Getting started with Simulis® Thermodynamics

Use Case 6: Defining the decomposition of pure components in order to use group contribution models

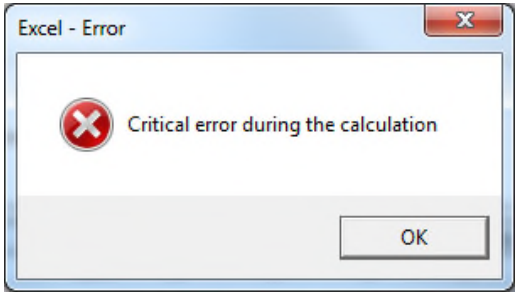
Software & Services In Process Simulation

We guide You to efficiency

ProSim

Introduction

The following message may appear when you are using a predictive thermodynamic model such as UNIFAC or PPR78:



In most of the cases, this message corresponds to missing information about the mixture, in particular concerning the decomposition of the mixture components.

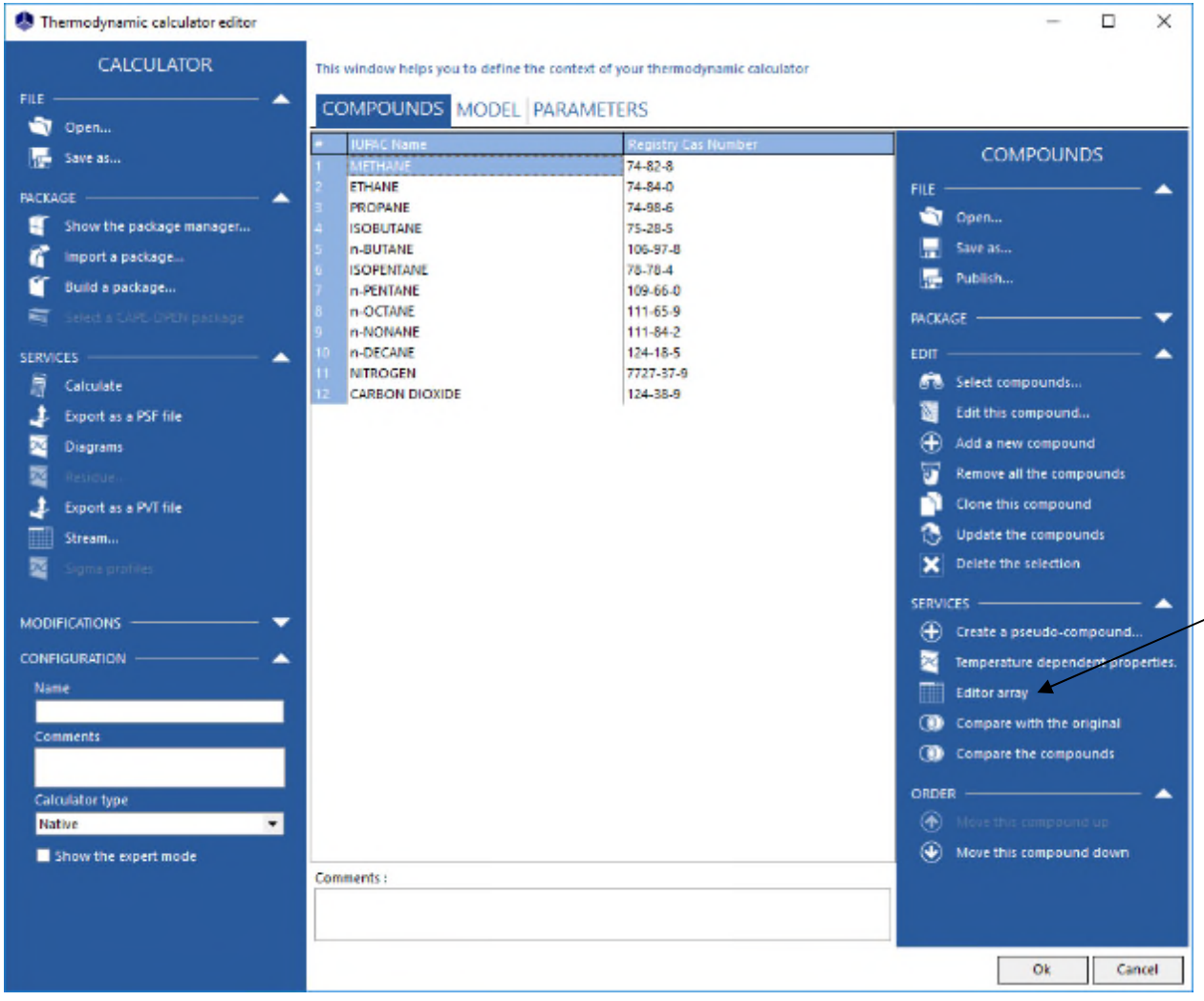
The following steps show how to add the required decomposition information.

