

# 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,
- RecPar:  $g^E$  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

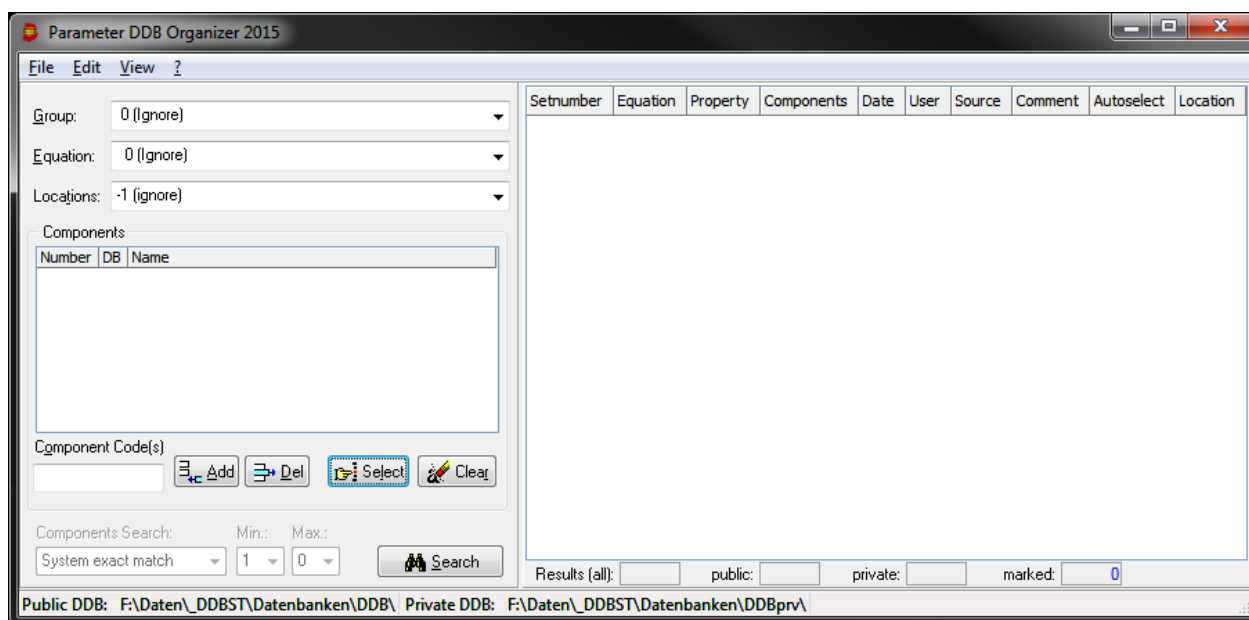
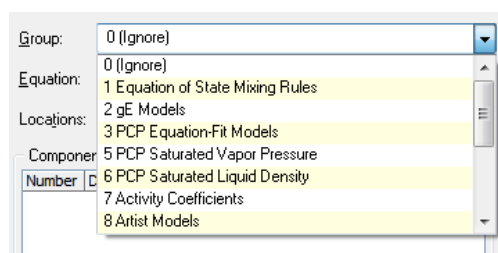


Figure 1: Opening dialog

## 2.1 Searching

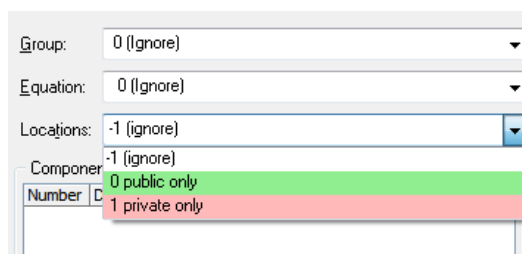
The Parameter DDB Organizer groups equations by their type. These groups determine which equations are shown in the Equation combo box.



**Figure 2:** Group selection.

Locations are

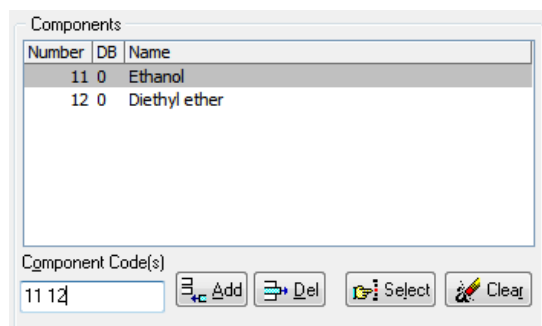
- public (DDBST delivered parameters)
- private (custom parameters)



