

GC Model Parameters

Editor for the Parameters of Group Contribution Methods

DDBSP - Dortmund Data Bank Software Package



DDBST Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 (0) 441 361819 0

Fax: +49 (0) 441 361819 10

E-Mail: support@ddbst.com

Web: www.ddbst.com

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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.

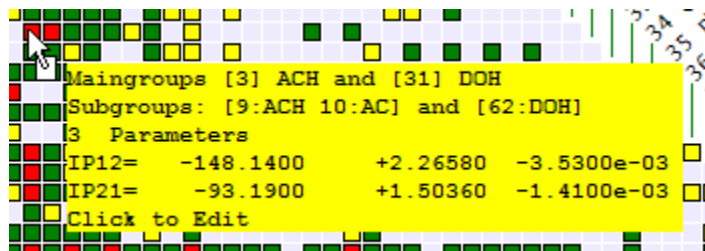
Overview

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

The screenshot displays the 'Group Contributions' software interface. The main window shows a matrix of interaction parameters between 30 chemical groups. The groups are listed on the left and right sides of the matrix, including CH2, C=C, ACH, ACCH2, OH, CH3OH, H2O, ACOH, CH2CO, CHO, CCOO, HCOO, CH2O, CH2NH2, CH2NH, (C)3N, ACNH2, PYRIDINE, CH2CN, COOH, CCL, CCL2, CCL3, CCL4, ACCL, ACNO2, CS2, CH3SH, and FURFURAL. The matrix cells are colored based on the number of parameters: white for 0, yellow for 1, green for 2, and red for 3. A legend indicates these color mappings. The interface includes a menu bar with options like Exit, Open, Save, Save As, Print, Compare, Export, and Import. A toolbar is located at the top right. A settings panel on the right allows for adjusting box size and gap width, and selecting colors for different parameter counts. A list of groups on the bottom right is used for editing group-specific data. Callouts identify the 'List of Models', 'Tool Bar', 'Settings', 'Group-Group Interaction Parameters', and 'Editor for Group Specific Data'. At the bottom, there is an 'Accept' button and a 'Main Groups' section with a 'Remove' button. The status bar at the very bottom shows the file path 'K:\DDB\PARAM.MOD' and the license server state 'Access granted'.

The Group-Group Interaction Parameters Triangle

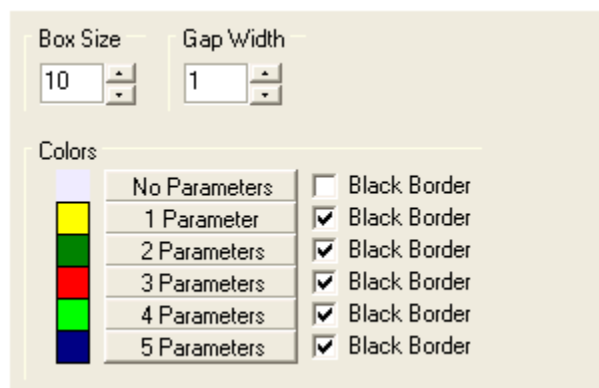
The triangle content is displayed in a hint window which follows the mouse cursor.



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

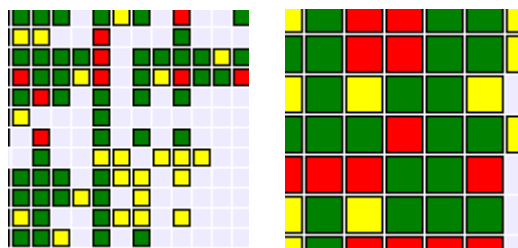
- main group names,
- the list of sub groups,
- the number of available parameters (interaction parameter can be temperature-dependent like in mod. UNIFAC, or temperature-independent like in original UNIFAC) and
- The interaction parameters (a_{ij} and a_{ji})

Settings



It is possible to

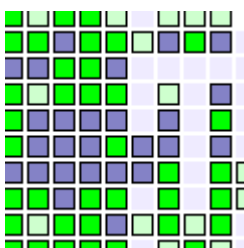
- modify the size of the boxes



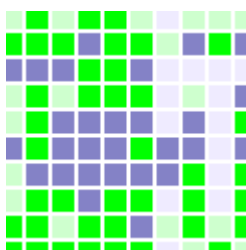
- modify the gap width



- change the color of the boxes



- display or hide borders



Editing Interaction Parameters

IP 18-38	197.9500	-0.33160	-4.00000E-0004	Main Groups	18	38
IP 38-18	-1052.5000	1.68540	2.70000E-0003		Remove	

Accept

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 to put the modified interaction parameters back in the grid but doesn't save automatically.

