Getting started with Simulis® Thermodynamics

Use Case 10: Use of the Predictive Models Editor

Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

This document presents the Predictive Models Editor that is used to configure predictive thermodynamic models based on group contributions.

- Editor presentation
- Use within Simulis Thermodynamics
- Installation of « private » matrices from the UNIFAC consortium

Presentation: models

- Simulis Thermodynamics (ProSim's thermodynamic calculation server) includes several predictive models based on group contributions.
  - UNIFACs (Original, Dortmund, Larsen, PSRK, VTPR, NIST, …)
  - PPR78
  - GC-PPC-SAFT
  - NRTL-PR
  - …

Presentation: groups and sub-groups

- A group can include several functional sub-groups
- Each sub-group has specific parameters that depend on the model
- Interaction coefficients between groups allow to describe the influence of the groups on each other
- In order for the model to work, it must be possible to do group assignment for each molecule

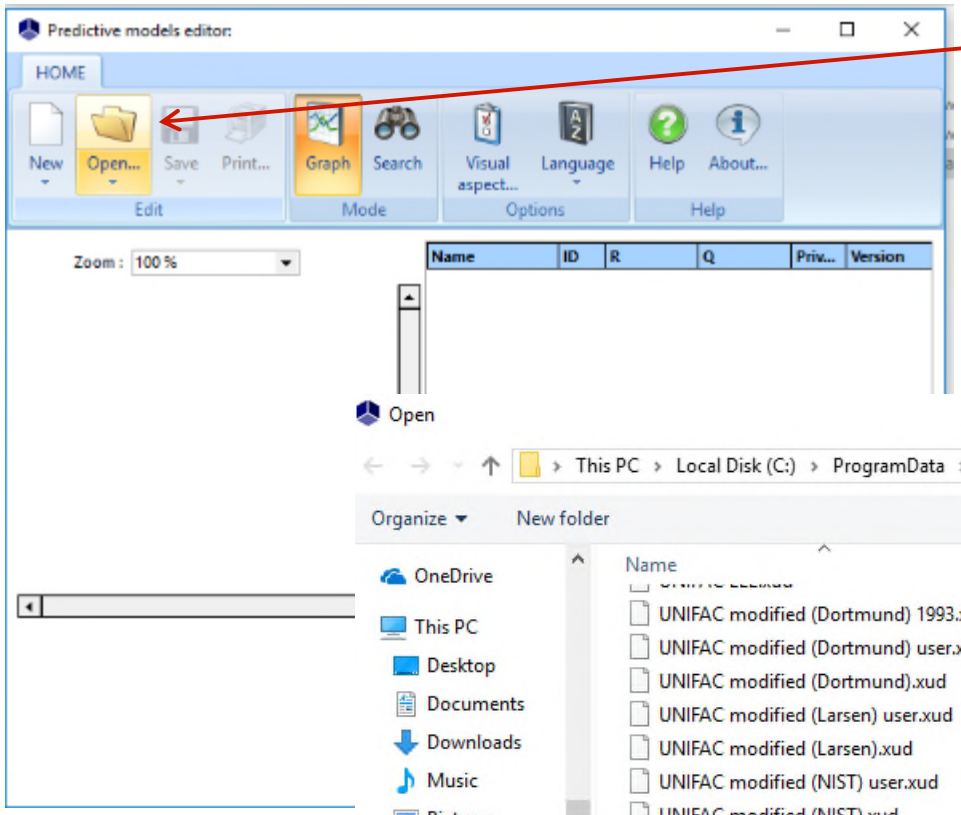
Presentation: the software

- Accessible from the start menu in the ProSim directory, under the name: « predictive models editor »

- Open the files containing the groups and sub-groups information and their interaction parameters (.xud) located in the default directory:

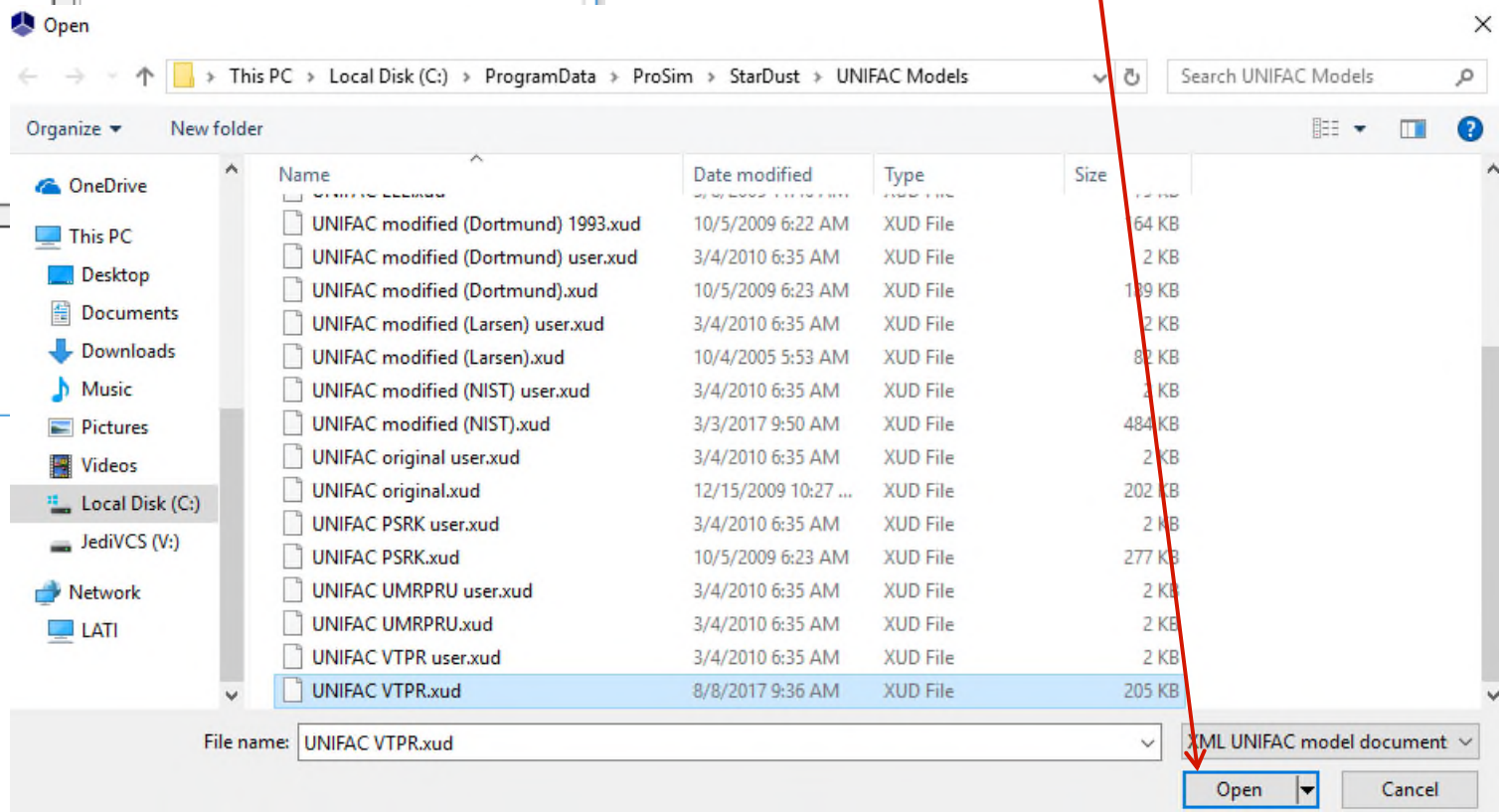
  « C:\ProgramData\ProSim\StarDust\UNIFAC Models »

