Group Interaction Parameters and Contributions

Editor for the Parameters of Group Contribution Methods

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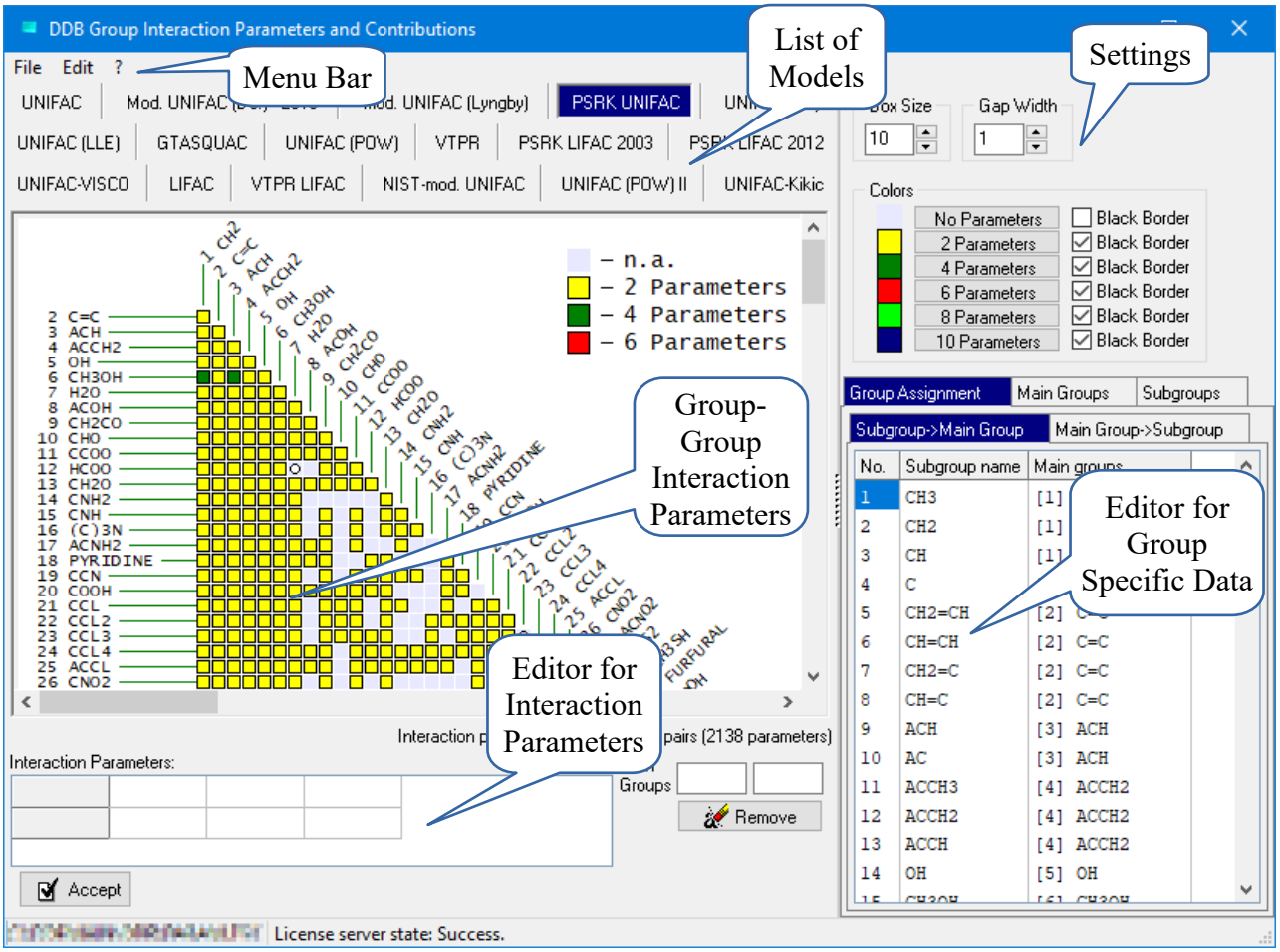
1 Introduction

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.

