ParameterDDB Organizer

DDBSP – Dortmund Data Bank Software Package

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1 Introduction 3
2 Getting Started 3
2.1 Searching 4
2.2 Search Result 6
3 Single Data Set Display 7
4 Statistics 8
4.1 Statistics (Summary) 8
4.2 Show Triangle for Binary Sets 8
5 Import Parameter Sets 9
6 Export Parameter Sets 9
7 Special Views 9
8 Edit Menu Entries 10
9 Read Aspen Components 11

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 of more different types of parameters.

Sources for the parameters in the DDB software package are:

- PCPEquationFit: Pure component properties equation parameters,
- RecPar: g^E model and EOS mixing rule interaction parameters (simultaneous fit to different data types),
- MixCalc: g^E model interaction parameters (simple T independent fit),
- GenMixRulesParameters: equation of state mixing rule parameters (based on VLE data only).

2 Getting Started

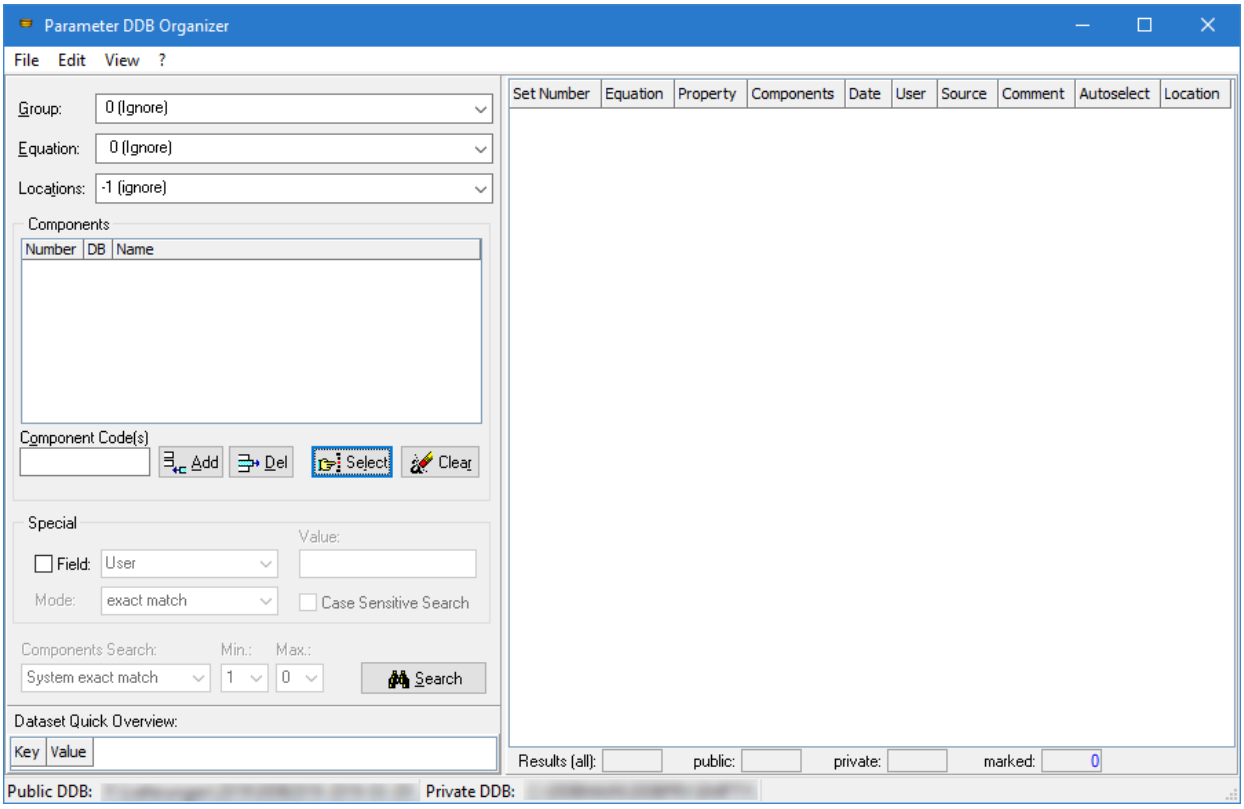


Figure 1: Opening dialog

2.1 Searching

The Parameter DDB Organizer groups equations by their type. These groups determine which equations are shown in the Equation combo box.