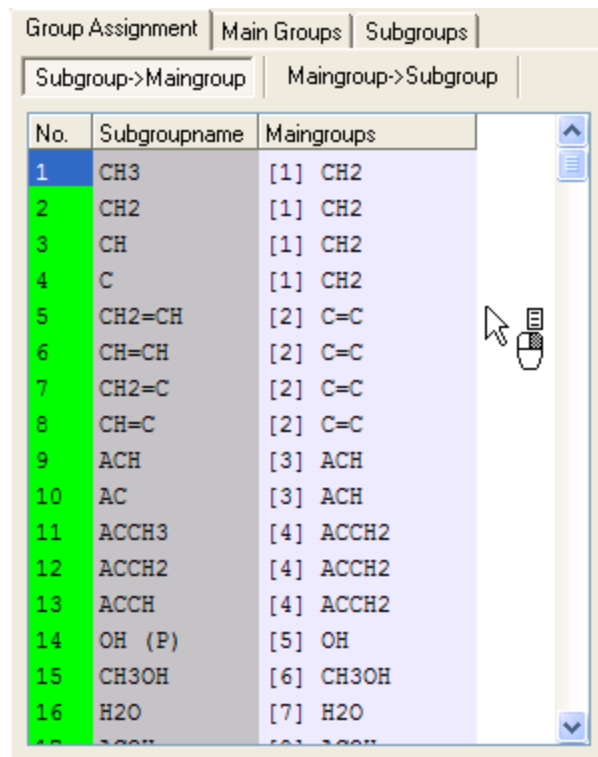
Removing Interaction Parameters

IP 18-38	9000	0	0
IP 38-18	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 $a_{12}=a_{21}=9000$ because zeros can be valid interaction parameters.

Group Specific Data



No.	Subgroupname	Maingroups
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
13	ACCH	[4] ACCH2
14	OH (P)	[5] OH
15	CH3OH	[6] CH3OH
16	H2O	[7] H2O

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

List of Main and Sub Groups

Group Assignment		Main Groups	Subgroups
No.	Maingroupname		
1	CH2		
2	C=C		
3	ACH		
4	ACCH2		
5	OH		
6	CH3OH		
7	H2O		
8	ACOH		
9	CH2CO		
10	CHO		
11	CCOO		

Figure 1: List of Main Groups

Group Assignment		Main Groups	Subgroups
No.	Subgroupname	r	q
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

Figure 2: List of Sub Groups

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

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

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->Maingroup” table:

No.	Subgroupname	Maingroups
1	CH3	[1] CH2
2	CH2	1
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
13	ACCH	[4] ACCH2
14	OH (P)	[5] OH
15	CH3OH	[6] CH3OH

Figure 3: Sub to Main Group Assignment

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

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
7	H2O	[16] H2O
8	ACOH	[17] ACOH
9	CH2CO	[18] CH3CO [19] CH2CO
10	CHO	[20] CHO
11	CCOO	[21] CH3COO [22] CH2COO
12	HCOO	[23] HCOO
13	CH2O	[24] CH3O [25] CH2O [26] CHO
14	CH2NH2	[28] CH3NH2 [29] CH2NH2 [30] CHNH2 [85] CNH2

Opening and Saving Parameter Files

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)
psu, psx	PSRK (Predictive Soave-Redlich-Kwong)
vtp, vtx	VTPR (Volume-translated Peng-Robinson)
uow	UNIFAC (POW)
gtq	GTASQUAC
fei	UNIFAC (Fei)

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



Opening Other Files

Parameter files from other locations than the DDB folder or other parameter files can be opened by the

 **Open** button:

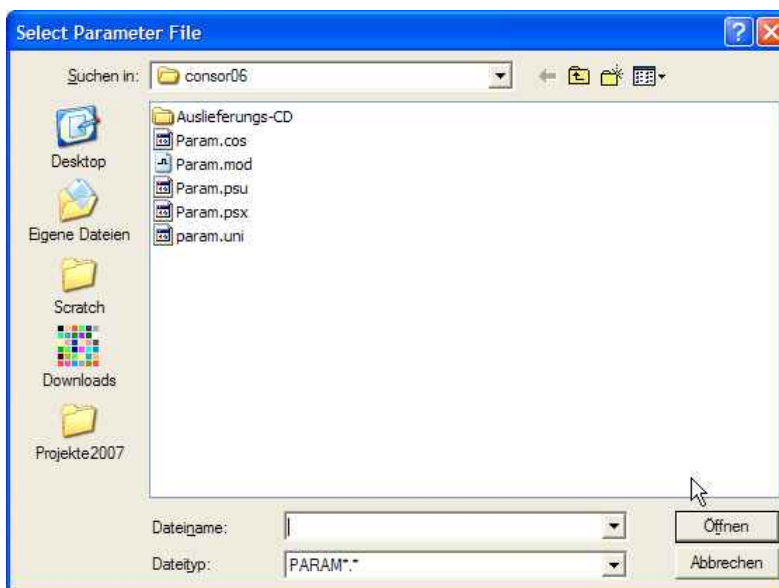
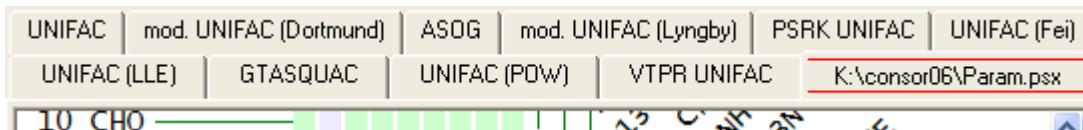




