Getting started with Simulis® Thermodynamics

Use Case 7: Plotting residue curves

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ProSim

Introduction

This document presents the different steps to follow in order to plot residue curves with Simulis Thermodynamics.

The steps are the following:

- Step 1: Set the thermodynamic system
- Step 2: Plot the ternary diagram
- Step 3: Plot the residue curves

The ternary system used in this example is a mixture of acetone, methanol and methyl-ethyl-ketone (MEK).

Before studying this case, it is recommended to consult "Getting Started with Simulis Thermodynamics, Case 1" .

About residue curves...

Residue curves map (RCM) are useful, for example, to visualize and investigate entrainers that can facilitate distillation by breaking an azeotrope.

Because the choice of an entrainer determines the separation sequence, its selection is a critical step in the synthesis and conceptual design of azeotropic distillation processes.

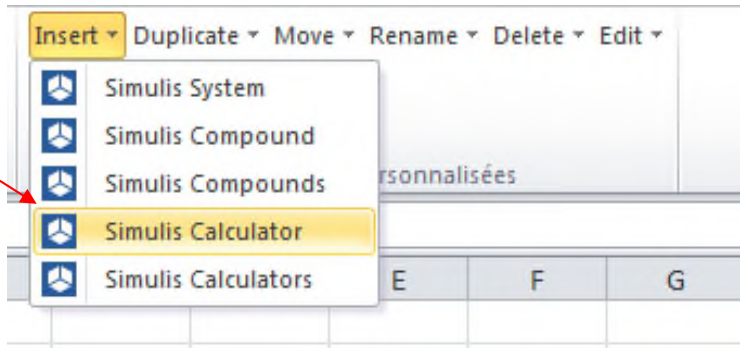
Residue curves are obtained by plotting the evolution through time of the composition of the liquid residue at vapor equilibrium for a simple batch distillation (Rayleigh distillation), starting with the initial composition of the boiler. The path of the liquid compositions starting from the initial point (charge composition) is called a *residue curve*.

Step 1: Set the thermodynamic system

ACCESS THE THERMODYNAMIC CALCULATOR EDITOR:

- **<u>If you are using Simulis Thermodynamics in Excel</u>:**

Create the calculator object in a spreadsheet



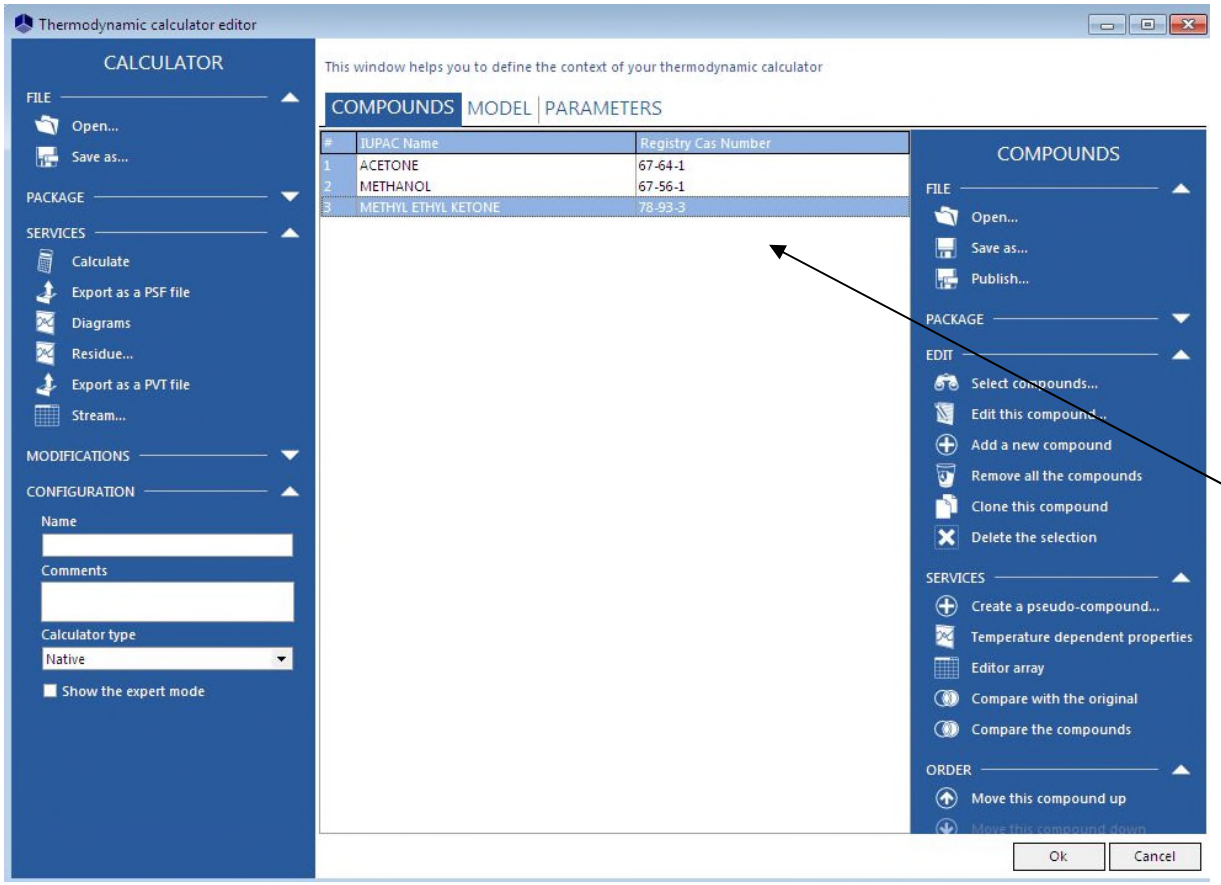
- **<u>If you are using Simulis Thermodynamics within another ProSim environment</u> (ProSimPlus, BatchReactor, BatchColumn etc…):**