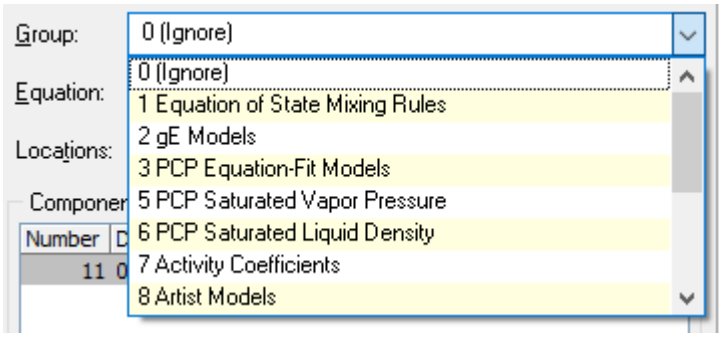


Figure 2: Group selection

Locations are

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

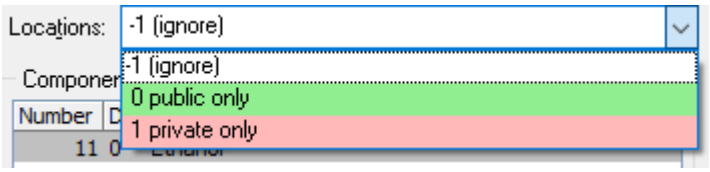


Figure 3: Locations

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

This search can be restricted to specific components or systems.

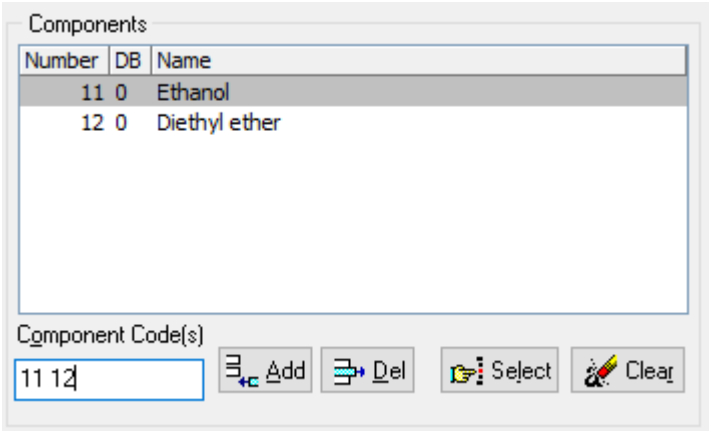


Figure 4: Component resp. system specification

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

- The *Add* button will read and display the component basic information.
- The *Del* button removes 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:

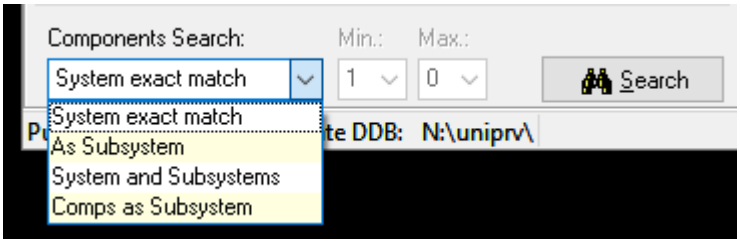


Figure 5: Component search options

- *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 built from the component list will match.
- *Comps as Subsystems*: Every parameter set is found where a single component of the defined components is available.

2.2 Search Result

The search result grid contains the following columns:

Setnumber	Equation	Property	Components	Date	User	Source
11	Wagner Equation (2.5-5-Form)	PCP - Saturated Vapor Pressures	11	1996-05-15	Cordes	PCP
668	Antoine Equation	PCP - Saturated Vapor Pressures	11	2001-02-15	Horstma	
2384	DIPPR Equation 106	PCP - Surface Tensions	11	2009-01-07	cordes	PCP
2866	PPDS Equation 15	PCP - Liquid Heat Capacities	11	2009-01-16	cordes	PCP
4025	Antoine Equation	PCP - Saturated Vapor Pressures	11	2001-02-15	Horstma	
5839	Cox Equation	PCP - Saturated Vapor Pressures	11	1994-06-23	AC	PCP
6737	Andrade Equation	PCP - Saturated Liquid Viscosities	11			PCP
7247	Extended Andrade (LVIS)	PCP - Liquid Viscosity	11	2011-10-12	cordes	PCP
8411	Second Vir. Coeff. DIPPR 104	PCP - Second Virial Coefficient	11	2012-08-01	cordes	DIPPR
8610	Vogel Equation	PCP - Saturated Liquid Viscosities	11			PCP
10208	DIPPR Equation 105	PCP - Liquid Saturated Densities	11			PCP
12355	Polynomial (DNS)	PCP - Liquid Saturated Densities	11	2002-02-04	jk	PCP
13216	Polynomial (SFT)	PCP - Surface Tension	11	1999-09-22	KUHLMAN	PCP
14791	Polynomial (TCN)	PCP - Liquid Thermal Conductivity	11	1998-08-26		PCP
15200	DIPPR Equation 101	PCP - Saturated Vapor Pressures	11			DIPPR
16577	Mathias-Copeman Equation for Soave-Redlich-Kwong EOS	PCP - Saturated Vapor Pressures	11	1999-01-21	SRKC123	
17159	MelhemSG Equation for Peng-Robinson EOS	PCP - Saturated Vapor Pressures	11	2003-11-25	Gardeler	STOFF1
17381	Polynomial (HCP)	PCP - Liquid Heat Capacities	11	2002-10-24	BECKER	PARAM.HCP
18703	TwuBCC Equation for Peng-Robinson EOS	PCP - Saturated Vapor Pressures	11	2013-09-27	Jabloniec	twu.dat
19405	DIPPR Equation 102	PCP - Vapor Viscosity	11	2003-07-17	Cordes	PCP
20322	Mathias-Copeman Equation for Peng-Robinson EOS	PCP - Saturated Vapor Pressures	11	2003-11-25	Gardeler	STOFF1
21631	Radius of Gyration	Radius of Gyration	11		AC	
39355	Polynomial (ICP)	PCP - Ideal Gas Heat Capacities	11	2005-05-26	AC	PARAM.ICP
40453	DIPPR Equation 102	PCP - Vapor Viscosity	11	2010-09-01	Kleiber	Kleiber
40734	DIPPR Equation 101	PCP - Saturated Vapor Pressures	11	2007-06-10	cordes	PCP
42751	PPDS Equation 9	PCP - Liquid Viscosity	11	2010-09-01	Kleiber	Kleiber
42795	DIPPR Equation 116	PCP - Liquid Saturated Densities	11	2010-09-01	Kleiber	Kleiber
42839	DIPPR Equation 106	PCP - Surface Tensions	11	2010-09-01	Kleiber	Kleiber
42883	PPDS Equation 12	PCP - Heat of Vaporization	11	2010-09-01	Kleiber	Kleiber
42918	PPDS Equation 2	PCP - Ideal Gas Heat Capacity	11	2010-09-01	Kleiber	Kleiber
42971	PPDS Equation 15	PCP - Liquid Heat Capacities	11	2010-09-01	Kleiber	Kleiber

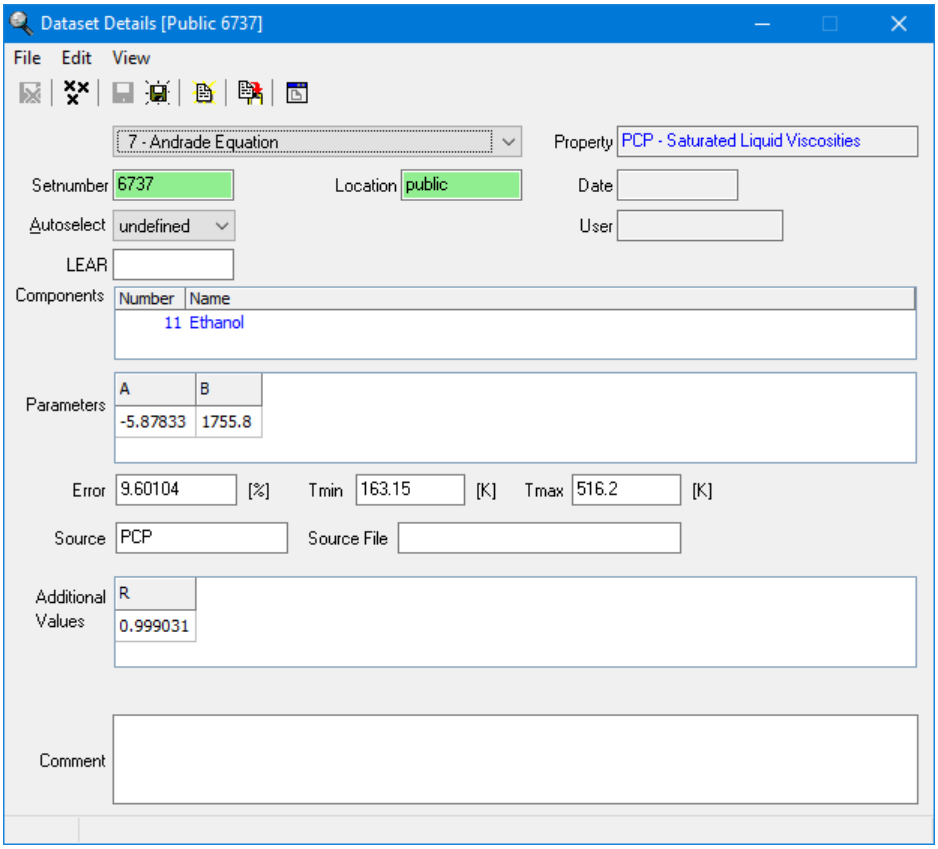
Results (all): 45 public: 45 private: 0 marked: 1

