

GC Model Parameters

Editor for the Parameters of Group Contribution Methods

DDBSP – Dortmund Data Bank Software Package



DDBST - Dortmund Data Bank Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 441 36 18 19 0

Fax: +49 441 36 18 19 10

support@ddbst.com

www.ddbst.com

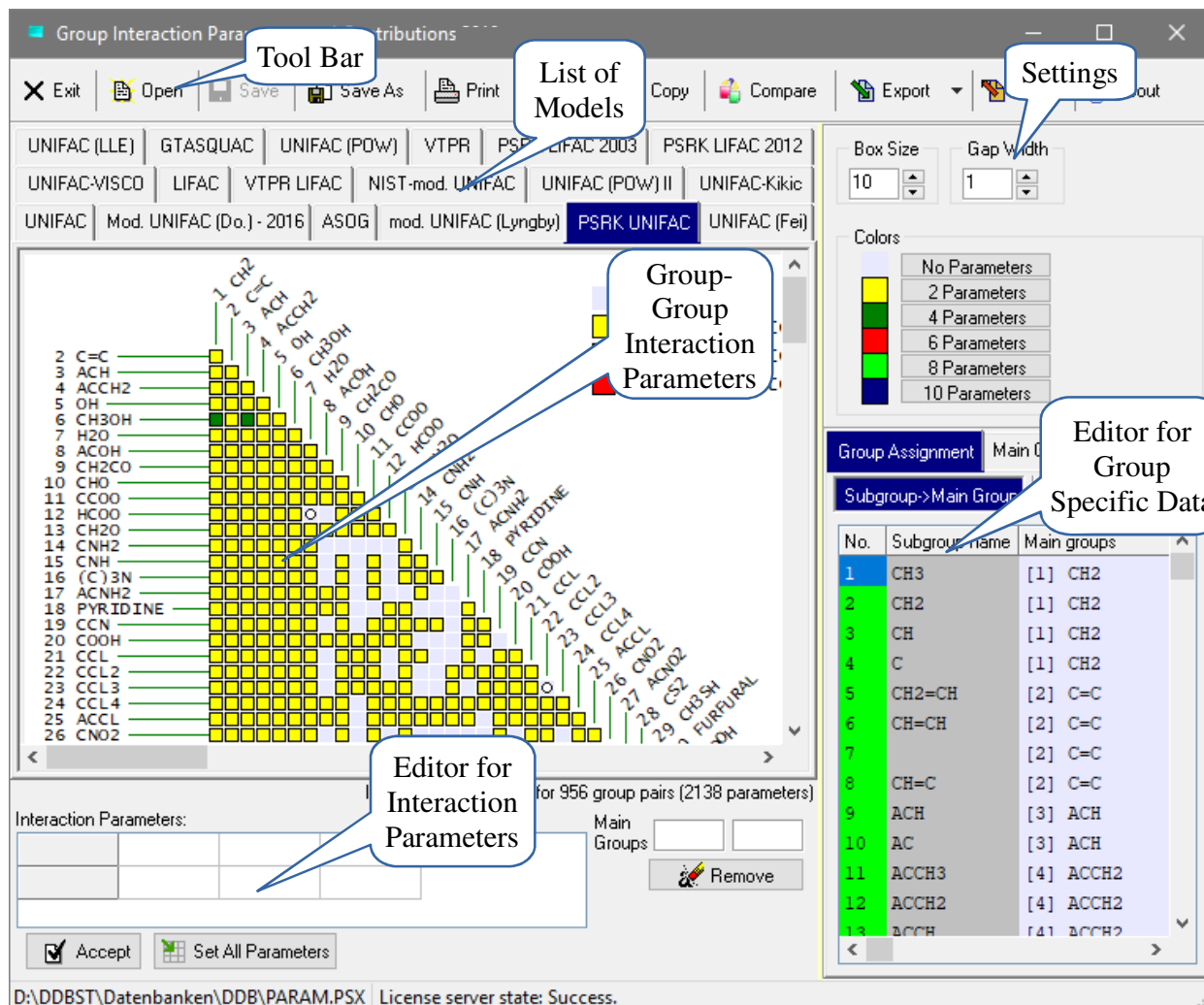
1	Introduction.....	3
2	Overview.....	3
3	The Group-Group Interaction Parameters Triangle.....	3
3.1	Settings.....	4
4	Editing Interaction Parameters.....	4
4.1	Removing Interaction Parameters.....	4
5	Group Specific Data.....	5
5.1	List of Main and Sub Groups.....	5
5.2	Relations between Sub and Main Groups.....	5
6	Opening and Saving Parameter Files.....	6
6.1	Standard Files.....	6
6.2	Opening Other Files.....	7
6.3	Saving Parameter Files.....	7
7	Printing.....	8
8	Compare Matrices.....	8
9	Export.....	9
9.1	Text Export.....	9
9.2	Aspen.....	10
9.3	Compact Parameter Lists.....	10
10	Import.....	10

1 Introduction

The program described in this tutorial displays and modifies the group-group interaction parameters and the group-specific parameters for the group contribution methods implemented in the DDB software package.