Editor: open a « xud » file



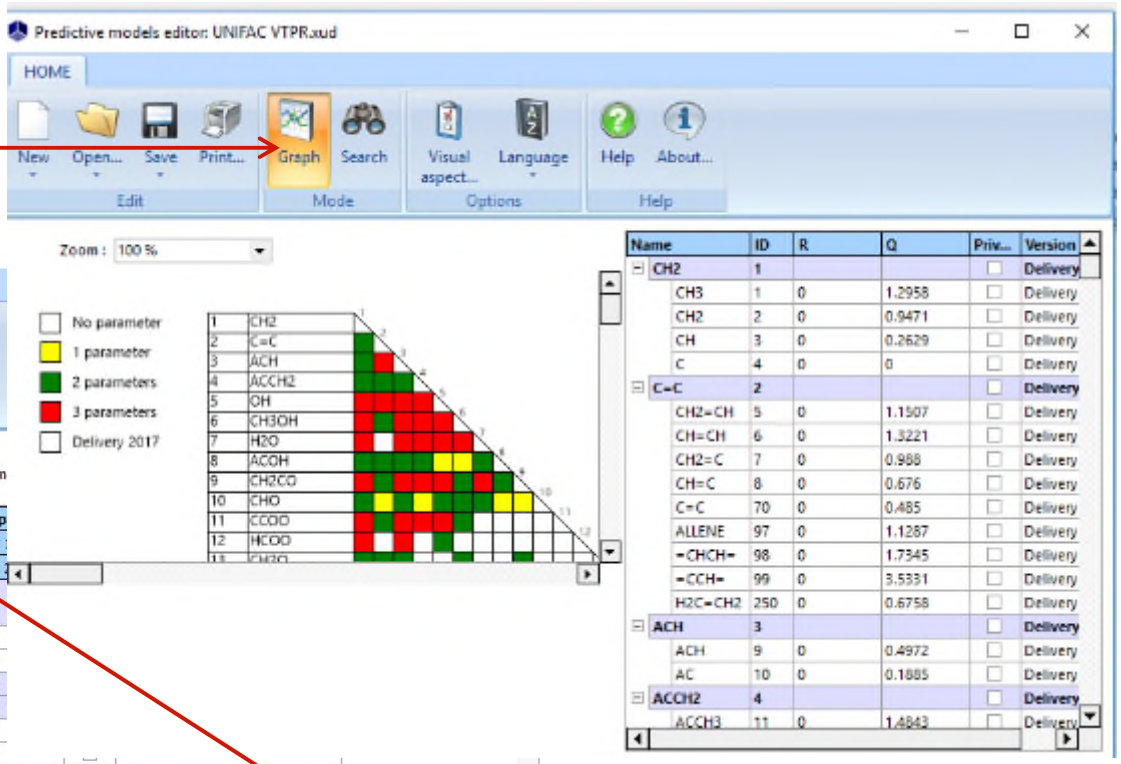
1. Click on « open »

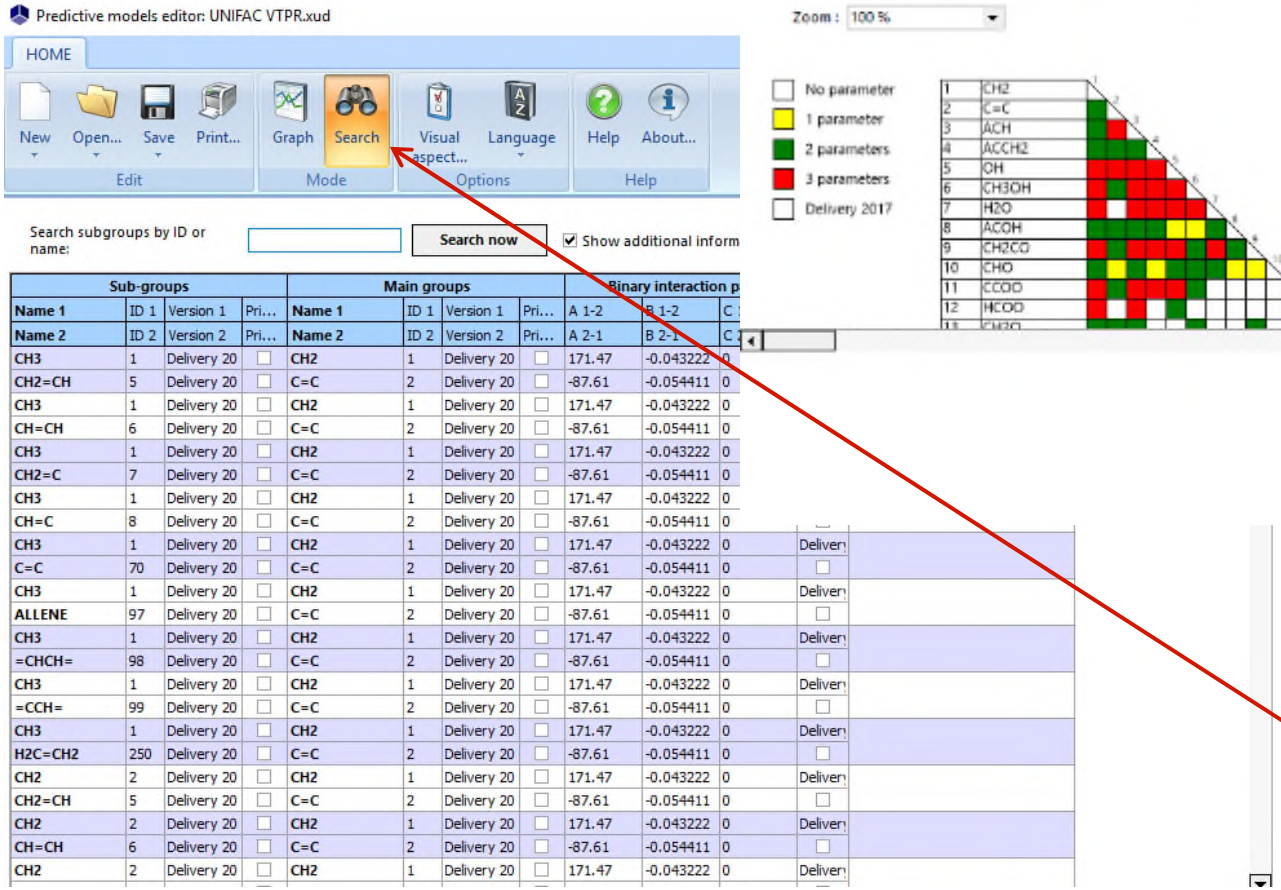
2. You can choose for example « UNIFAC VTPR.xud » and click on « open ».
Note: the default directory is the directory that contains « .xud » files