Click on the thermodynamic icon to open the calculator editor:

or

Simulis Thermodynamics is a « software component » that you can integrate into different applications: ProSim software, Excel, Matlab, your own software, etc…

Step 1: Set the thermodynamic system

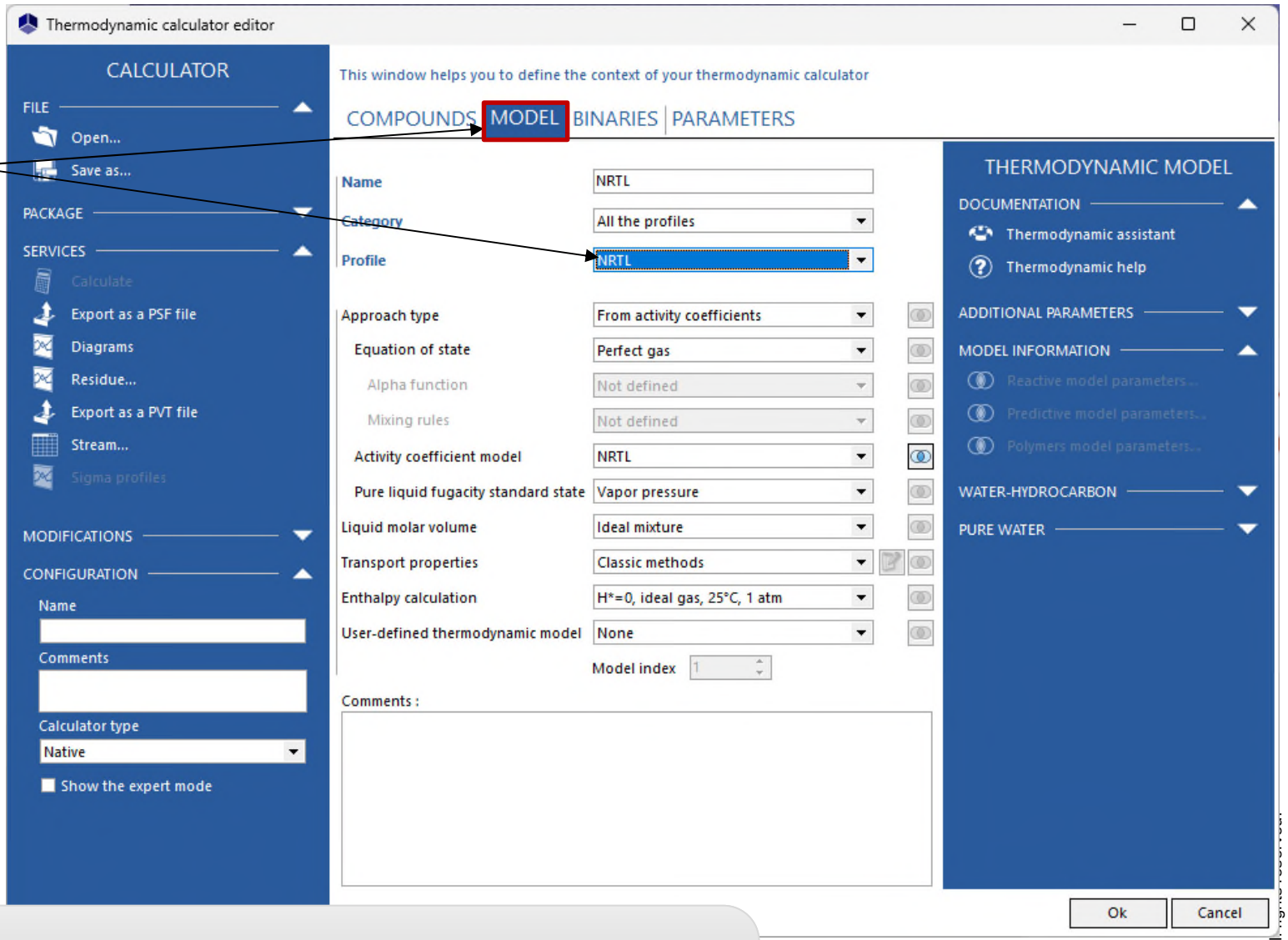


Select Acetone, Methanol and Methyl-Ethyl-Ketone in the standard pure components database (click on "*Select compounds*").