In this example, the mixture contains the following components: methane, ethane, propane, isobutane, n-butane, isopentane, n-pentane, n-heptane, n-octane, n-nonane, n-decane, nitrogen and carbon dioxide.

The Unifac VTPR thermodynamic model is selected.

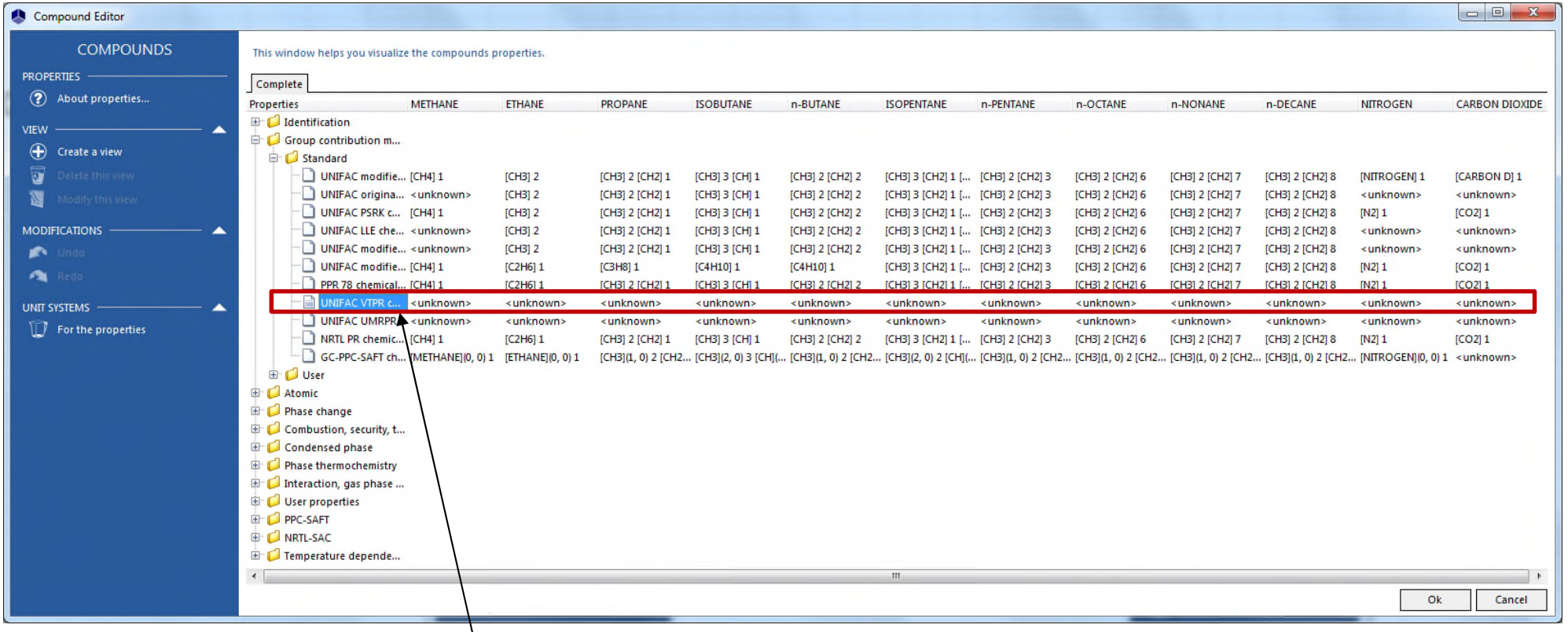
At this stage, it is assumed that components and thermodynamic models were already selected. For more information on this step, please consult "*Getting started with Simulis Thermodynamics, Case 1*".