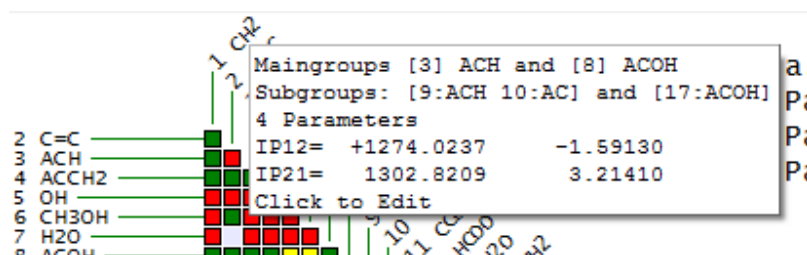
2 Overview

The interaction parameters are displayed as triangle and the number of interaction parameters for every pair of groups is encoded by colors.



3 The Group-Group Interaction Parameters Triangle

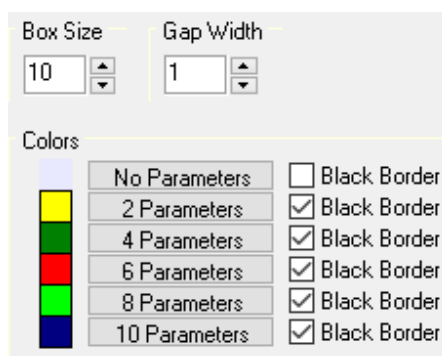
The triangle content is displayed in a hint window which follows the mouse cursor.



This hint window displays the interaction parameters of the group pair just below the mouse cursor. It displays the

- main group names,
- the list of sub groups,
- the number of available parameters (interaction parameter can be temperature-dependent like in mod. UNIFAC, or temperature-independent like in original UNIFAC) and
- The interaction parameters (a_{ij} and a_{ji})

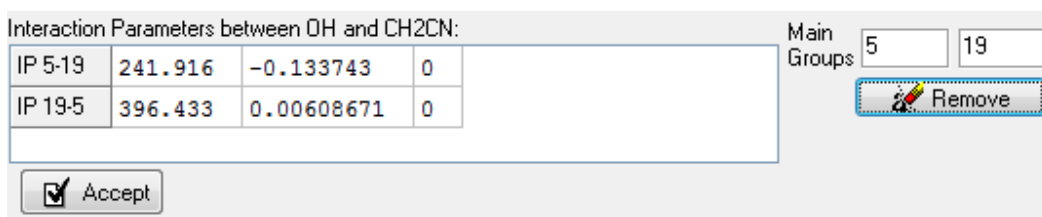
3.1 Settings



It is possible to

- modify the size of the boxes
- modify the gap width
- change the color of the boxes
- display or hide borders

4 Editing Interaction Parameters



The grid below the triangle is used for editing the interaction parameters. This grid is filled when an element in the triangle is left-clicked. The “Accept” button allows putting the modified interaction parameters back in the grid but doesn't save automatically. The “Set All Parameter” initializes the entire triangle with the entered values.

4.1 Removing Interaction Parameters

IP 38-49	9000	0	0
IP 49-38	9000	0	0

The “Remove” button can be used to delete all interaction parameters for a specified group pair. Removing the parameters creates the entries $a_{mm} = a_{mm} = 9000$ because zeros can be valid interaction parameters.

5 Group Specific Data

Group Assignment		
Subgroup->Main Group		Main Group->Subgroup
No.	Subgroup name	Main groups
1	CH3	[1] CH2
2	CH2	[1] CH2
3	CH	[1] CH2
4	C	[1] CH2
5	CH2=CH	[2] C=C
6	CH=CH	[2] C=C
7	CH2=C	[2] C=C
8	CH=C	[2] C=C
9	ACH	[3] ACH
10	AC	[3] ACH
11	ACCH3	[4] ACCH2
12	ACCH2	[4] ACCH2

All the group contribution methods in the DDB software package differentiate between main and sub groups. The interaction parameters shown in the triangle are always parameters of main group pairs.