Refer to "*Getting Started with Simulis Thermodynamics, use case 1*" for details on these operations.

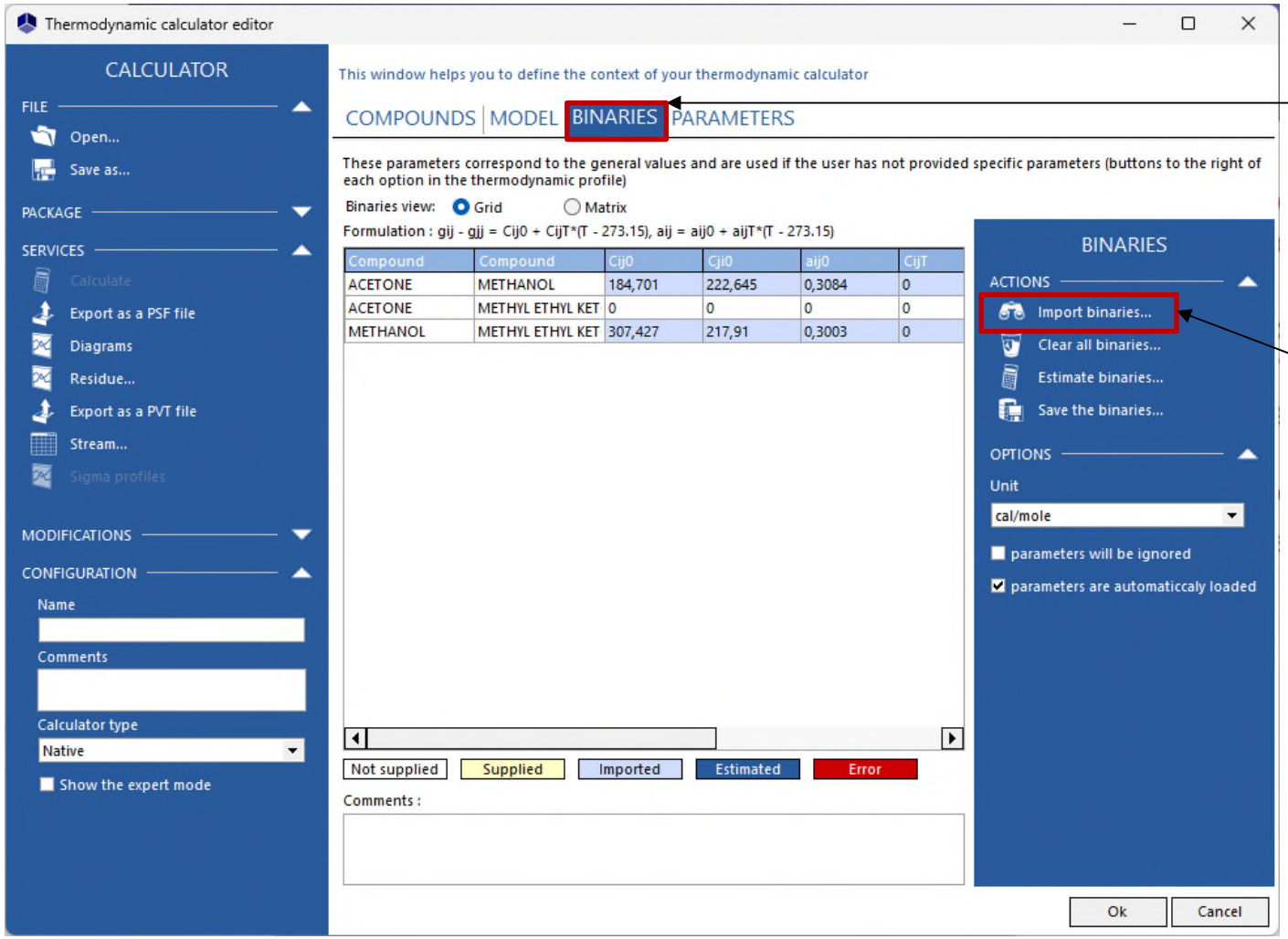
Step 1: Set the thermodynamic system

Select the NRTL profile in the "*Model*" tab



Refer to "*Getting Started with Simulis Thermodynamics, use case 1*" for details on these operations.