Step 1: Edit the calculator



Open the *Thermodynamic calculator editor* and click on *"Editor array"*.

Step 1: Edit the calculator

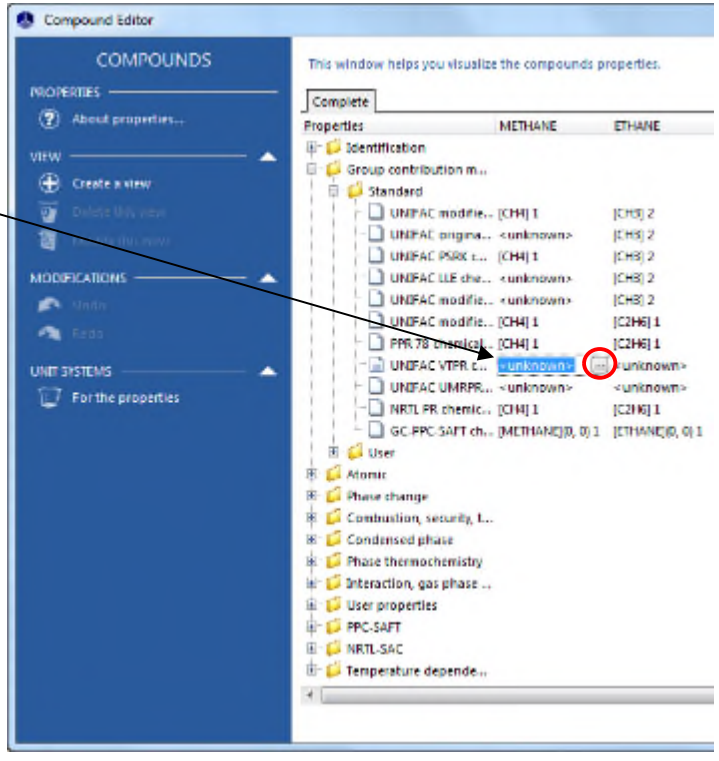


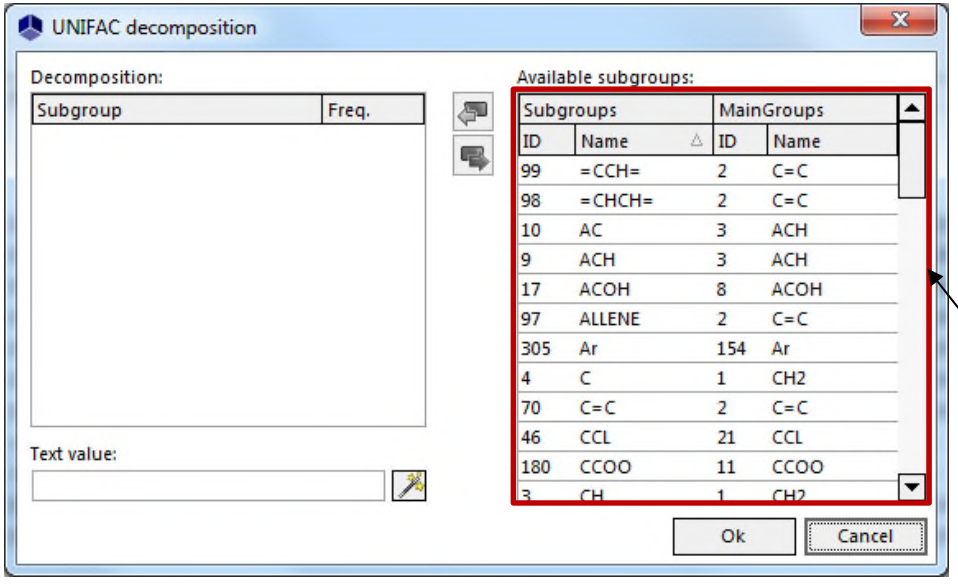
The decompositions that are available for the different thermodynamic models are displayed in the “Group contribution model" tab.

