor Pressures | 11 | 2001-02-15 | Horstma | Antoine-Low from S | undef. | public |
| 679 | Antoine Equation | PCP - Saturated Vapor Pressures | 22 | 2001-02-15 | Horstma | Antoine-Low from S | undef. | public |
| 4025 | Antoine Equation | PCP - Saturated Vapor Pressures | 11 | 2001-02-15 | Horstma | Antoine-High from S | undef. | public |
| 4033 | Antoine Equation | PCP - Saturated Vapor Pressures | 22 | 2001-02-15 | Horstma | Antoine-High from S | undef. | public |
| 5839 | Cox Equation | PCP - Saturated Vapor Pressures | 11 | 1994-06-23 | AC | | undef. | public |
| 5850 | Cox Equation | PCP - Saturated Vapor Pressures | 22 | 1996-10-25 | AC | | undef. | public |
| 6737 | Andrade Equation | PCP - Saturated Liquid Viscosities | 11 | | | | undef. | public |
| 6748 | Andrade Equation | PCP - Saturated Liquid Viscosities | 22 | | | | undef. | public |
| 8610 | Vogel Equation | PCP - Saturated Liquid Viscosities | 11 | | | | undef. | public |
| 8621 | Vogel Equation | PCP - Saturated Liquid Viscosities | 22 | | | | undef. | public |
| 10208 | DIPPR Equation 105 | PCP - Liquid Saturated Densities | 11 | | | | undef. | public |
| 10219 | DIPPR Equation 105 | PCP - Liquid Saturated Densities | 22 | | | | undef. | public |
| 12355 | Polynomial (DNS) | PCP - Liquid Saturated Densities | 11 | 2002-02-04 | jk | | undef. | public |
| 12365 | Polynomial (DNS) | PCP - Liquid Saturated Densities | 22 | 2002-02-04 | jk | | undef. | public |
| 13216 | Polynomial (SFT) | PCP - Surface Tension | 11 | 1999-09-22 | KUHLMAN | | undef. | public |
| 13227 | Polynomial (SFT) | PCP - Surface Tension | 22 | 1999-09-22 | KUHLMAN | | undef. | public |
| 14791 | Polynomial (TCN) | PCP - Liquid Thermal Conductivity | 11 | 1998-08-26 | | | undef. | public |
| 14797 | Polynomial (TCN) | PCP - Liquid Thermal Conductivity | 22 | 1998-08-26 | | | undef. | public |
| 15200 | DIPPR Equation 101 | PCP - Saturated Vapor Pressures | 11 | | | | undef. | public |
| 15211 | DIPPR Equation 101 | PCP - Saturated Vapor Pressures | 22 | | | | undef. | public |
| 16577 | Mathias-Copeman Equation f | PCP - Saturated Vapor Pressures | 11 | 1999-01-21 | SRKC123 | | undef. | public |

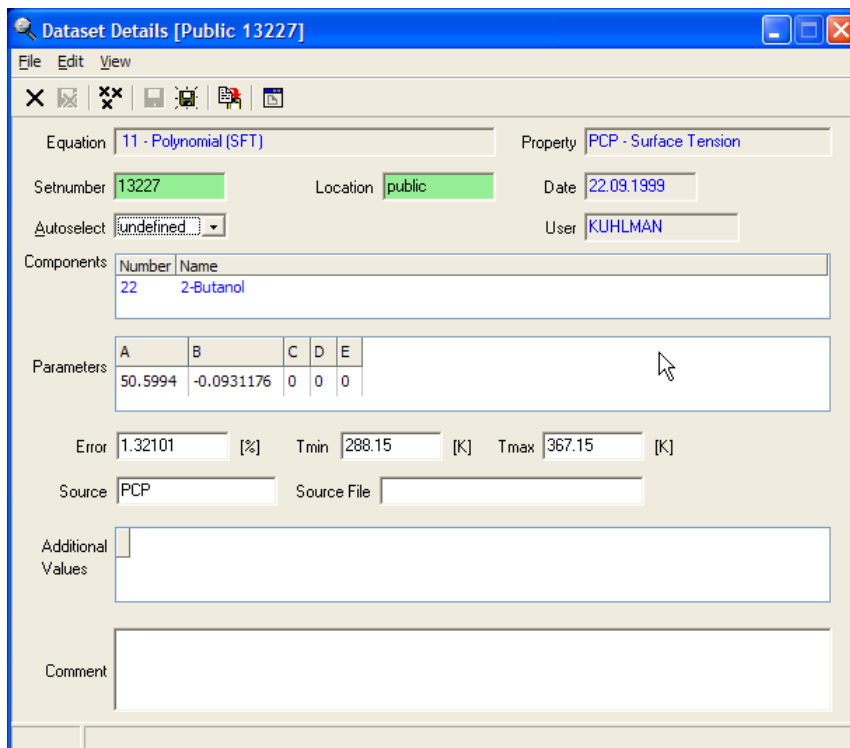
Results (all): 38 public: 38 private: 0 marked: 1