Step 1: Set the thermodynamic system

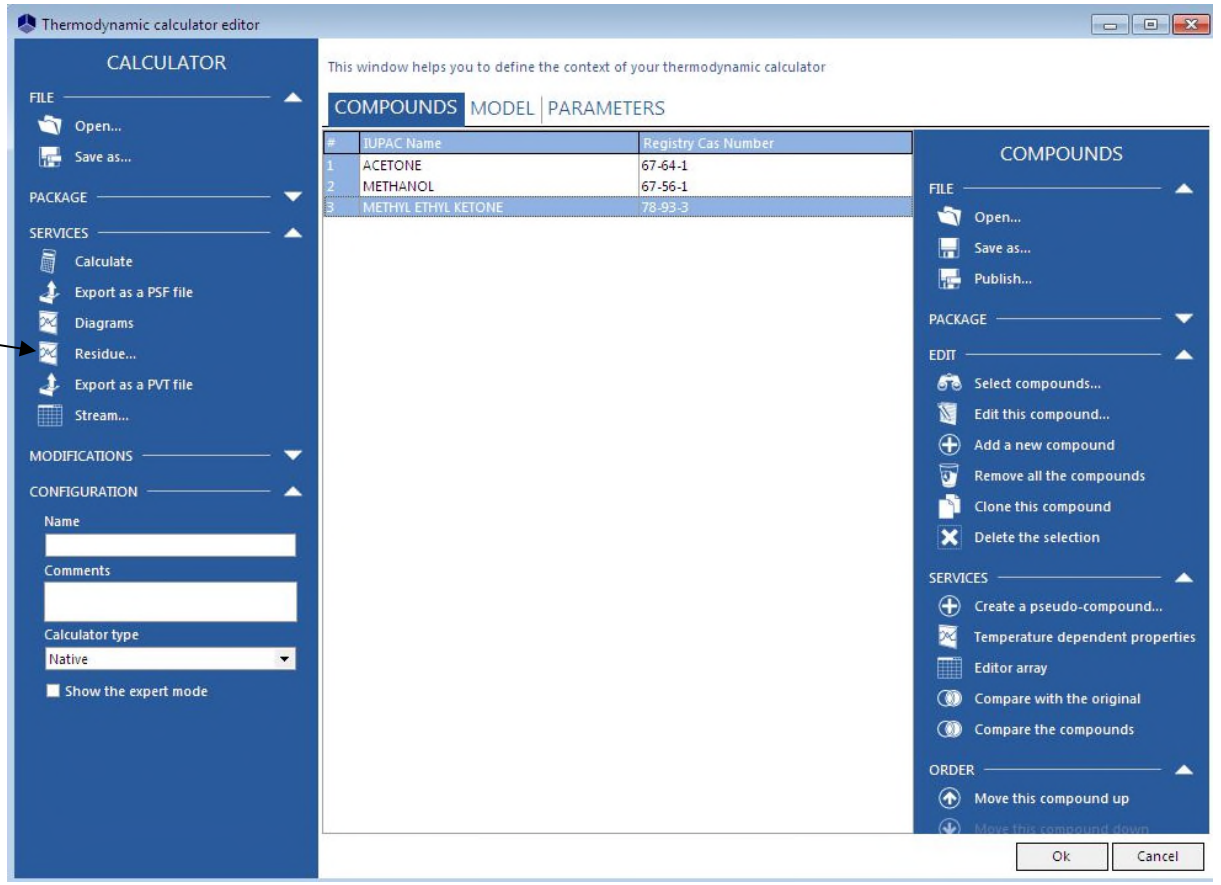


Click on the "*Binaries*" tab (which appears when you select the NRTL model). The binaries interaction parameters (BIPs) available in the Standard database are automatically loaded.

Refer to "*Getting Started with Simulis Thermodynamics, use case 1*" for details on these operations.

Step 2: Plot the ternary diagram

Click on “Residue” to open the residue curve calculation service.