Editor: indication of use

Graph mode



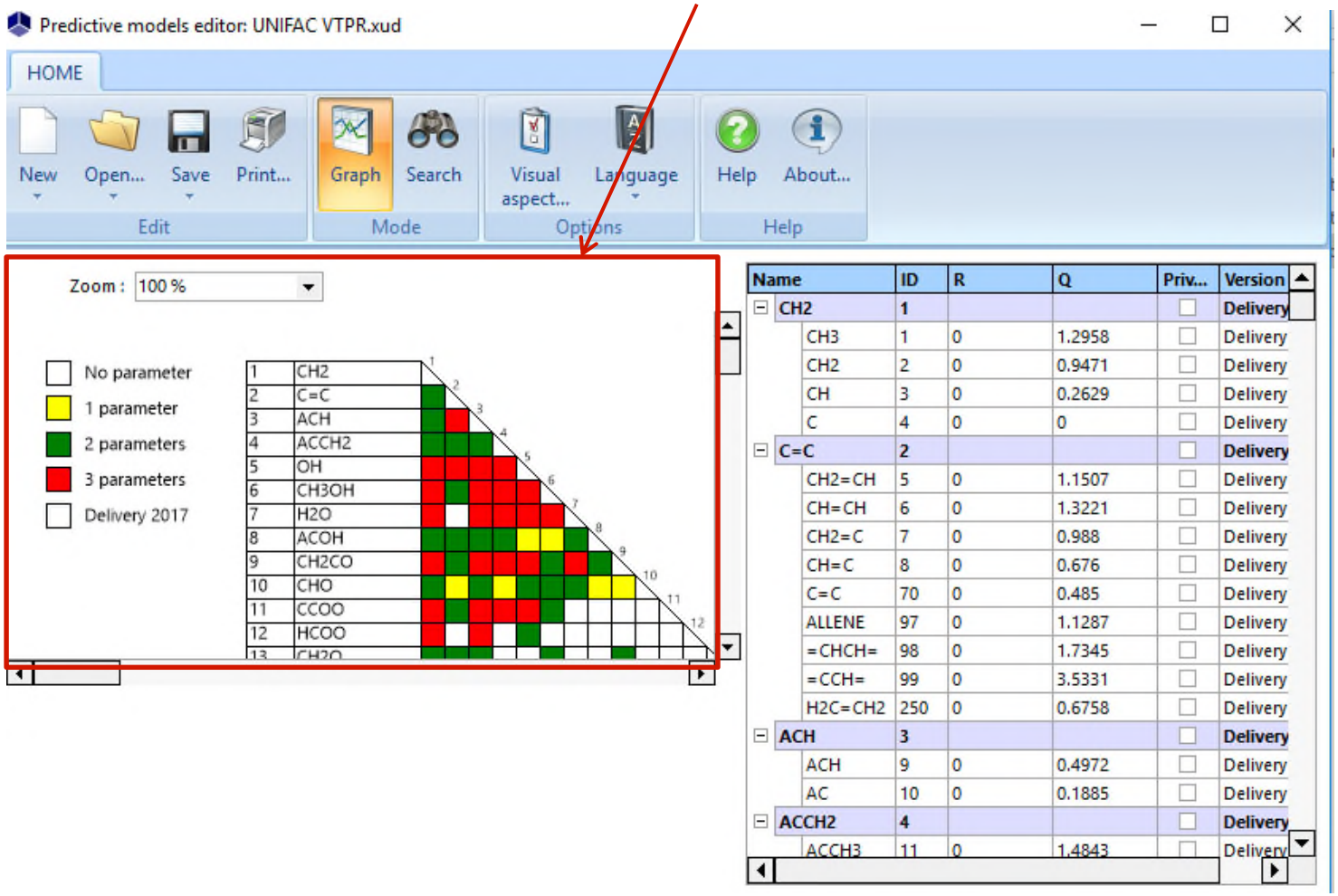


Search mode

Editor: data visualization

Group interactions matrix

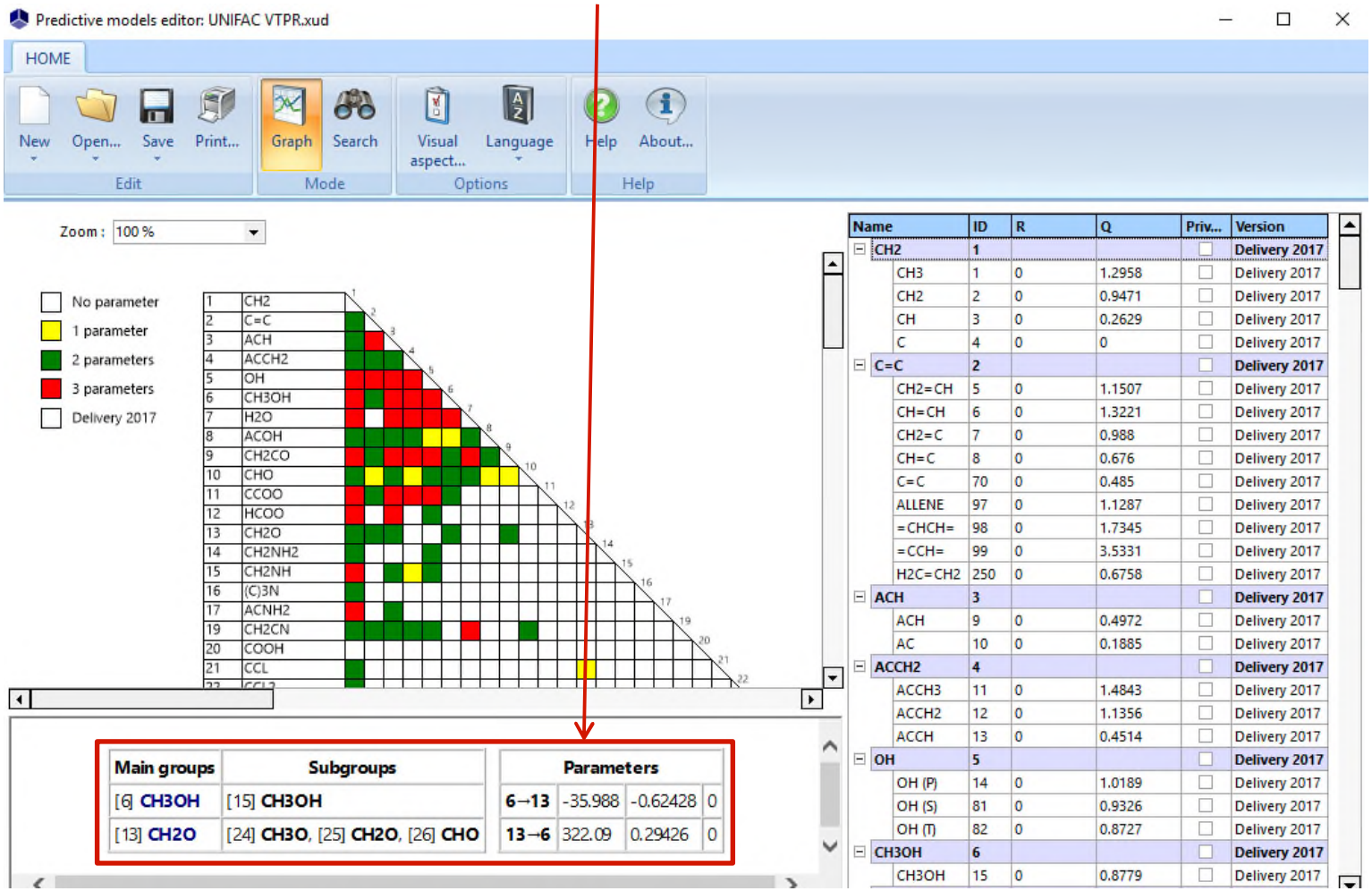
- The color code indicates the number of parameters available for each interaction.
  - In the absence of parameters, the reliability of the predictive model is questionable.