We can see that the decompositions are missing (marked as “unknown”) for the UNIFAC VTPR model.

Step 2: fill out the missing information

Click on the "*unknown*" field, then click on the 3 dots that appear.





The decomposition window opens.

The available subgroups for this specific thermodynamic model are presented on the right side of the window.

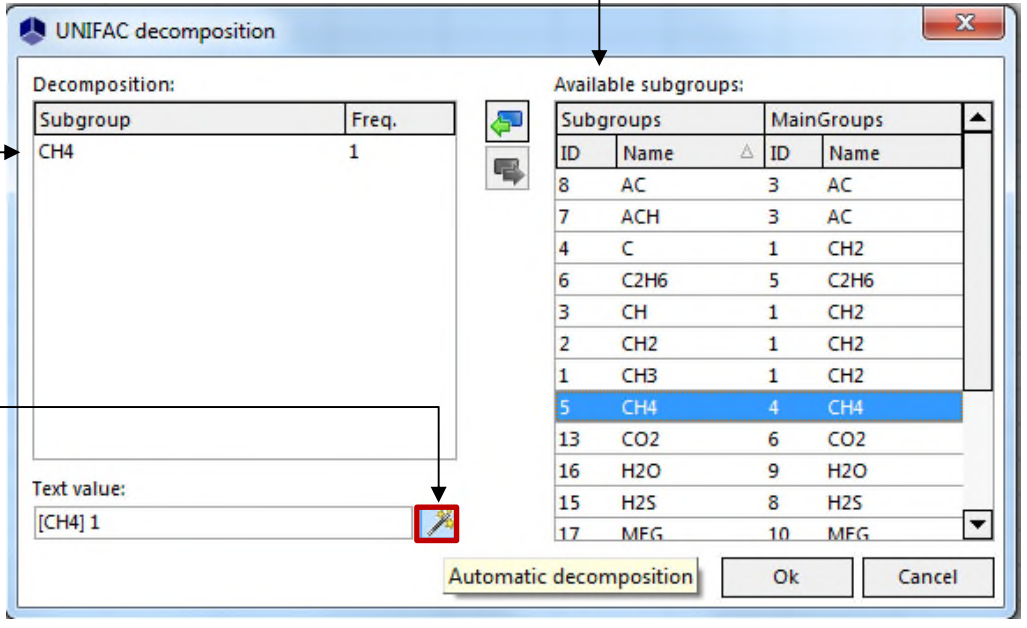
Step 2: fill out the missing information

There are 2 different methods to obtain the group decomposition of a compound:

Manual method:
Double-click on the subgroups corresponding to the chemical structure of the component.

The subgroups that are selected, along with their frequency in the molecule, are displayed on the left part of the window.