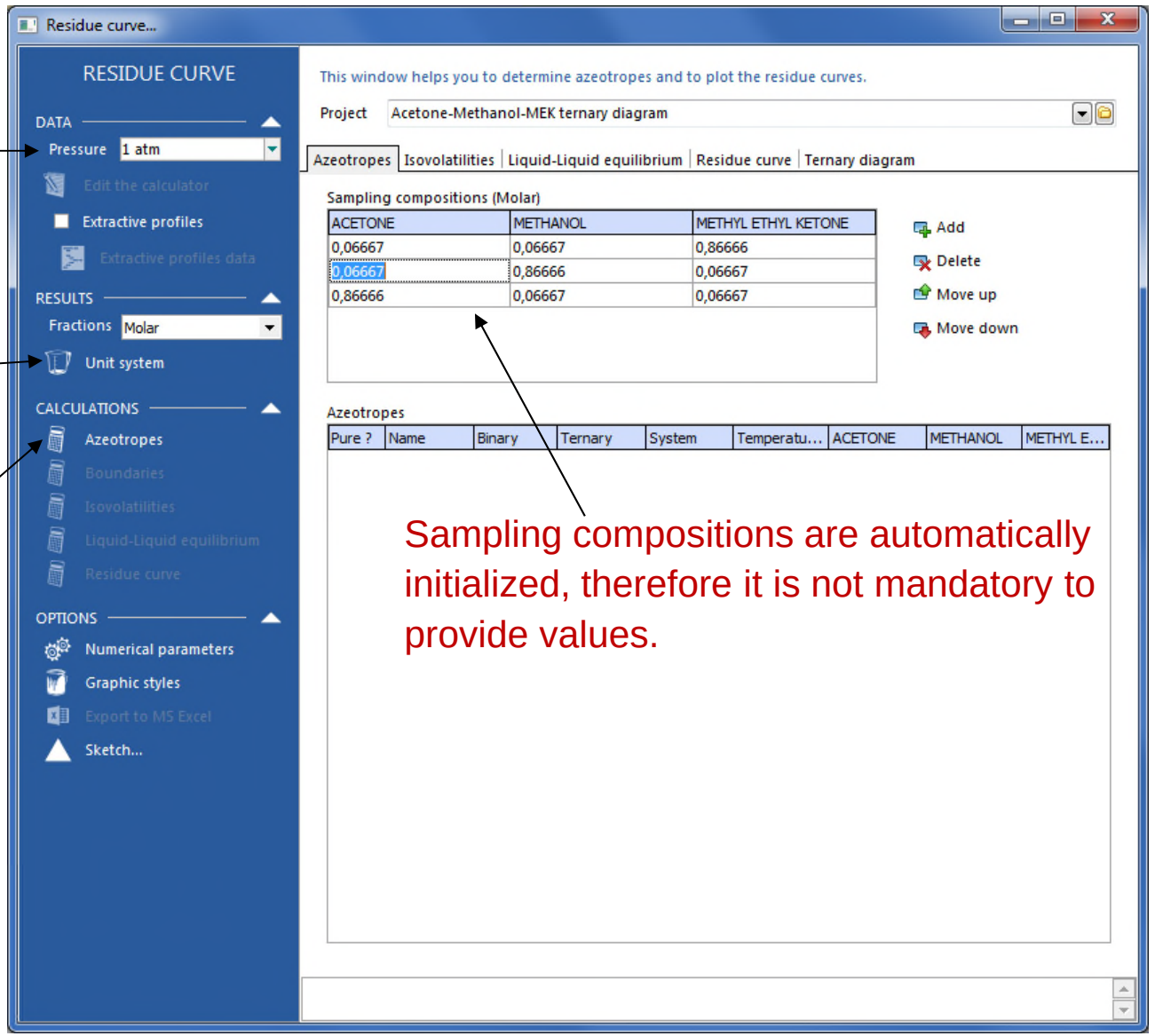
The residue curve calculation service is only available when 3 components have been selected.

Step 2: Plot the ternary diagram

Set the pressure to 1 atm (default value).

Change the temperature units from Kelvin to Celsius in the unit system.

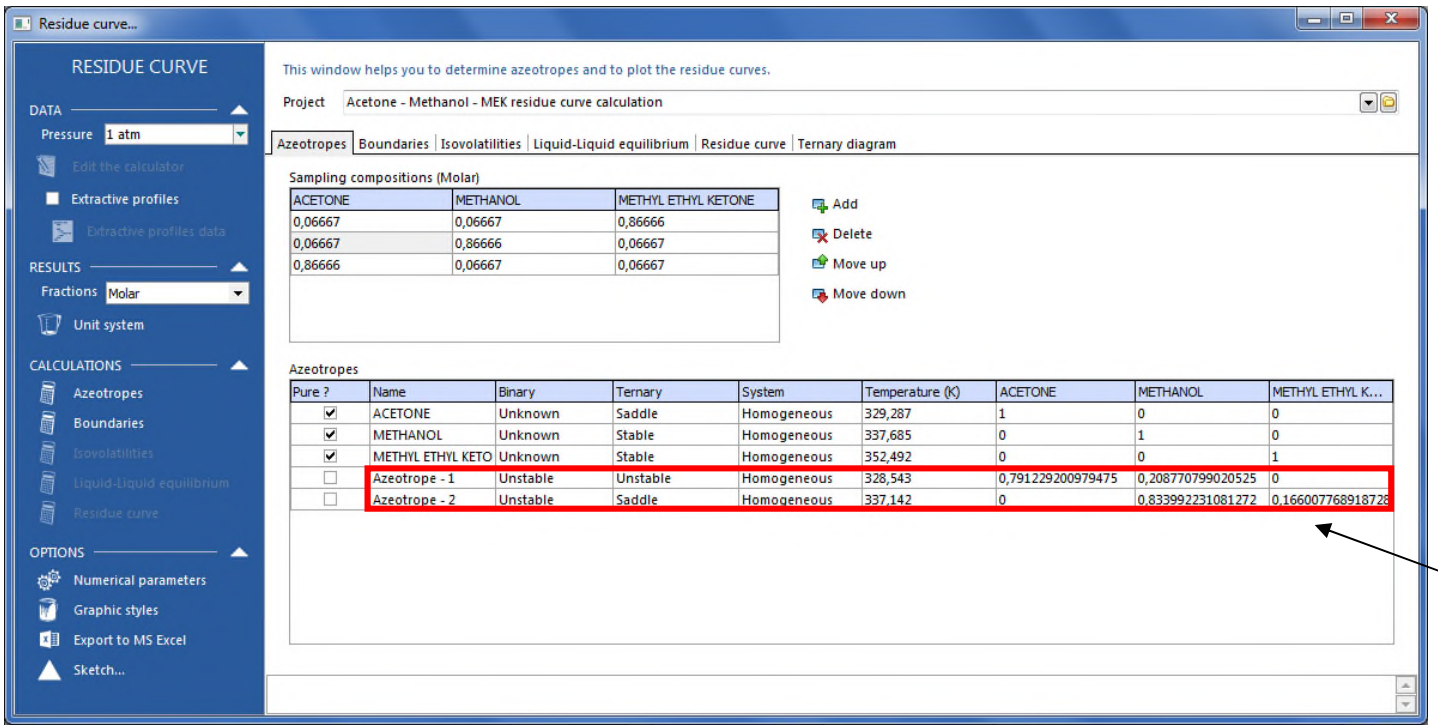
Click on "*Azeotropes*" to identify the possible azeotropes in the mixture.