Editor: data visualization

By hovering the mouse on a colored box:

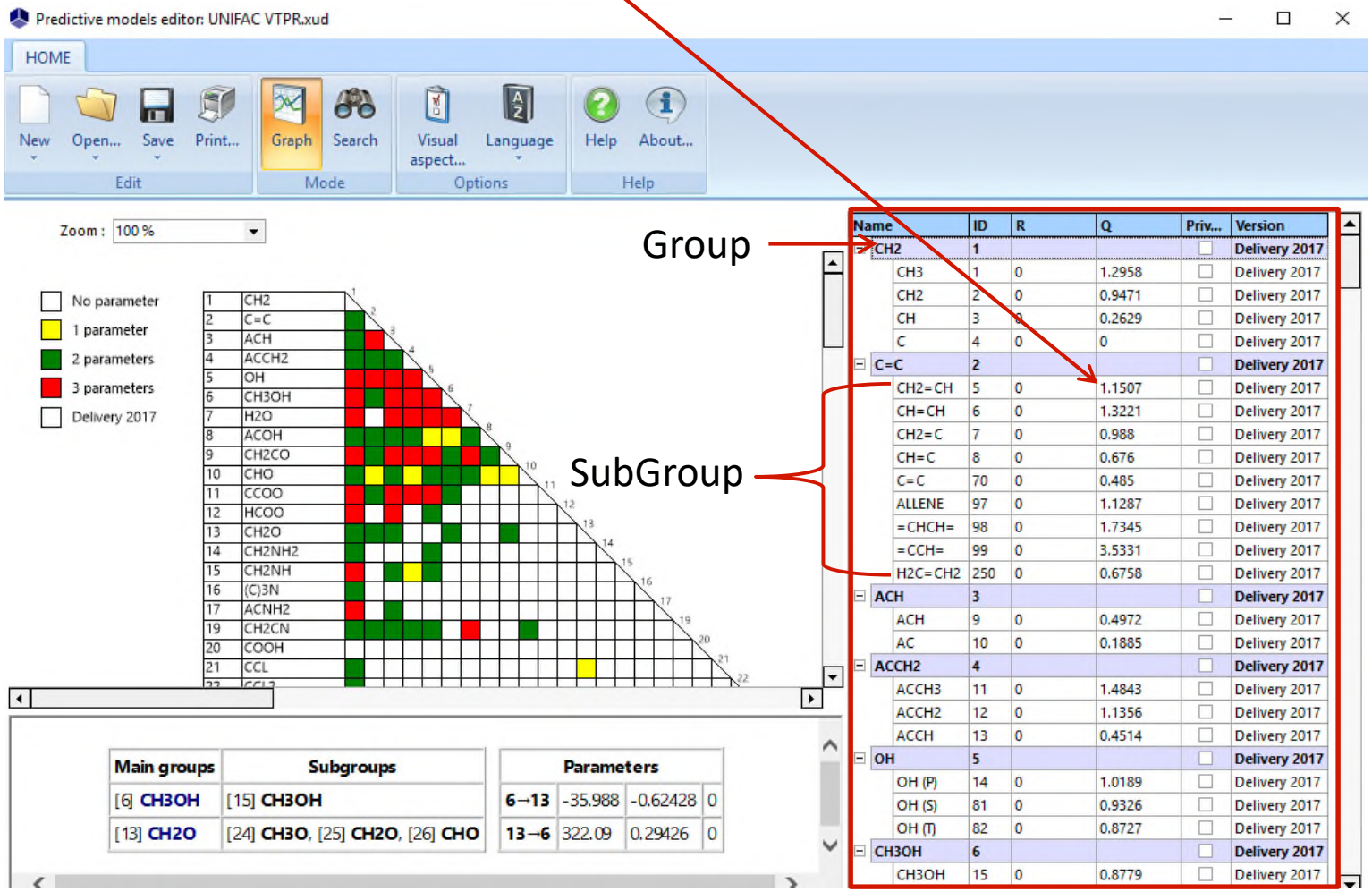
- Display the available parameters for the corresponding groups binary and therefore for associated sub-groups.



Editor: data visualization

Groups and sub-groups description

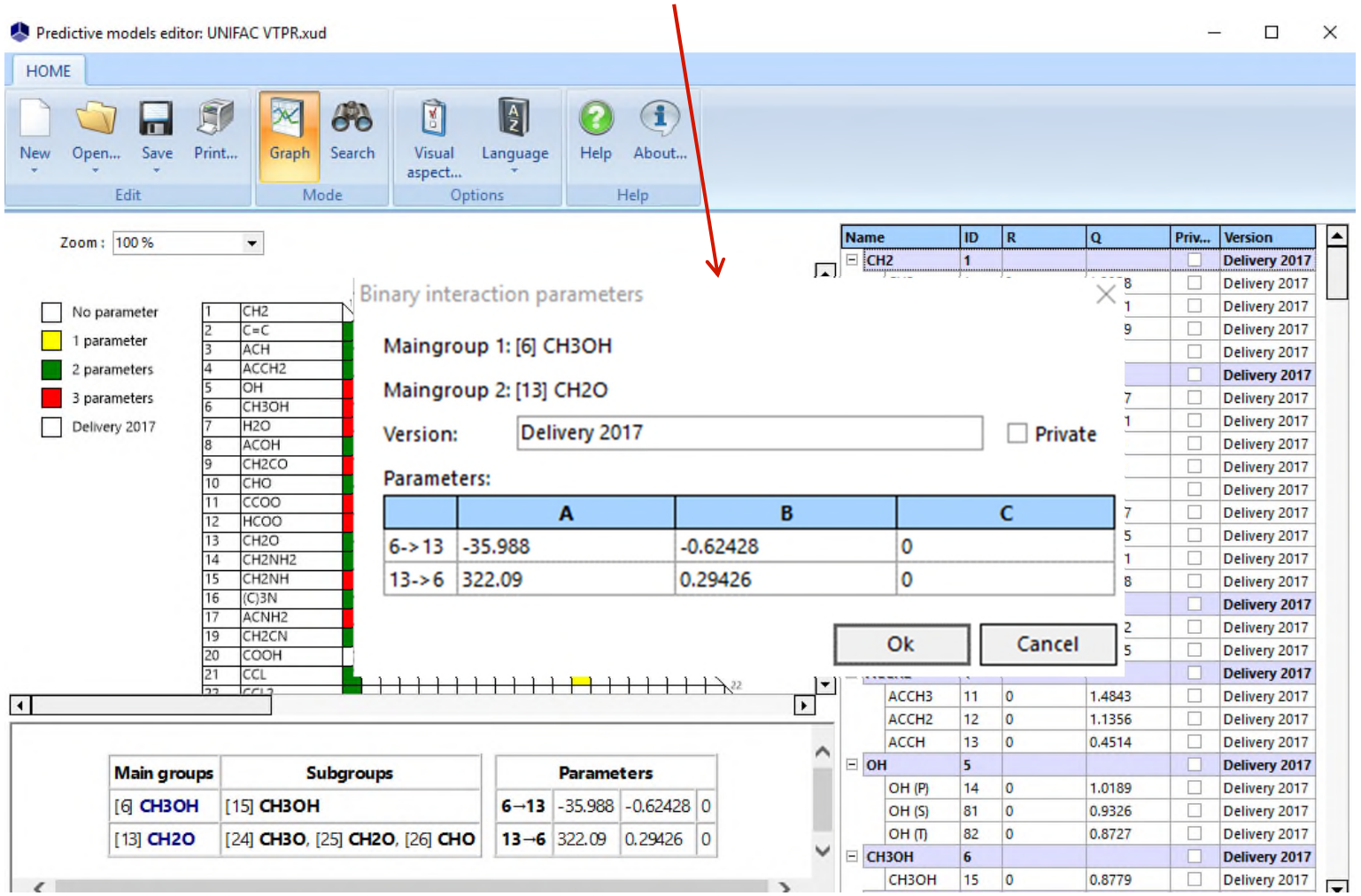
- Groups and sub-groups number
- Sub-groups parameters



Editor: modifications

By clicking on a box, colored or not:

- Open a window for editing group interaction parameters
  - The parameters are not necessarily symmetrical



Editor: modifications

All fields are editable by following the procedure below:

- Select the field
  - In this example, the property R (Van der Waals volume) of CH3 sub-group is selected