**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.

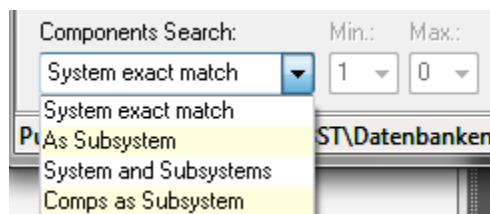


**Figure 4:** Component resp. system specification.

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	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 ST	undef.	public
679	Antoine Equation	PCP - Saturated Vapor Pressures	22	2001-02-15	Horstma	Antoine-Low from ST	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 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”
- “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 tool bar buttons and the corresponding menu entries

Dataset Details [Public 4523]

File Edit View

Equation: 16-Wilson gE model Property: Activity Coefficients

Setnumber: 4523 Location: public Date: User:

Autoselect: undefined

Components:

Number	Name
11	Ethanol
174	Water

Vapor Mix. Model: (undefined)

Temp. Dep.: 0 Aij = aij Tmin: 248.14 [K] Tmax: 458.65 [K]

Parameters [cal/mol]:

	A
11, 174	250.032
174, 11	949.419

Obj. Function: 0.14 Additional Component Values:

	V (Wilson) [ccm/mol]
11	58.6866
174	18.0692

Source File: WILSON.RDA

Data Source: 552 553 554 1028 1029 1033 1434 1435 1717

Comment:

## 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

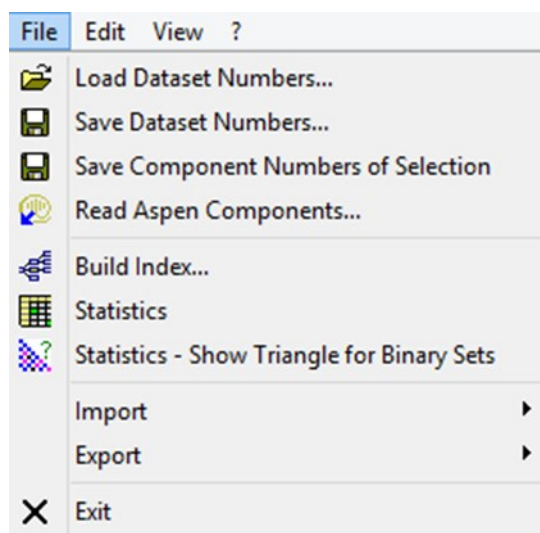
- Equation
- Property
- Set number
- Date
- User

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.

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

## 4 Statistics



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

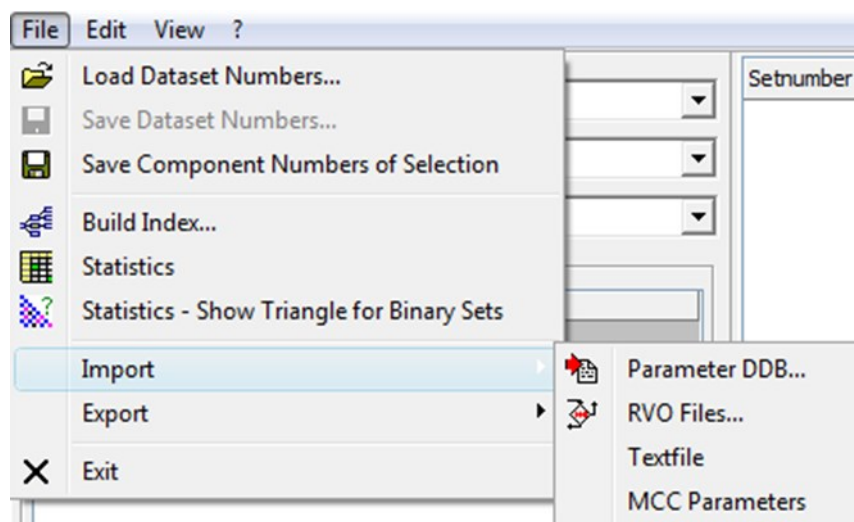
Equation ID	Count	Systems/Components	Equation Short Term	Property	Description
1	82	82	EOS-MR	Vapor-liquid Equilibria	Equation of State Mixing Rules
2	723	676	WAG25	PCP - Saturated Vapor Pressures	Wagner Equation (2.5-5-Form)
3	6	6	WAG36	PCP - Saturated Vapor Pressures	Wagner Equation (3-6-Form)
4	5861	4859	ANT	PCP - Saturated Vapor Pressures	Antoine Equation
5	904	904	COX	PCP - Saturated Vapor Pressures	Cox Equation
6	1710	1710	VOGEL	PCP - Saturated Liquid Viscosities	Vogel Equation

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 statistics.