Sampling compositions are automatically initialized, therefore it is not mandatory to provide values.

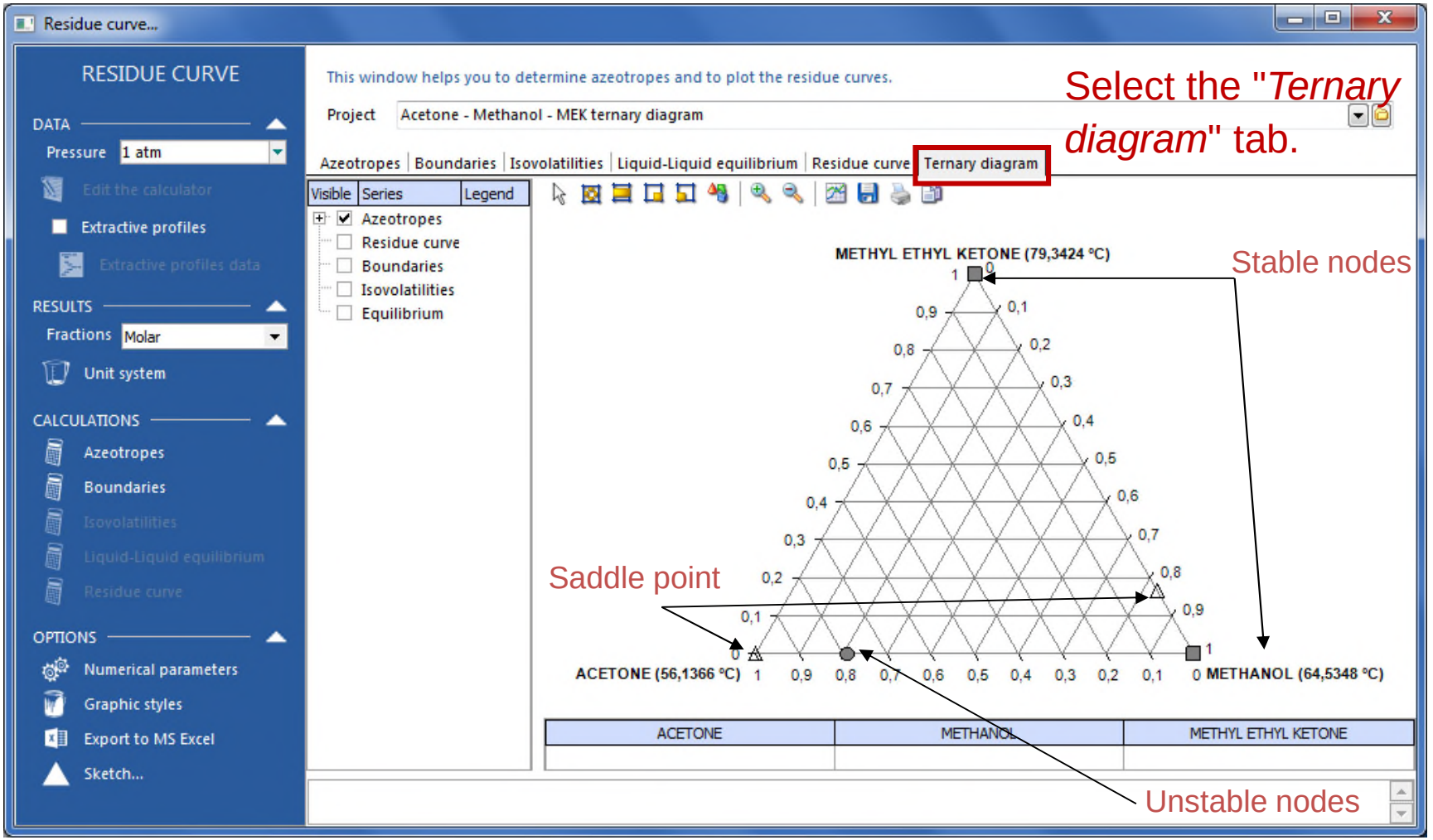
Step 2: Plot the ternary diagram

The following table appears and displays boiling points of pure components as well as binary and ternary azeotropes.