5.1 List of Main and Sub Groups

Group Assignment	
Main Groups	
No.	Main group name
1	CH2
2	C=C
3	ACH
4	ACCH2
5	OH
6	CH3OH
7	H2O
8	ACOH
9	CH2CO
10	CHO
11	CCOO
12	HCOO
13	CH2O
14	CH2NH2

Figure 1: List of sub groups

Group Assignment			
Main Groups		Subgroups	
No. i	Subgroup name	Ri	Qi
1	CH3	0.6325	1.0608
2	CH2	0.6325	0.7081
3	CH	0.6325	0.3554
4	C	0.6325	0.0000
5	CH2=CH	1.2832	1.6016
6	CH=CH	1.2832	1.2489
7	CH2=C	1.2832	1.2489
8	CH=C	1.2832	0.8962
9	ACH	0.3763	0.4321
10	AC	0.3763	0.2113
11	ACCH3	0.9100	0.9490
12	ACCH2	0.9100	0.7962
13	ACCH	0.9100	0.3769
14	OH (P)	1.2302	0.8927

Figure 2: List of sub groups

The main groups are simply a list of groups where a short name of the group can be edited.

The sub group is also a list of groups with some specific name but in this grid sub group (and model) specific data can be entered and modified.

5.2 Relations between Sub and Main Groups

The sub groups are related to main groups but describe the group with more details. A main group is normally split into several different sub groups. The relation between sub and main groups can be entered or modified in the "Subgroup -> Main group" table:

Group Assignment		
Subgroup->Main Group		Main Groups
No.	Subgroup name	Main groups
1	CH3	[1] CH2
2	CH2	[1]
3	CH	[1] CH2
4	C	[1] CH2

Figure 3: Sub to main group assignment

The second list (“Main group -> Subgroup”) is the reverse display but this table can't be edited.

Group Assignment		
Subgroup->Main Group		Main Group->Subgroup
No.	Main group name	Subgroups
1	CH2	[1] CH3 [2] CH2 [3] CH [4] C
2	C=C	[5] CH2=CH [6] CH=CH [7] CH2=C
3	ACH	[9] ACH [10] AC
4	ACCH2	[11] ACCH3 [12] ACCH2 [13] ACCH
5	OH	[14] OH (P) [81] OH (S) [82] OH (T)
6	CH3OH	[15] CH3OH
7	H2O	[16] H2O
8	ACOH	[17] ACOH
9	CH2CO	[18] CH3CO [19] CH2CO

Figure 4: Main to subgroup assignment

6 Opening and Saving Parameter Files

6.1 Standard Files

Parameter files are named – for some historic reason – “PARAM.*”. The extension describes the model. The standard extensions are

Extension	Model
mod	Modified UNIFAC (Dortmund)
uni	Original UNIFAC
asg	ASOG
lyn	Modified UNIFAC (Lyngby)
psx	PSRK (Predictive Soave-Redlich-Kwong)
vtx	VTPR (Volume-translated Peng-Robinson)
uow	UNIFAC (POW)
gtq	GTASQUAC
fei	UNIFAC (Fei)
ull	UNIFA (LLE)

eps PSRK LIFAC 2003
 psl PSRK LIFAC 2012
 nist NIST-modified UNIFAC

These parameter files are all located in the public DDB folder and are opened automatically and displayed as pages above the triangle.

6.2 Opening Other Files

Parameter files from other locations than the DDB folder or other parameter files can be opened by the *Open* button:

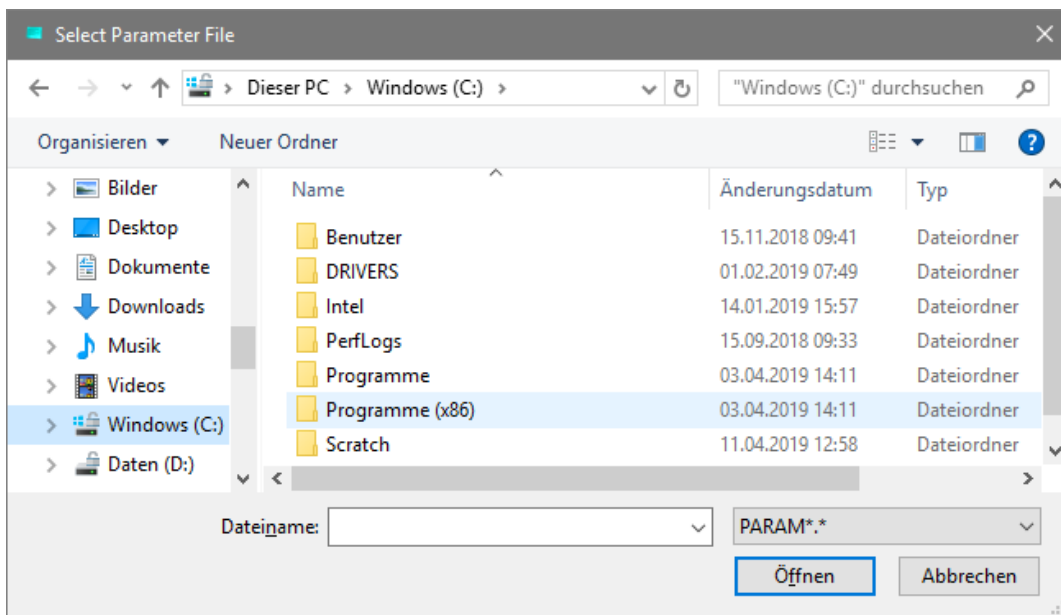


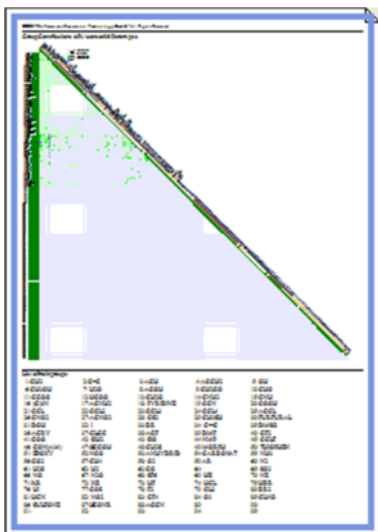
Figure 5: UNIFAC Consortium parameter files.

The loaded files are appended to the standard pages.

6.3 Saving Parameter Files

The function “Save” stores the modified parameter file at the original location whereas the “Save As” opens a save dialog where a different folder and filename can be selected.

7 Printing



The triangle plus a list of main groups is printed. For a complete list of parameters – which can be printed – please take a look at the export functions.

8 Compare Matrices

This function allows identifying

- newly added interaction parameters
- modified interaction parameters
- deleted interaction parameters

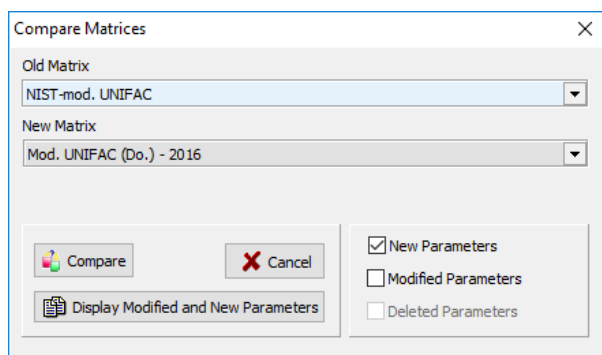


Figure 6: Comparison Dialog

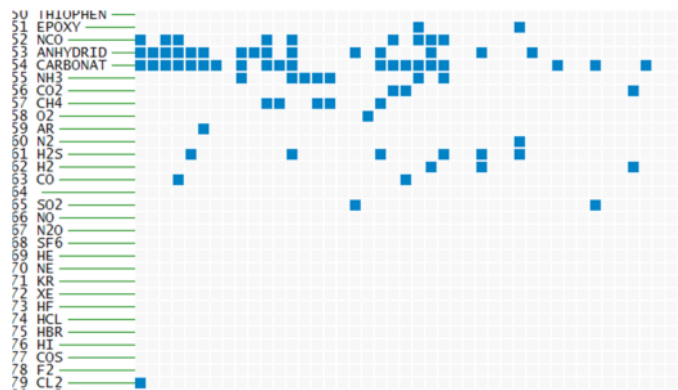
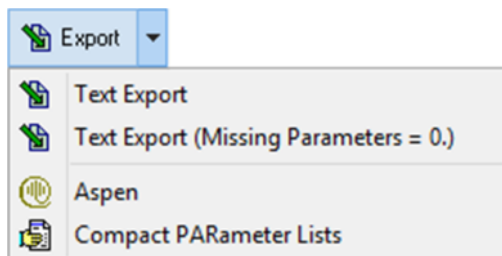


Figure 7: Comparison Result

This function creates a triangle where only the new, the modified, or the deleted parameters are shown.