Figure 7: Search Result Grid

- “Setnumber”: ParameterDDB set number
- “Equation”: Description of the equation
- “Property”: Property which can be calculated by the parameters
- “Components”: DDB component numbers
- “Date”: Date of storage
- “User”
- “Comment”: Can be everything, often some source description
- “AutoSelect”: Flags recommended parameter sets (useful if more than one parameter set is available)
- “Location”: Public or private DDB folder

3. Single Data Set Display

The single sets look a little different for every equation because of the different forms. Always the same are the menu entries



1. File
 1. "Save": Saves changes
 2. "Append to...": Appends the data set to either the private or public parameter data base.
 3. "Save and Close": Save changes and closes the dialog
 4. "Close": Closes the dialog without saving
2. Edit
 1. "Copy": Copies the parameter set to the Windows clipboard
3. View
 1. "Show Main Window": Brings the main window to the front

and the corresponding tool bar buttons.

Additional the

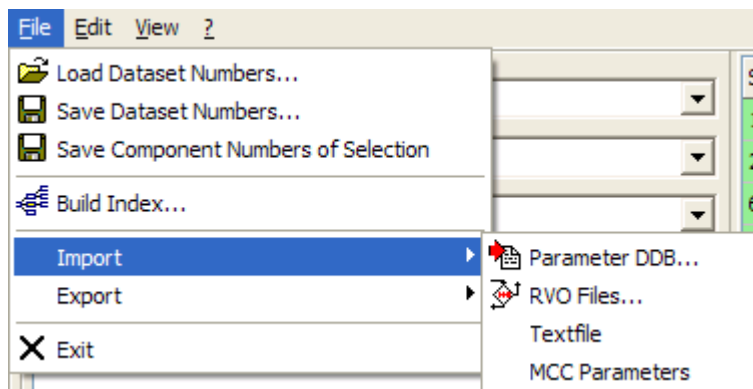
- Equation
- Property
- Set number
- Date
- User

| Key | Value |
|----------|------------|
| A | 50.5994 |
| B | -0.0931176 |
| C | 0 |
| C1 | 22 |
| COUNT | 1 |
| D | 0 |
| DateD | 1 |
| DateM | 6 |
| DateY | 2007 |
| E | 0 |
| EQID | 11 |
| Error | 1.32101 |
| LOCATION | 0 |
| SETNUM | 13227 |
| Source | PCP |
| Tmax | 367.15 |
| Tmin | 288.15 |
| User | cordes |

Figure 8: Copied Parameter Data Set

are always present. These five entries cannot be modified. The set number, the date and the user are set automatically by the program and the equation and property are the core identifiers of the set.

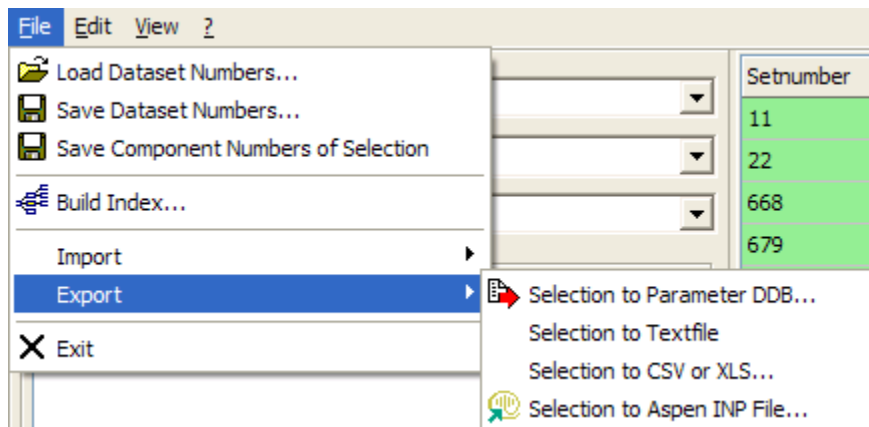
4. Import Parameter Sets



The Parameter DDB Organizer can import from

- other parameter data banks
- RVO files. RVO files are result files of the g^E model fit program RecVal.
- Text files: These text files have to be exported from the Parameter DDB Organizer
- MCC Parameters: Internally used for an import of file with Mathias-Copeman constants (used in PSRK)