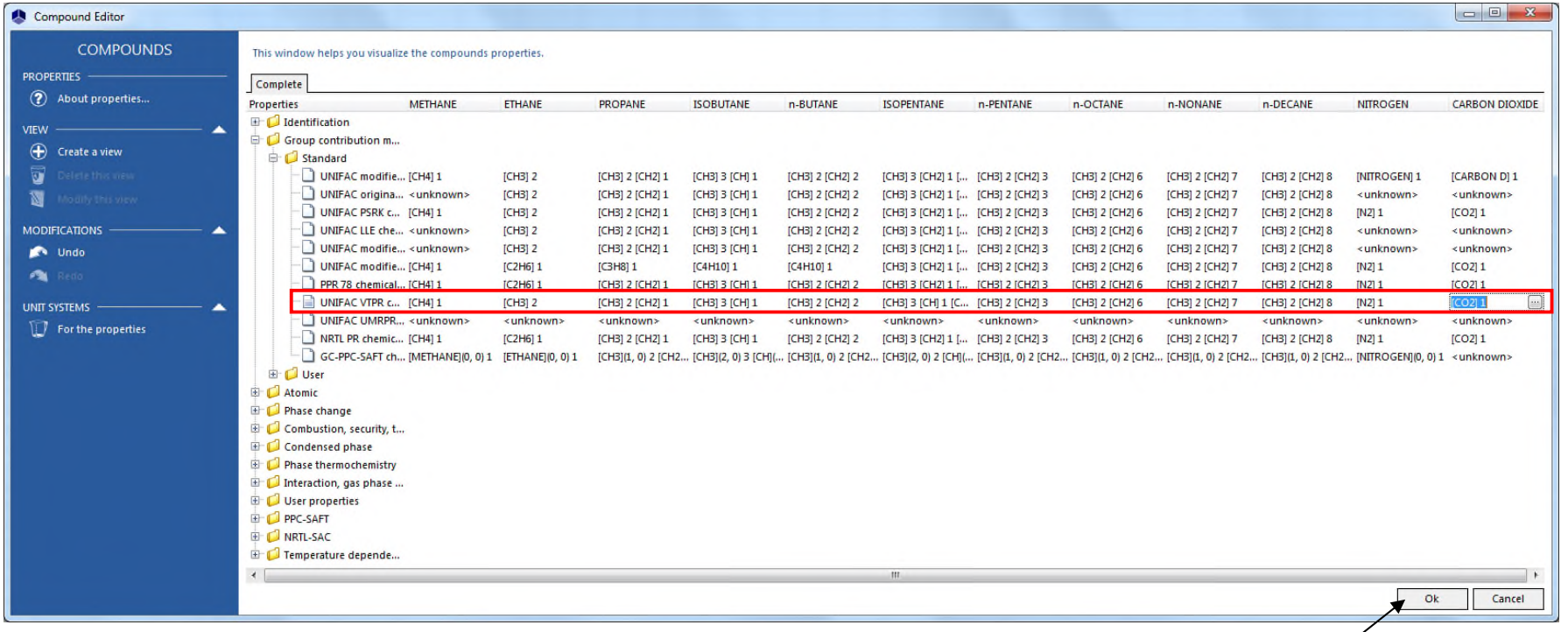
Automatic method:
Click on the wand icon. The group decomposition will be automatically generated from the SMILES.



The automatic method can be used if the SMILES of the compound has been provided and if the corresponding subgroups are available for the selected thermodynamic model.

Step 3: complete the operation and confirm

Repeat the operation until all the fields are defined for the selected model.