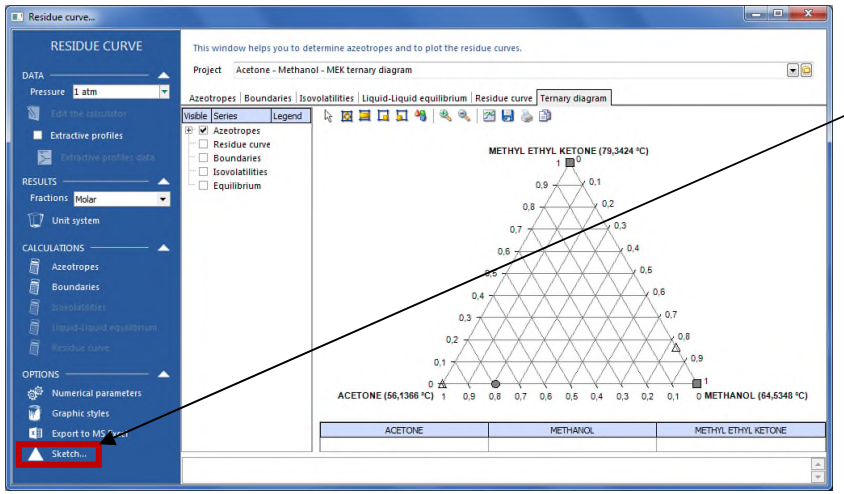
This system presents two homogeneous azeotropes (acetone-methanol and methanol-MEK) and no ternary azeotrope.

Step 2: Plot the ternary diagram

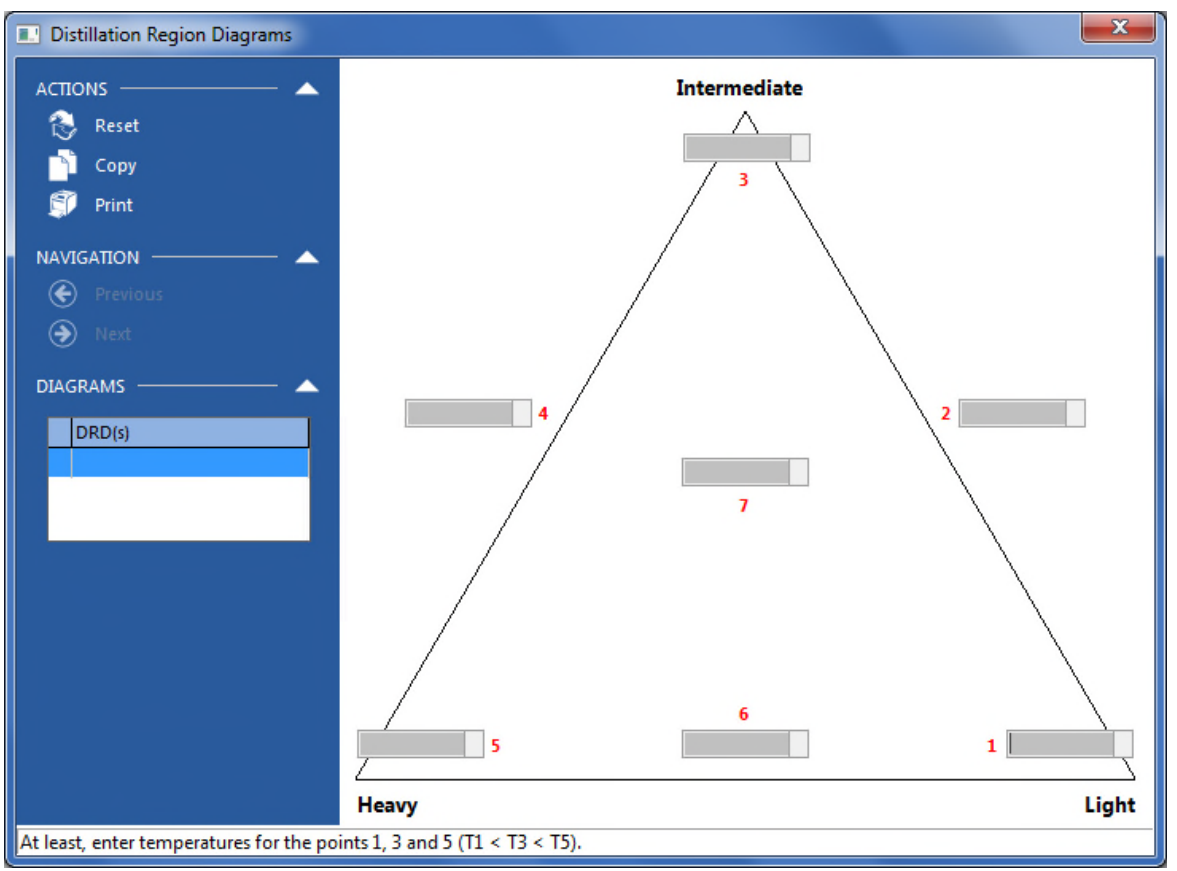


- Stable nodes are represented by a square (MEK and methanol).
- Unstable nodes are represented by a circle (acetone-methanol azeotrope).
- Saddle points are represented by a triangle (MEK-methanol azeotrope and acetone).