5. Export Parameter Sets

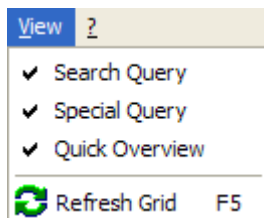


The Parameter DDB Organizer can export parameter sets to

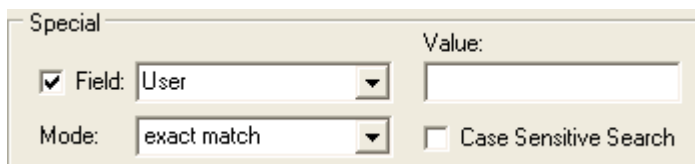
- another parameter data banks
- export to a text file

- to a CSV or XLS file (CSV: comma-separated values, XLS: Microsoft Excel file)
- Aspen INP files. These INP are project files for the Aspen simulator.

6. Special Views



These function allow to hide and show some parts of the main window. The “Search Query” has already been explained in an earlier chapter. The “Special Query” shows an extra search panel



where the parameter data set fields “User” and “Comment” can be searched.

The “Quick Overview” display a grid where the currently selected parameter set is shown in a very compact grid display.

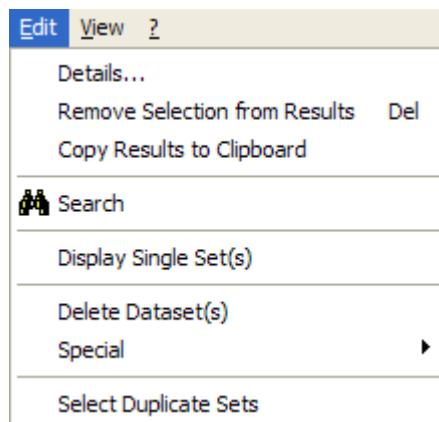
```
@BEGIN
A=3.87644
B=0.0619661
C=547.994
C1=22
COUNT=1
D=0.109738
EQID=9
Error=0.226752
LOCATION=0
RStat=0.999499
SETNUM=10219
Source=PCP
Tmax=520
Tmin=200
@END
@BEGIN
A=1012.17
Author=jk
....
```

Figure 9: Text Export

| Key | Value |
|----------|------------|
| A | 50.9775 |
| Author | KUHLMAN |
| B | -0.0975532 |
| C | 0 |
| C1 | 11 |
| COUNT | 1 |
| D | 0 |
| DateD | 22 |
| DateM | 9 |
| DateY | 1999 |
| E | 0 |
| EQID | 11 |
| Error | 8.74067 |
| LOCATION | 0 |
| SETNUM | 13216 |
| Source | PCP |
| Tmax | 513.15 |
| Tmin | 180.12 |

Figure 10: "Quick Overview" Display

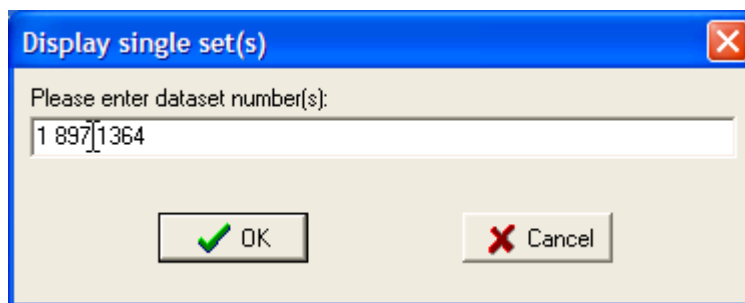
7. Edit Menu Entries



The edit menu allows to

- display the selected sets (for single sets it's same as double-clicking a line in the result grid)
- remove data sets from the result grid
- copy the result grid content to the Windows clipboard
- start a search (same as "Search" button)
- delete selected sets from the parameter data bank (requests confirmation)

- display single sets (parameter data set number have to be entered)



- select duplicate sets (same equation and same system)