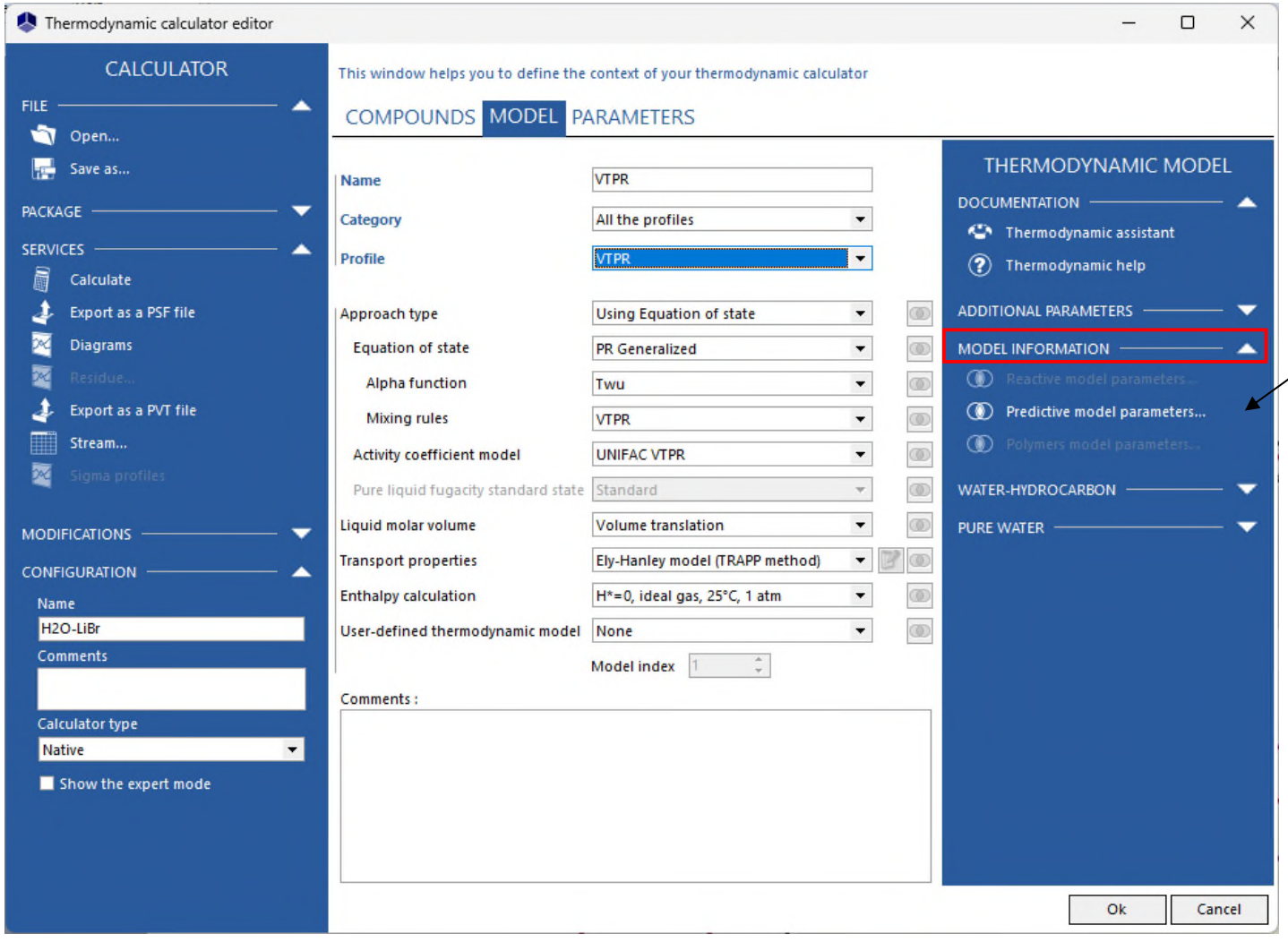


Click on "*OK*" to confirm. You can now use UNIFAC VTPR thermodynamic model for this mixture.

In order to use a group contribution model, the decomposition of all the compounds must be provided for this specific model.