Name	ID	R	Q	Priv...	Version
CH2	1				Delivery 201
CH3	1	0	1.2958		Delivery 2017
CH2	2	0	0.9471		Delivery 2017
CH	3	0	0.2629		Delivery 2017
C	4	0	0		Delivery 2017

- Press « Enter » or « F2 » to activate the edit mode
  - The property R (Van der Waals volume) of CH3 sub-group is now editable

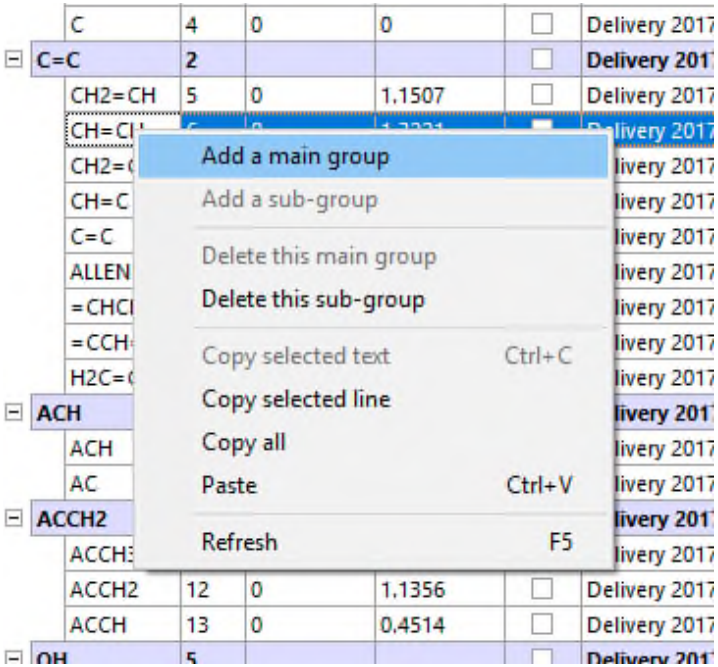
Name	ID	R	Q	Priv...	Version
CH2	1				Delivery 201
CH3	1	0	1.2958		Delivery 2017
CH2	2	0	0.9471		Delivery 2017
CH	3	0	0.2629		Delivery 2017
C	4	0	0		Delivery 2017

- Validate the modification by pressing « Enter ». Since edit mode is active, the next cell becomes editable if necessary

Editor: modifications

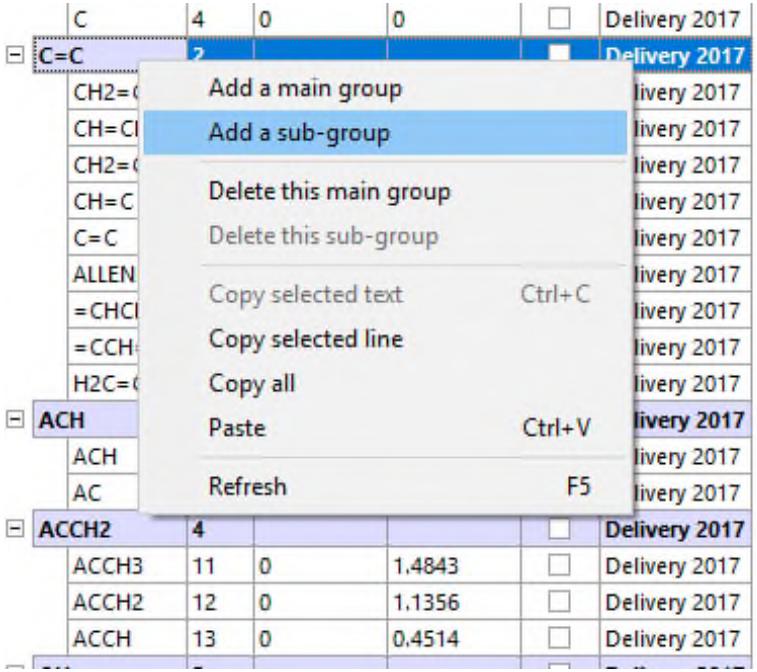
Adding a new main group:

- Right-click on any cell
- In the dropdown menu, choose« Add a main group »
  - The main group is automatically added at the end of the list



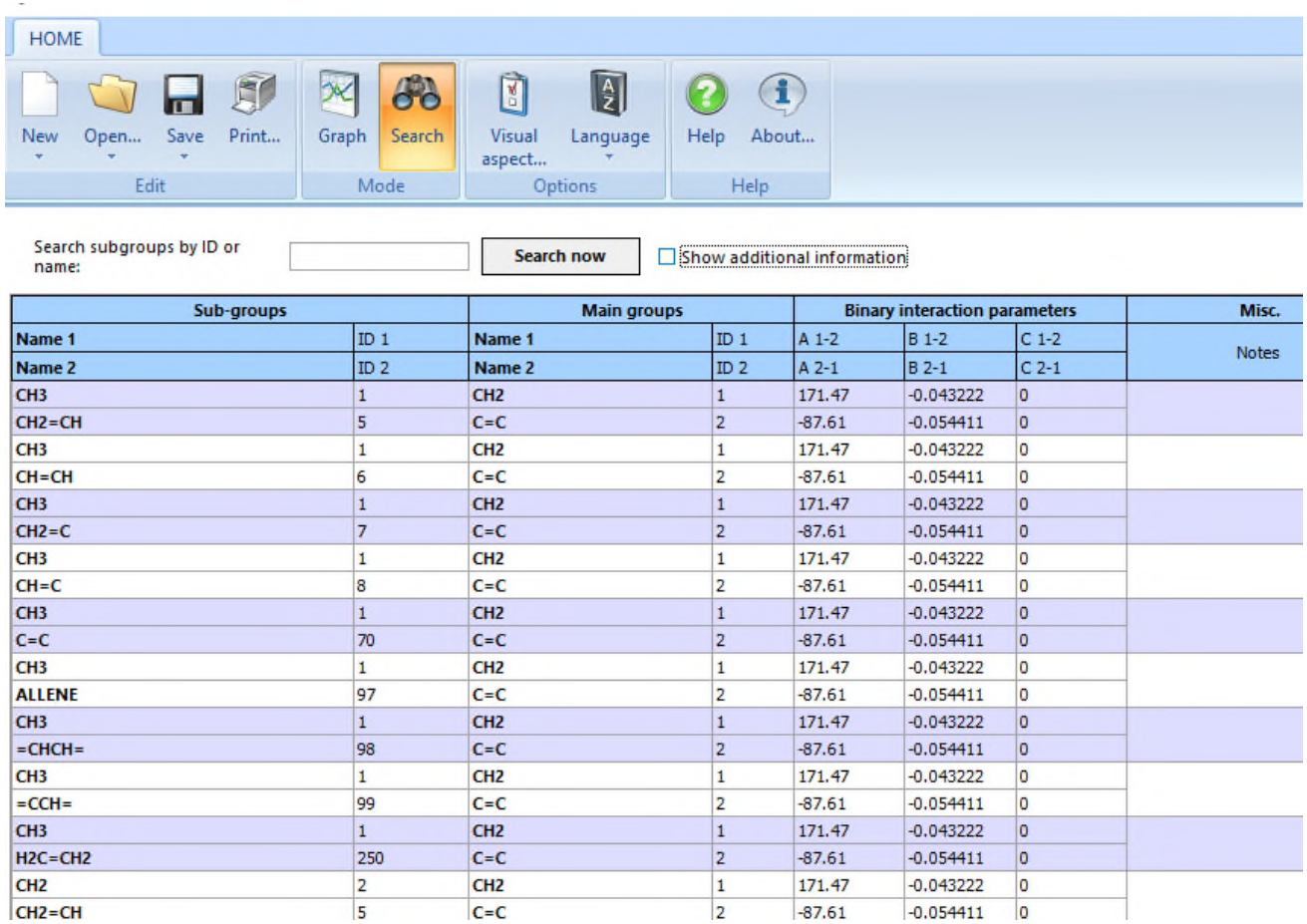
Adding a new sub-group:

- Right-click on the purple line of the desired main group
- In the drop down list, choose « Add a sub-group »



Editor: modifications

The « Search » mode allows to visualize the global set of parameters between a given group and the others, and easily edit them (rather than clicking on the corresponding cell of the triangular matrix presented previously).