Figure 6: 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"
- "Source": 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 tool bar buttons and the corresponding 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

Additionally the entries for

- 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
```

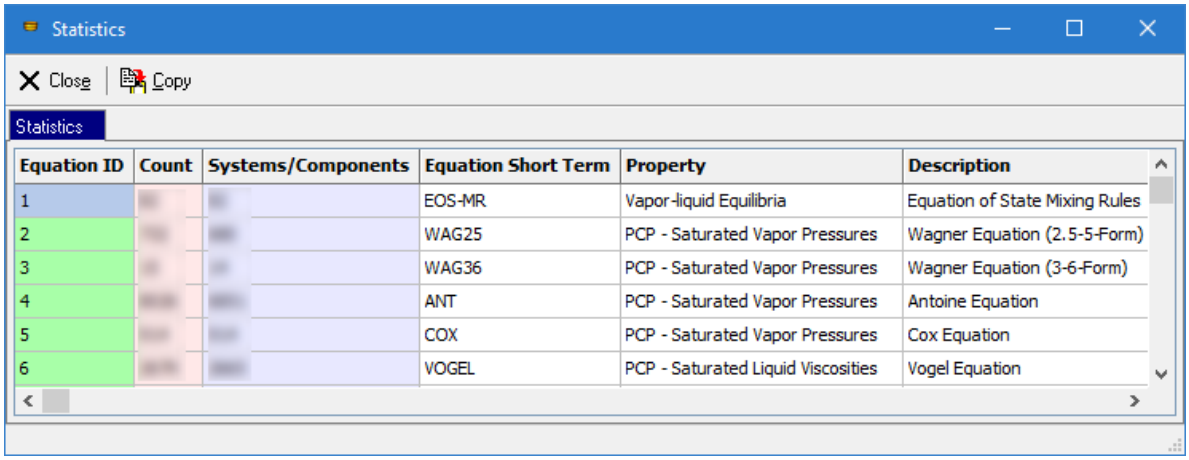
Figure 7: Copied parameter data set

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 Statistics

4.1 Statistics (Summary)

The “Statistics” function shows a table with a statistics about number of systems/components for which parameters are available.



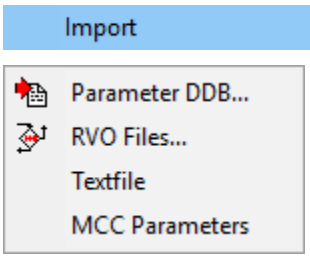
Equation ID	Count	Systems/Components	Equation Short Term	Property	Description
1	[illegible]	[illegible]	EOS-MR	Vapor-liquid Equilibria	Equation of State Mixing Rules
2	[illegible]	[illegible]	WAG25	PCP - Saturated Vapor Pressures	Wagner Equation (2.5-5-Form)
3	[illegible]	[illegible]	WAG36	PCP - Saturated Vapor Pressures	Wagner Equation (3-6-Form)
4	[illegible]	[illegible]	ANT	PCP - Saturated Vapor Pressures	Antoine Equation
5	[illegible]	[illegible]	COX	PCP - Saturated Vapor Pressures	Cox Equation
6	[illegible]	[illegible]	VOGEL	PCP - Saturated Liquid Viscosities	Vogel Equation

4.2 Show Triangle for Binary Sets

The “Show Triangle for Binary Sets” is used for displaying number of interaction parameters of g^E models like NRTL. It show the number of found data sets as triangle where the filled places and gaps can easily be identified. Data base is the list of found sets. For a complete overview, it is therefore necessary to find and selected all g^E model parameters before starting this statistic.

	Acetonitrile	Acetone	1,2-Ethanediol	Ethanol	Diethyl ether	Formic acid ethyl ester	Aniline