Step 3: complete the operation and confirm

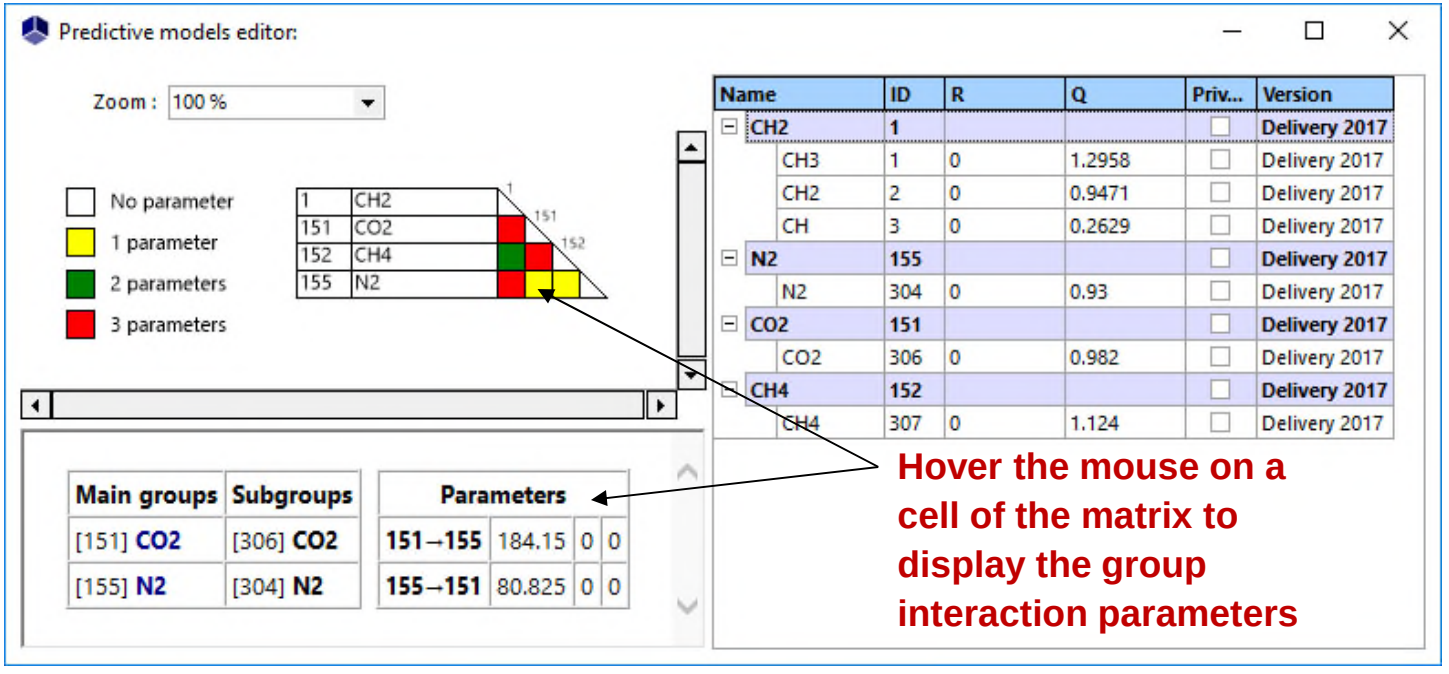
When a predictive model is selected in the "*Model*" tab, it is possible to access the parameters of the groups (and subgroups) corresponding to the compounds imported in the calculator.



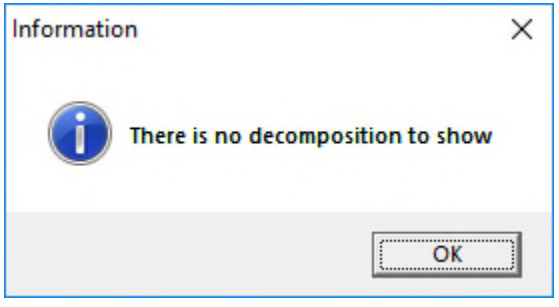
Click on "*Predictive model parameters*".

Step 3: complete the operation and confirm

The following window appears, displaying the decomposition obtained for the selected predictive model:



If, for the selected model, the decomposition has not been provided for all the compounds, the following error is displayed:



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

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

☎: +1 215 600 3759

www.prosim.net

info@prosim.net