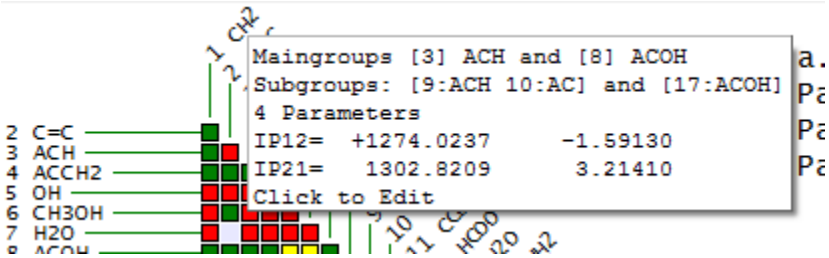
2 Overview

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

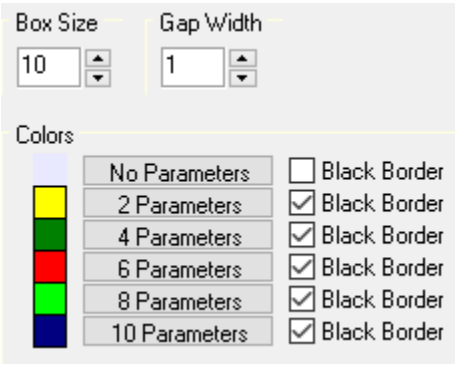
The triangle content is displayed in a hint window which follows the mouse cursor.



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})

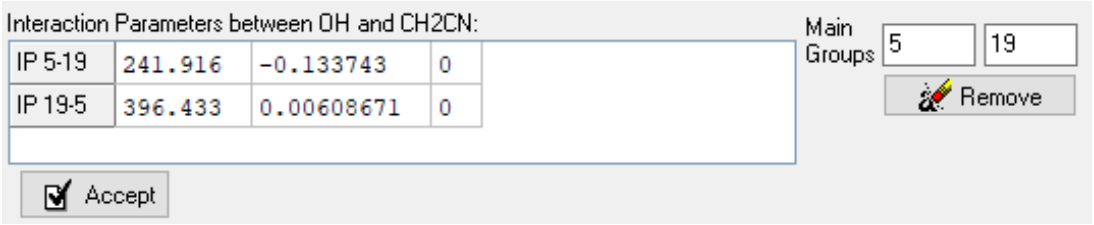
3.1 Settings



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



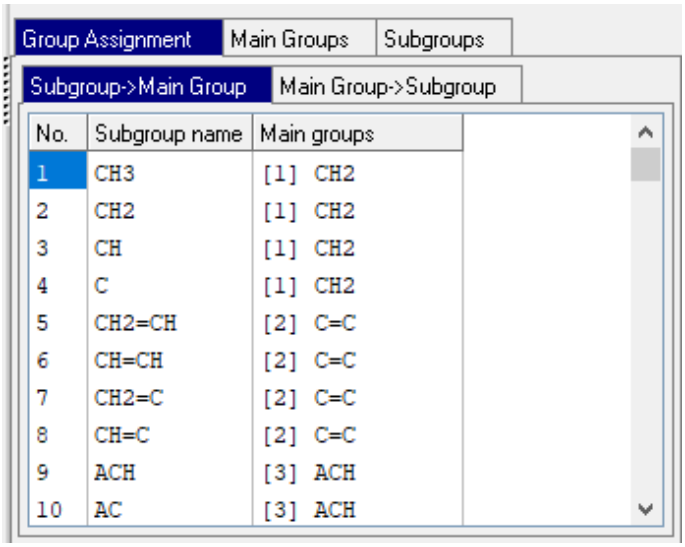
The grid below the triangle is used for editing the interaction parameters. This grid is filled when an element in the triangle is left-clicked. The “Accept” button allows putting the modified interaction parameters back in the grid but doesn't save automatically. The “Set All Parameter” initializes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

4.1 Removing Interaction Parameters

IP 37-38	9000	0	0
IP 38-37	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 $a_{nm} = a_{mn} = 9000$ because zeros can be valid interaction parameters.

5 Group Specific Data



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

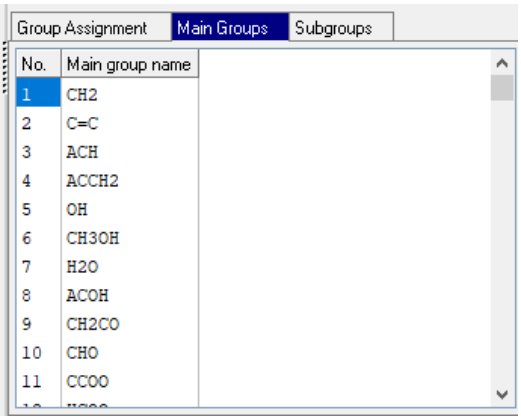


Figure 1: List of main groups

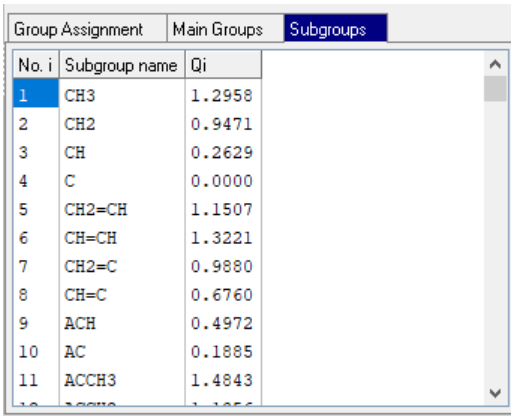


Figure 2: List of sub groups

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:

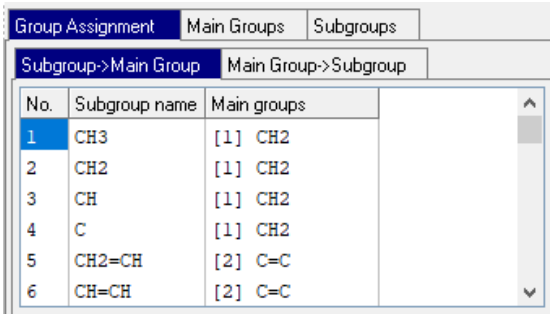


Figure 3: Sub to main group assignment

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

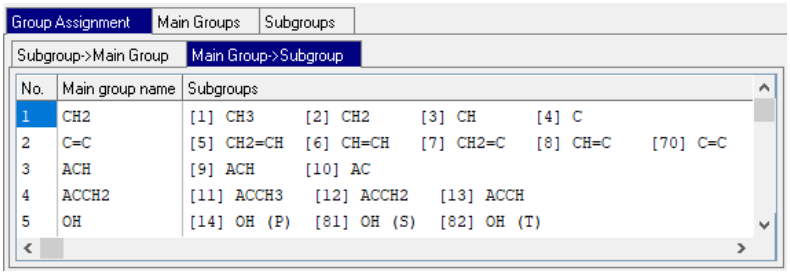


Figure 4: Main to subgroup assignment

6 File Menu

6.1 Standard Files

The 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

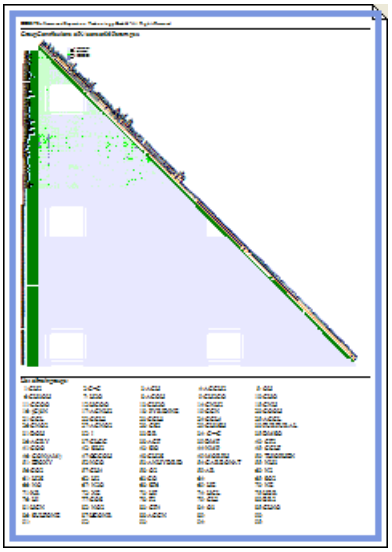
Parameter files from other locations than the DDB folder or other parameter files can be opened by the *Open* button.

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.

6.4 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.

6.5 Compare

This function allows identifying

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

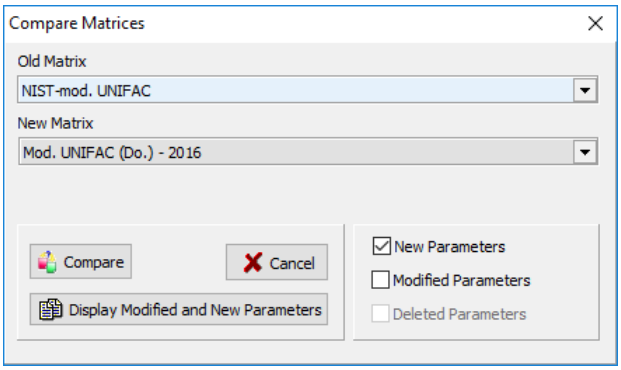


Figure 5: Comparison Dialog

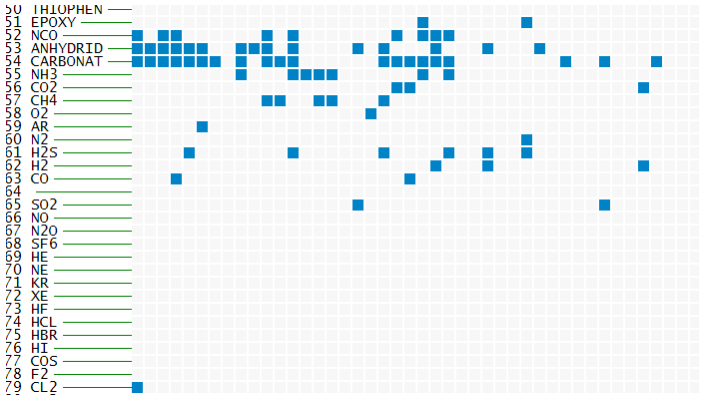
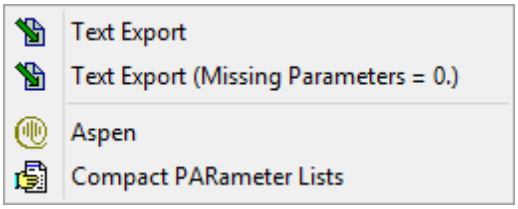