Acetone	1						
1,2-Ethanediol	0	0					
Ethanol	3	3	0				
Diethyl ether	0	0	0	2			
Formic acid ethyl ester	0	0	0	1	0		
Aniline	0	0	2	0	0	0	
Ethyl acetate	1	1	0	3	0	0	0
Filled: 9			Empty: 19				

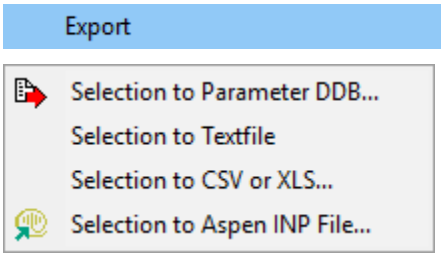
5 Import Parameter Sets



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 a file with Mathias-Copeman constants (used in PSRK)

6 Export Parameter Sets



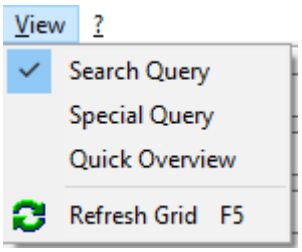
The Parameter DDB Organizer can export parameter sets to

- 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.

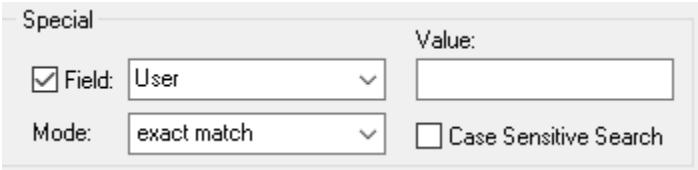
```
@BEGIN
A=3.87644
B=0.0619661
C=547.994
C1=22
COUNT=1
D=0.109738
EQID=9
Error=0.226752
LOCATION=0
RStat=0.999499
SETNUM=10219
Source=PCP
Tmax=520
Tmin=200
@END
@BEGIN
A=1012.17
Author=jk
....
```

Figure 8: Text Export

7 Special Views



These functions allow hiding and showing 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.

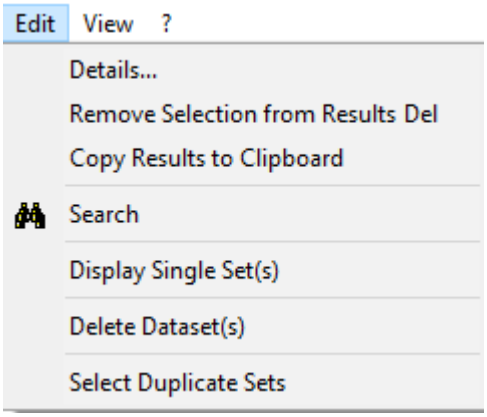
The “Quick Overview” displays a grid where the currently selected parameter set is shown in a very compact grid display.

Dataset Quick Overview:

Key	Value
COUNT	1
EQID	7
Error	9.60104
LOCATION	0
RStat	0.999031
SETNUM	6737
Source	PCP
Tmax	516.2
Tmin	163.15

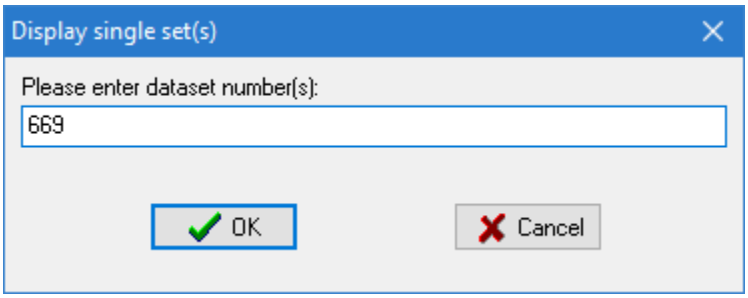
Figure 9: "Quick Overview" Display

8 Edit Menu Entries

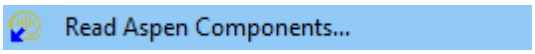


The edit menu allows to

- 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)



9 Read Aspen Components



This function opens an Aspen simulator project and searches it for the components.

It then opens a dialog where the Aspen components can be assigned to DDB components and add the DDB number to the search query.