

# DDB Parameter Organizer



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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 of more different types of parameters.

Sources for the parameters in the DDB software package are:

- DDB Predict Pure: Pure component properties equation parameters,
- DDB Predict Mix:  $g^E$  model and EOS mixing rule interaction parameters (simultaneous fit to different data types),
- MixCalc:  $g^E$  model interaction parameters (simple T independent fit),

# 2 Getting Started

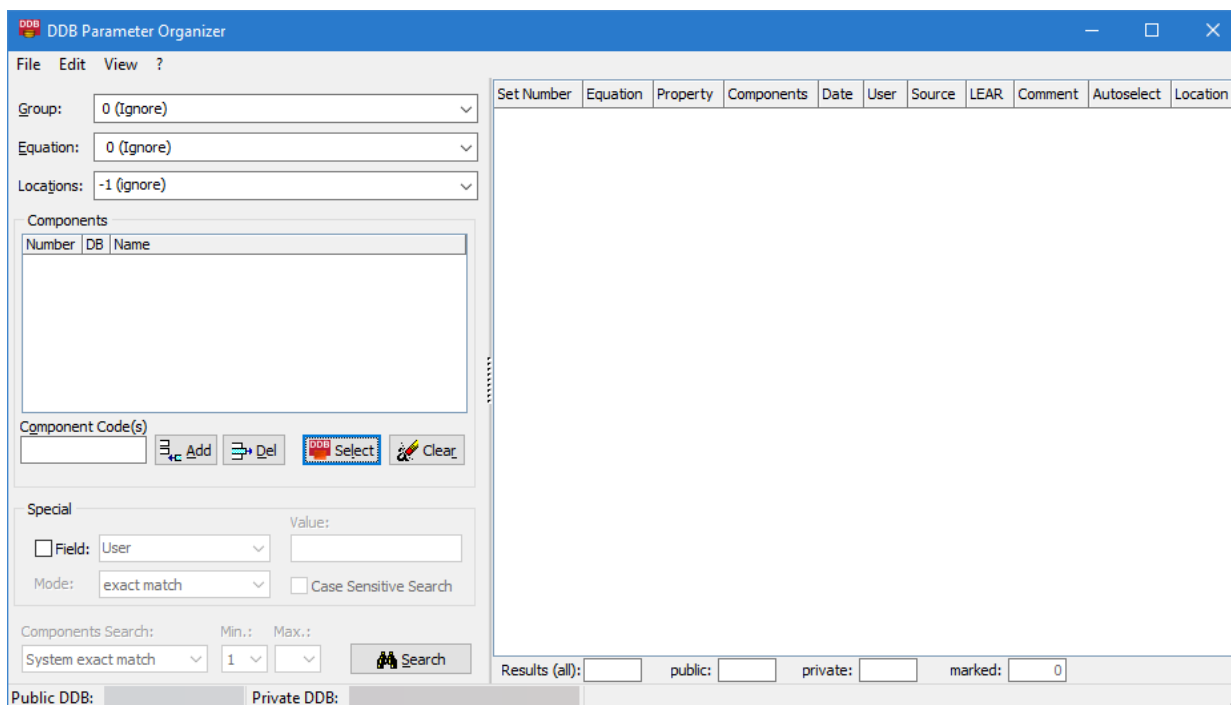


Figure 1: Opening dialog

## 2.1 Searching

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

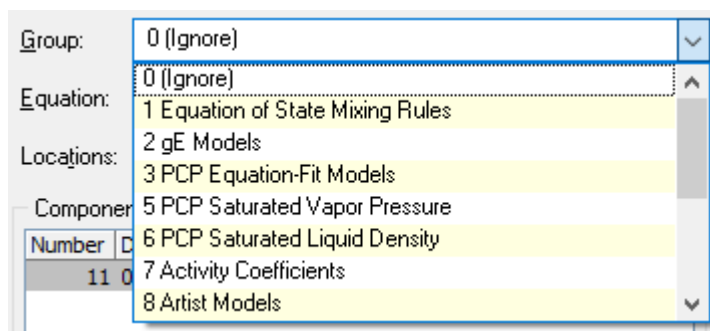


Figure 2: Group selection

Locations are

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

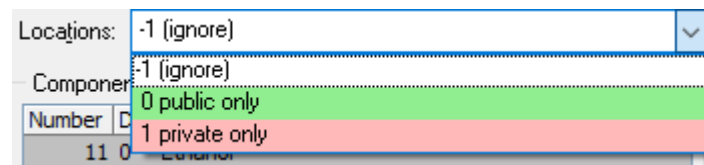


Figure 3: Locations

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.

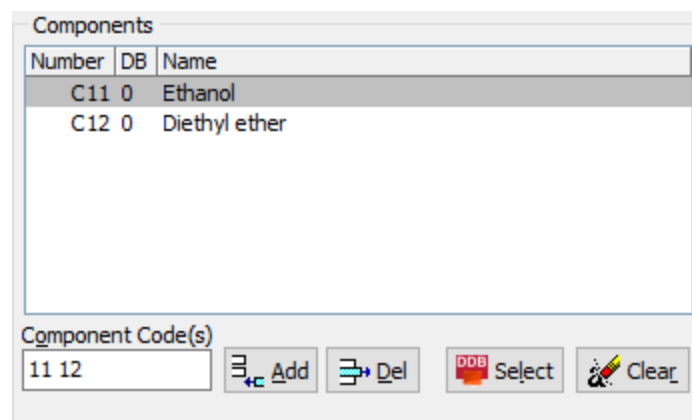


Figure 4: Component resp. system specification

This search can be restricted to specific components or systems.

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 DDB Components 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:

- *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”: 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, there are 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.

## 4 Statistics

### 4.1 Statistics (Summary)



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

Equation ID	Count	Systems/Components	Equation Short Term	Property	Description
1			EOS-MR	Vapor-liquid Equilibria	Equation of State Mixing Rules
2			WAG25	PCP - Saturated Vapor Pressures	Wagner Equation (2.5-5-Form)
3			WAG36	PCP - Saturated Vapor Pressures	Wagner Equation (3-6-Form)
4			ANT	PCP - Saturated Vapor Pressures	Antoine Equation
5			COX	PCP - Saturated Vapor Pressures	Cox Equation
6			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 shows 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 DDB Parameter 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 DDB Parameter Organizer
- MCC Parameters: Internally used for an import of a file with Mathias-Copeman constants (used in PSRK)

## 6 Export Parameter Sets

The DDB Parameter 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

These *View* 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

Special

Field: User

Mode: exact match  Case Sensitive Search

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 5: “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.