Figure 6: Comparison Result

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

6.6 Export



Three different formats are supported:

Text Export

The text export displays 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 Export

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...
```

Compact Parameter Lists Export

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...
```

6.7 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	

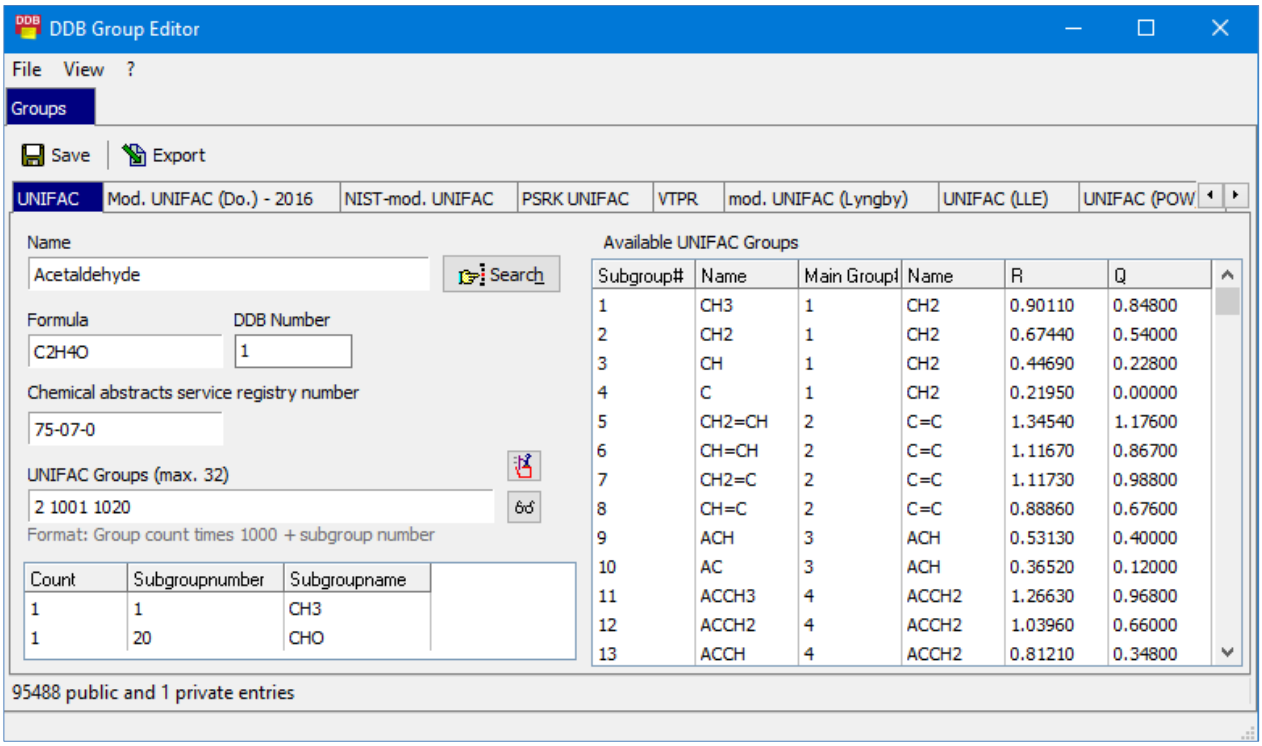
The title line can be omitted.

7 Edit Menu

7.1 Copy triangle

The program has the possibility to copy the triangle as metafile or bitmap to the clipboard

7.2 Group Assignments



The “Groups” page allows editing group list for the implemented mixture group contribution methods.

This dialog displays the name, formula, CAS-RN and the DDB number of the currently edited component.

The group assignment is displayed in a read-only field because editing the list of groups is performed in the grid below that display field.

The grid allows entering the group count directly in the left column. Adding subgroups is done by dragging a line from the group list to editing grid. Lines are removed by double-clicking.

The “Groups” page can also be used for the original UNIFAC and modified UNIFAC (Dortmund) group assignments.