	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					

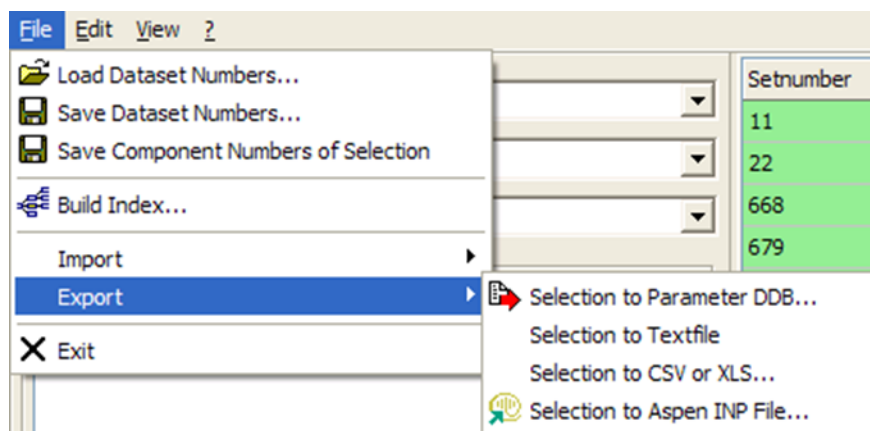
## 5 Import Parameter Sets



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)

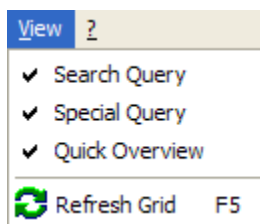
## 6 Export Parameter Sets



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.

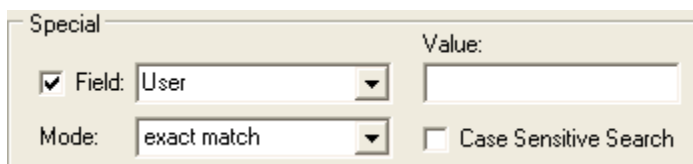
## 7 Special Views



```
@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**

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.

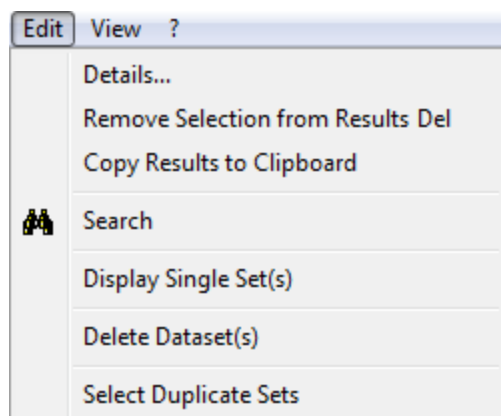
The “Quick Overview” displays a grid where the currently selected parameter set is shown in a very compact grid display.

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

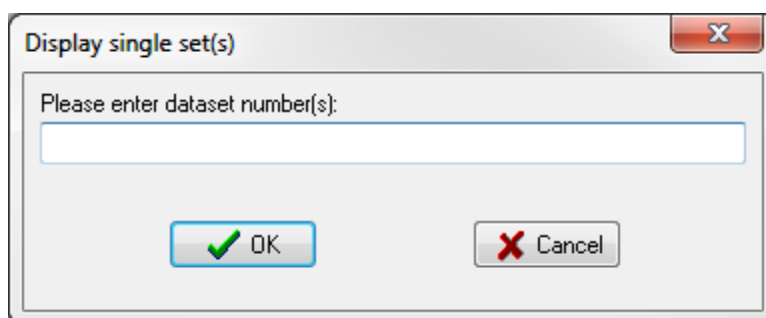
**Figure 10: "Quick Overview" Display**

## 8 Edit Menu Entries

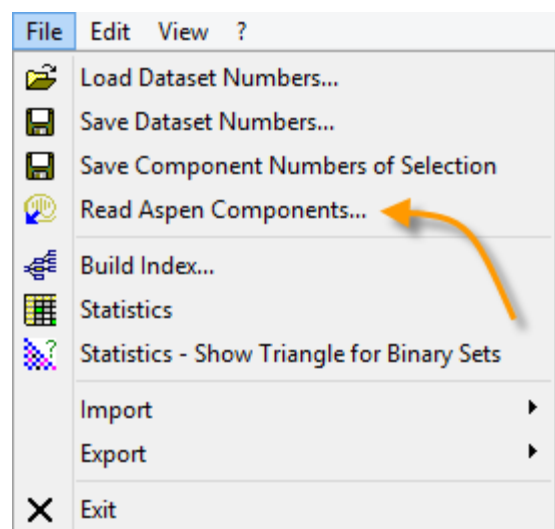
The edit menu allows to



- 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.