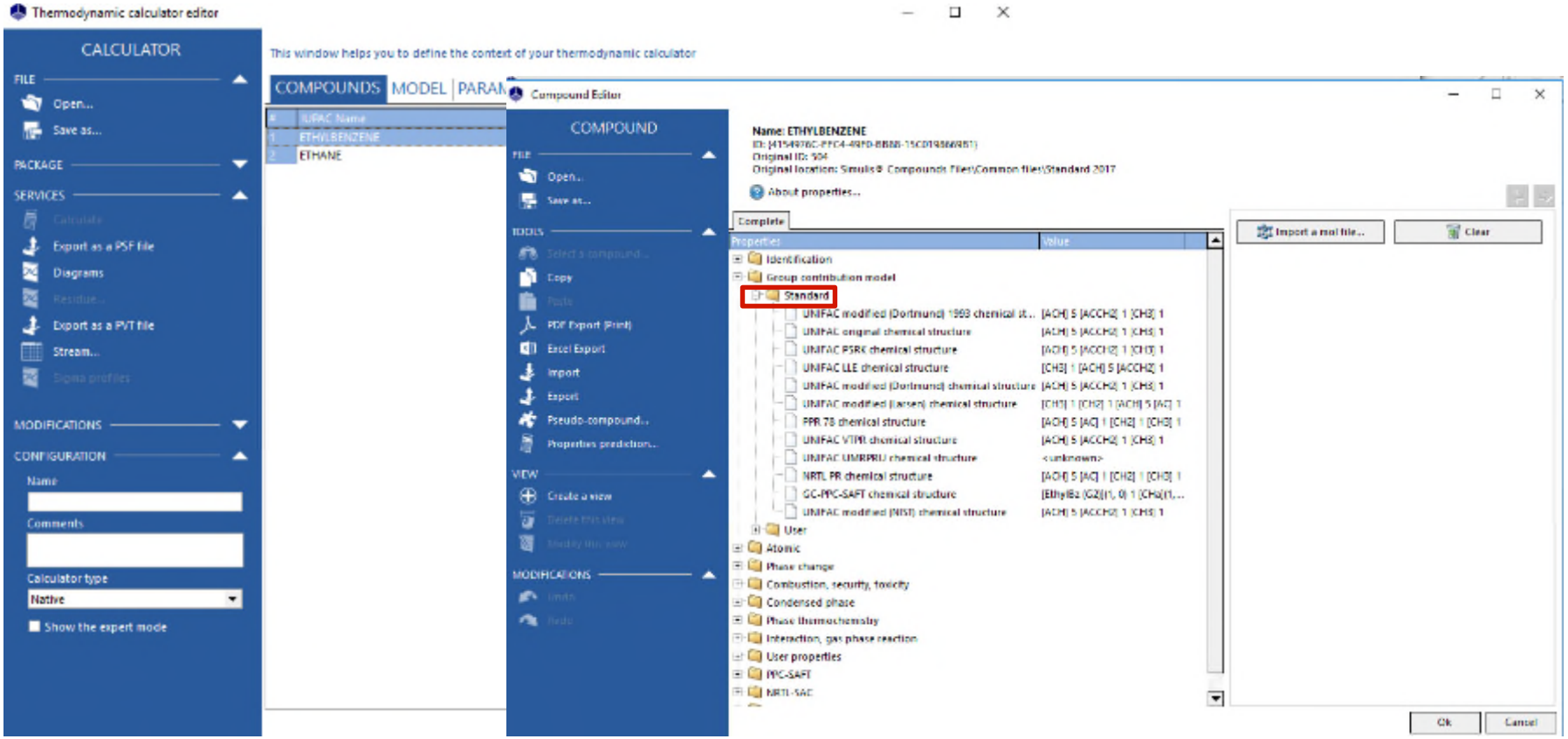


Sub-groups		Main groups		Binary interaction parameters			Misc.
Name 1	ID 1	Name 1	ID 1	A 1-2	B 1-2	C 1-2	Notes
Name 2	ID 2	Name 2	ID 2	A 2-1	B 2-1	C 2-1	
CH3	1	CH2	1	171.47	-0.043222	0	
CH2=CH	5	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH=CH	6	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH2=C	7	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH=C	8	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
C=C	70	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
ALLENE	97	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
=CHCH=	98	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
=CCH=	99	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
H2C=CH2	250	C=C	2	-87.61	-0.054411	0	
CH2	2	CH2	1	171.47	-0.043222	0	
CH2=CH	5	C=C	2	-87.61	-0.054411	0	

Simulis Thermodynamics

For a group contribution model to work, the decomposition of the molecules must involve sub-groups that are available in that model (if the decomposition of the molecules involves a sub-group not recognized by the model, that predictive model cannot be used).

In Simulis Thermodynamics, the decomposition of a molecule must be specified in the « Compounds » tab of the calculator, using the « Standard » sub-folder of the « Group contribution model » folder in the compound editor.

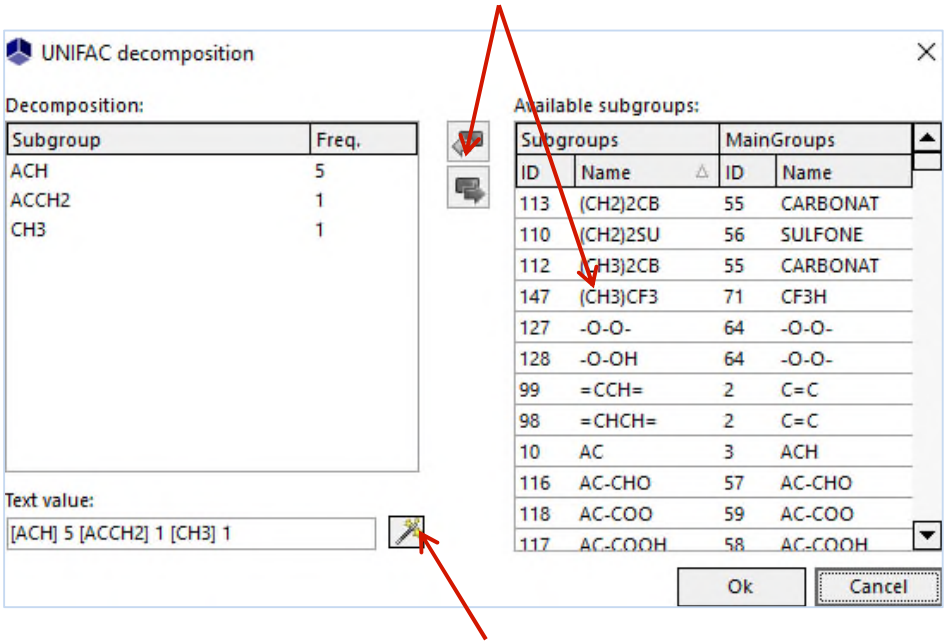


Simulis Thermodynamics

Create the decomposition specification by clicking on the « … » button located at the end of the line for each decomposition