9 Export



Three different formats are supported:

9.1 Text Export

The text export display a text triangle showing the availability of interaction parameters:

```
mod. UNIFAC (Dortmund)
12.06.2007 15:48:33
C=C      2   +
ACH      3  ++
ACCH2    4  +++
OH       5  ++++
CH3OH    6  +++++
H2O      7  ++++++
ACOH     8  ++++++
CH2CO    9  ++++++
CHO      10 ++++++
...continued...
```

The list of the interaction parameters follows:

Group1	Group2	A12	B12	C12	A21	B21	C21
1	2	189.6600	-0.2723		-95.4180	0.0617	
1	3	114.2000	0.0933		16.0700	-0.2998	
1	4	7.3390	-0.4538		47.2000	0.3575	
1	5	2777.0000	-4.6740	1.5510e-03	1606.0000	-4.7460	9.1810e-04
1	6	2409.3999	-3.0099		82.5930	-0.4857	
1	7	1391.3000	-3.6156	1.1440e-03	-17.2530	0.8389	9.0210e-04

...continued...

The next part is the main to sub group relation list:

No.	Maingroupname	Subgroups
1	CH2	[1] CH3 [2] CH2 [3] CH [4] C
2	C=C	[5] CH2=CH [6] CH=CH [7] CH2=C [8] CH=C [70] C=C
3	ACH	[9] ACH [10] AC
4	ACCH2	[11] ACCH3 [12] ACCH2 [13] ACCH
5	OH	[14] OH (P) [81] OH (S) [82] OH (T)
6	CH3OH	[15] CH3OH

...continued...

The last block is the list of sub groups with the sub group specific parameters:

No.	Subgroupname	Maingroup	R	Q
1	CH3	[1] CH2	0.6325	1.0608
2	CH2	[1] CH2	0.6325	0.7081
3	CH	[1] CH2	0.6325	0.3554
4	C	[1] CH2	0.6325	0.0000

...continued...

The second text output (missing parameter = 0.) differs only slightly in the interaction parameter table by filling

the gaps with zeros.

Group1	Group2	A12	B12	C12	A21	B21	C21
1	2	189.6600	-0.2723	0.	-95.4180	0.0617	0.
1	3	114.2000	0.0933	0.	16.0700	-0.2998	0.
1	4	7.3390	-0.4538	0.	47.2000	0.3575	0.
1	5	2777.0000	-4.6740	1.5510e-03	1606.0000	-4.7460	9.1810e-04
1	6	2409.3999	-3.0099	0.	82.5930	-0.4857	0.

9.2 Aspen

This export writes are parameter file which can be used in the Aspen simulator.

```
PPGRPBI  REPLACE      GMUFDMD
1
UNIFDM   6
639
CH2      C=C          1.89660e+02  -9.54180e+01  -2.72320e-01
          6.17080e-02  0.00000e+00  0.00000e+00
CH2      ACH          1.14200e+02  1.60700e+01  9.33000e-02
          -2.99800e-01  0.00000e+00  0.00000e+00
CH2      ACCH2        7.33900e+00  4.72000e+01  -4.53800e-01
          3.57500e-01  0.00000e+00  0.00000e+00
...continued...
```

9.3 Compact Parameter Lists

This export is a compact text output omitting the 'graphical' triangle output. Another difference is that the sub to main group assignment is integrated in the sub group parameters list.

```
111
1 CH3      0.6325      1.0608      1      CH2
2 CH2      0.6325      0.7081      1      CH2
3 CH       0.6325      0.3554      1      CH2
4 C        0.6325      0.0000      1      CH2
...continued...
```

10 Import

Interaction parameters can be imported from simple Excel files (".xls" format) or files with comma-separated values (".csv" format). The tables must contain eight columns with

- both main group numbers
- a₁₂, b₁₂, c₁₂
- a₂₁, b₂₁, c₂₁

	A	B	C	D	E	F	G	H
1	Group1	Group2	a	b	c	a	b	c
2	17	22	37.33	0.13		909.96	-2.41	
3	15	22	22.98			-18.48		
4	14	22	-134.69			78.58		
5	15	21	89.88	-1.29		634.55	0.57	

The title line can be omitted.