Figure 4: UNIFAC Consortium Parameter Files

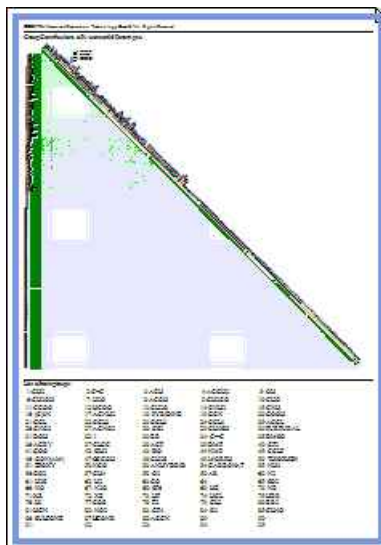
The loaded files is appended to the standard pages.



Saving Parameter Files

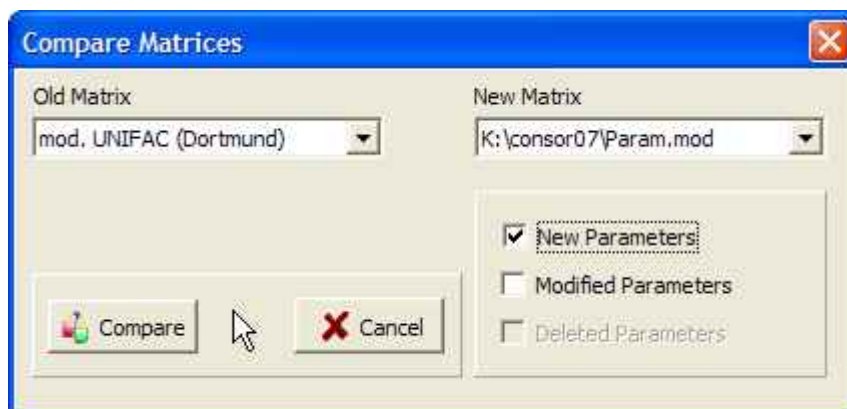
The function “Save” stores the (modified) parameter file at the original location whereas the “Save As” opens a save dialog where a different folder and filename can be selected ( Save  Save As).

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.

Compare Matrices



This function allows to identify

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

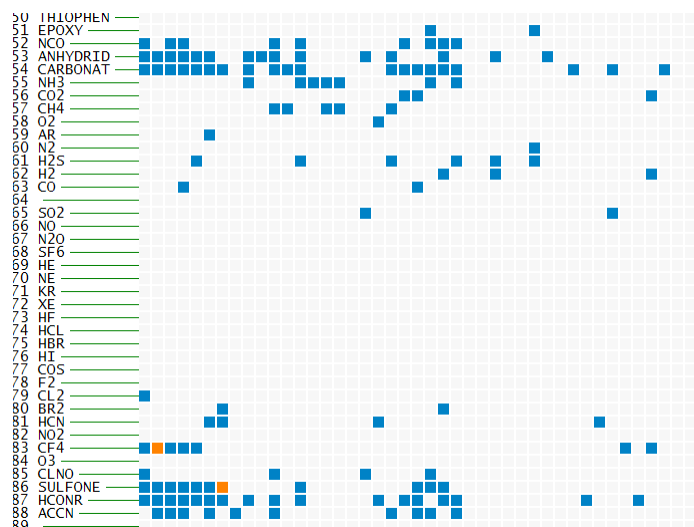
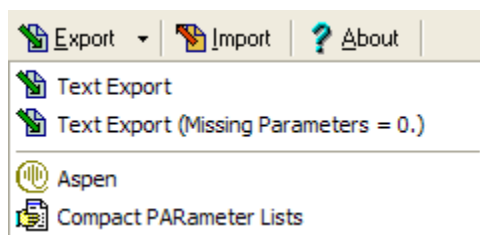


Figure 5: PSRK: New Parameters from the UNIFAC Consortium

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

Export



Three different formats are supported:

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.

Aspen

This export writes a 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...

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...

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
- a_{12} , b_{12} , c_{12}
- a_{21} , b_{21} , c_{21}

	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.