The editing window appears:

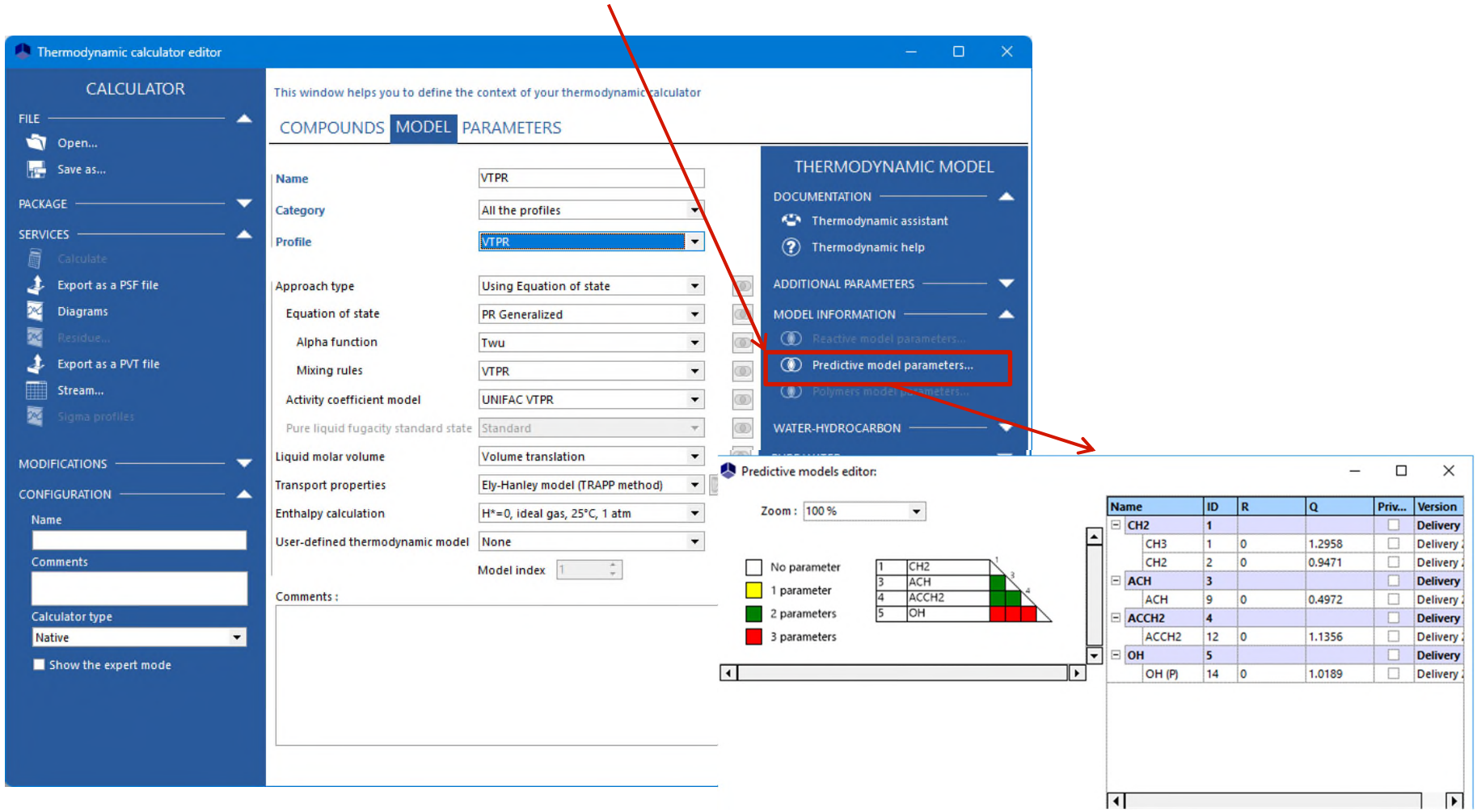
- Sub-groups are added by double clicking on the list located on the right or using the arrows located in the middle



- The magic wand allows an automatic prediction of the decomposition if it is possible and if the SMILES of the molecule has been provided (property available in the « identification » tab of the component).

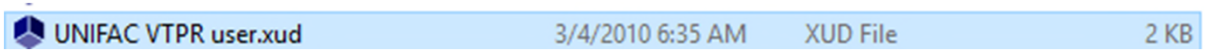
Simulis Thermodynamics

In a Simulis Thermodynamics « calculator », if a group contribution predictive model is selected (e.g. VTPR), click on “Predictive model parameters” to visualize the reduced matrix that only display the groups related to the components of the calculator.



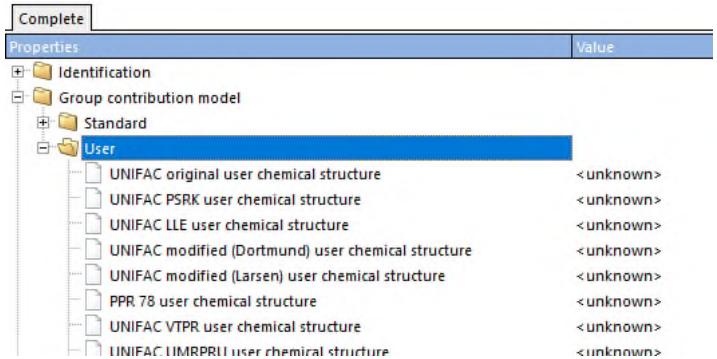
Simulis Thermodynamics

If the user wants to use a custom matrix it is possible to edit and import the « User » templates.
In the « C:\ProgramData\ProSim\StarDust\UNIFAC Models » folder, empty « .xud » files with the « User » indication are available for each model.



These files need to be fully configured by the user. The thermodynamic model to choose is the one with the « (User) » extension.

The molecules decompositions need to be defined in the « User » sub-folder**.**
For these models, automatic decomposition may not be consistent since it is based on the groups involved in original models.



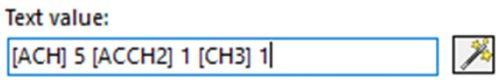
Private matrices

If the user is member of the UNIFAC consortium, private « .xud » files are provided by the consortium to all members. An installation tool provided by ProSim, in addition to Simulis Thermodynamics, allows to upgrade the ProSim public databases with the UNIFAC member's private databases.

« UNIFAC Private [year] for Simulis Setup.exe »

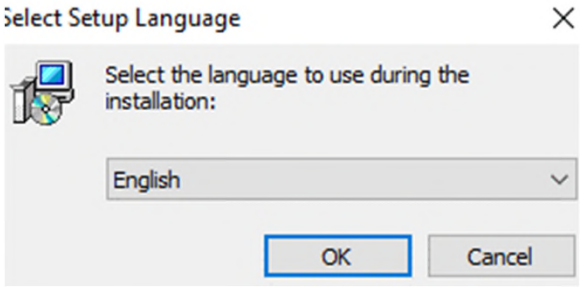
In order to compare the results, the public databases are conserved in the « Public » folder within the directory containing the « .xud » files.

WARNING: The use of private databases implies new parameters, but especially new groups! The molecules decompositions must be updated to correspond with the private databases. The automatic decomposition tool takes into account the type of database (public/private) in order to provide a consistent decomposition.

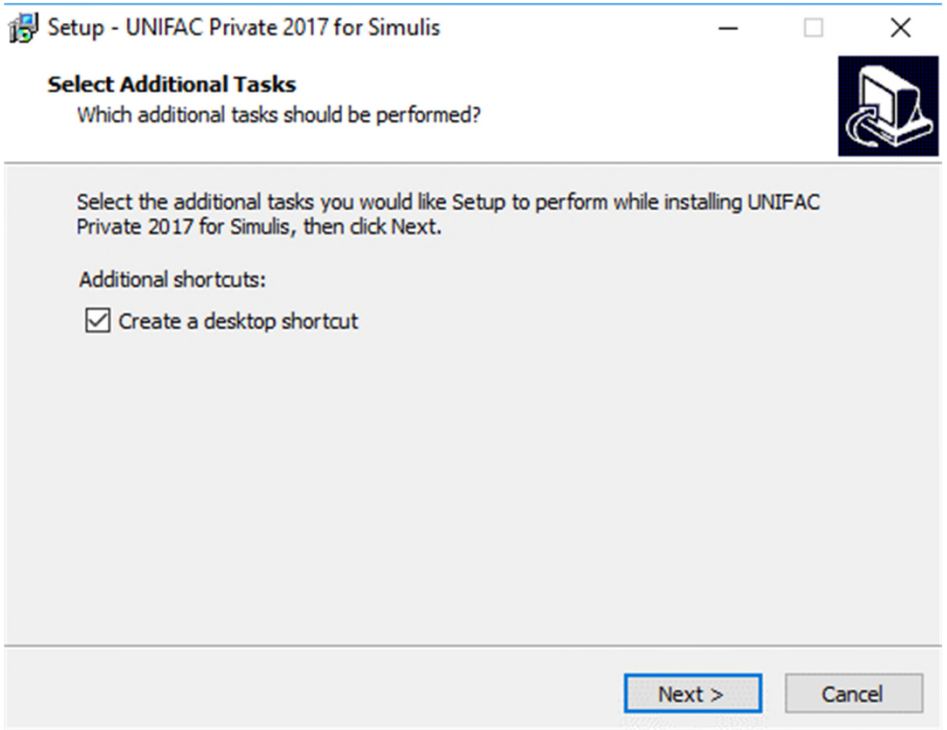


Private matrices

- Select the installation language and press « OK »

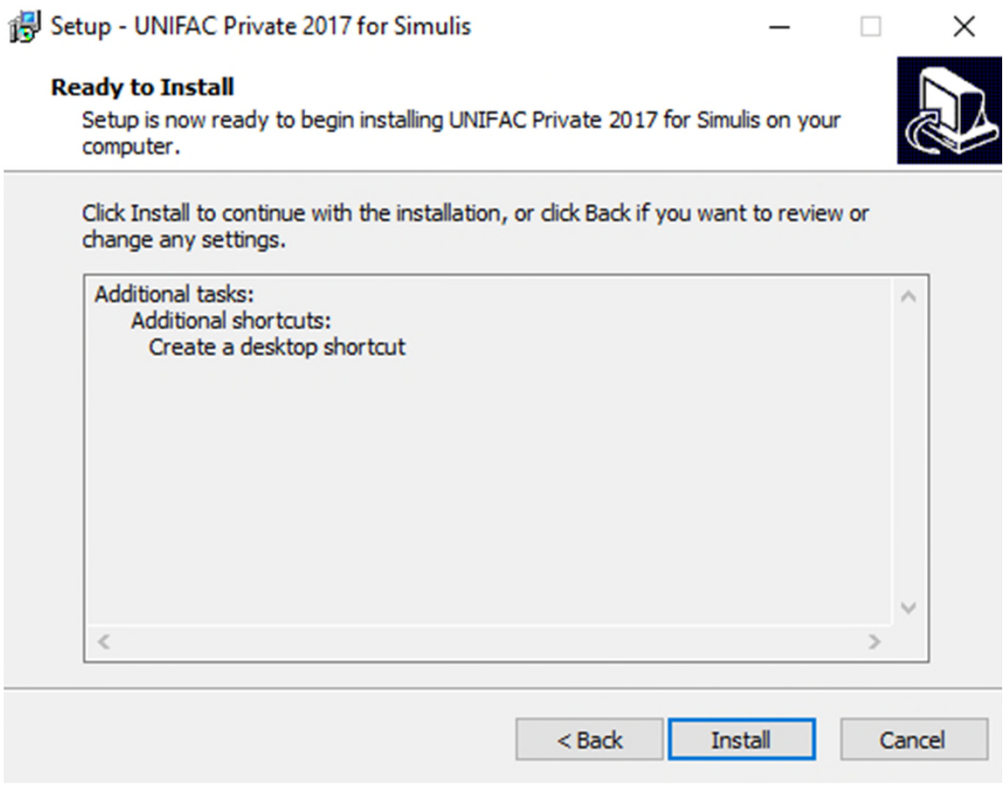


- Choose if a shortcut icon for the predictive model editor should be installed or not on the desktop and press « Next »



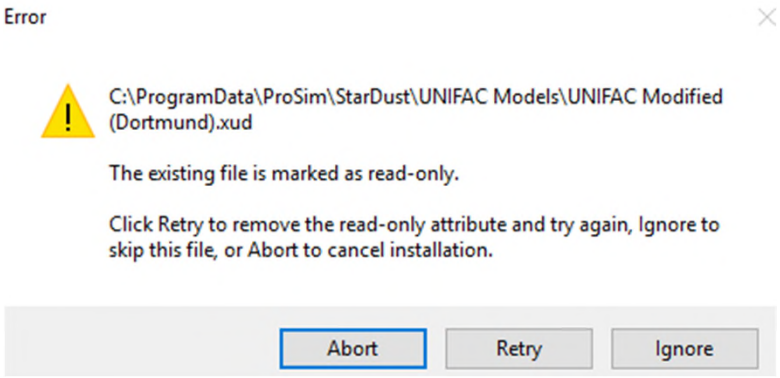
Private matrices

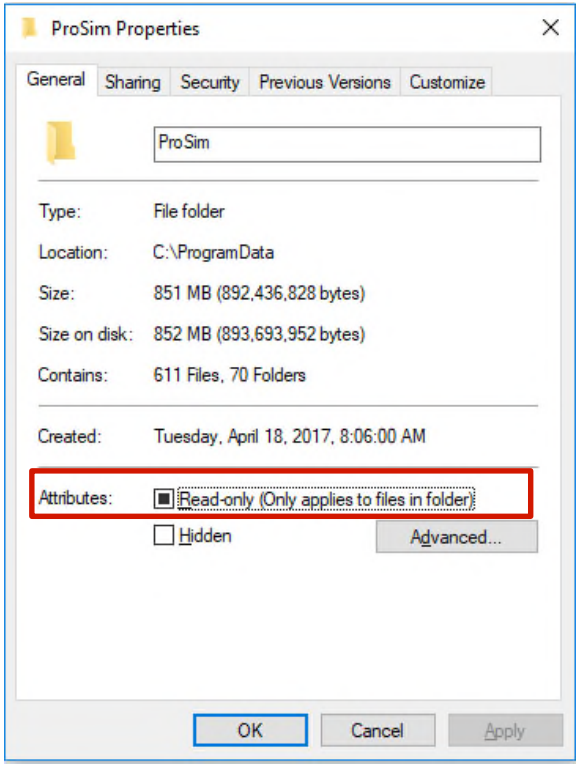
- Click on « Install »



Private matrices

- Note that in some cases, files are « read-only », therefore it is necessary to change the directory attribute « C:\ProgramData\ProSim »





Private matrices

- Once the installation is complete, the installer offers to immediately run the predictive models editor.

ProSim

Software & Services In Process Simulation

ProSim SA
51, rue Ampère
Immeuble Stratège A
F-31670 Labège
France

☎: +33 (0) 5 62 88 24 30

www.prosim.net

info@prosim.net

ProSim, Inc.
325 Chestnut Street, Suite 800
Philadelphia, PA 19106
U.S.A.

☎: +1 215 600 3759