Step 2: Plot the ternary diagram



Click on "*Sketch…*".



This graph gives a simplified representation of the ternary diagram.

In each relevant cells, enter the temperatures calculated in the previous table. In this example there is no ternary azeotrope (cell #7) and no binary azeotrope between heavy and light (cell #6). All other cells can be filled.

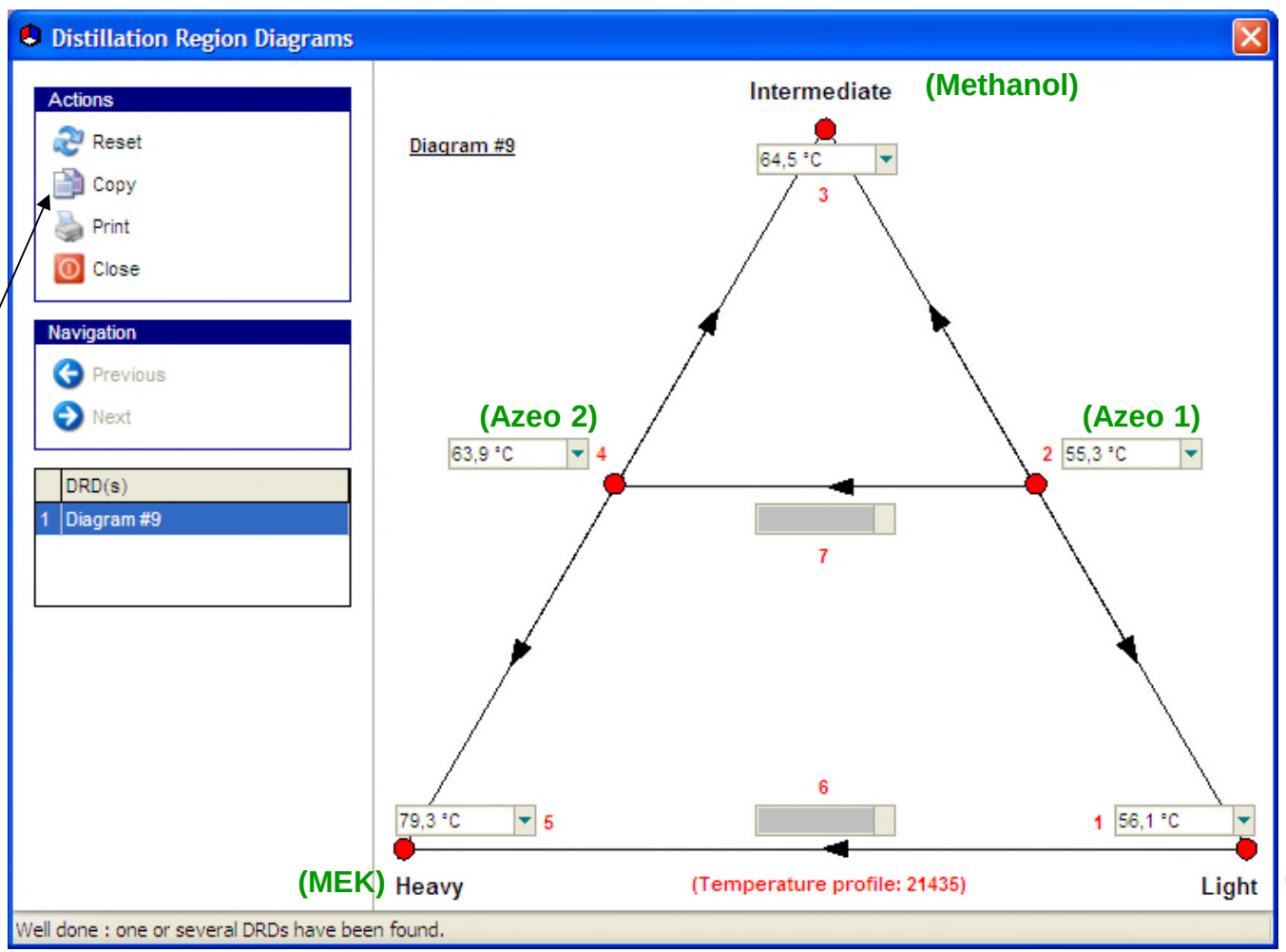
Step 2: Plot the ternary diagram

Azeotropes

Pure ?	Name	Binary	Ternary	System	Temperature (°C)	ACETONE	METHANOL	METHYL ETHYL K...
☑	ACETONE	Unknown	Saddle	Homogeneous	56,1366	1	0	0
☑	METHANOL	Unknown	Stable	Homogeneous	64,5348	0	1	0
☑	METHYL ETHYL KETC	Unknown	Stable	Homogeneous	79,3424	0	0	1
☐	Azeotrope - 1	Unstable	Unstable	Homogeneous	55,3933	0,791229200979474	0,208770799020526	0
☐	Azeotrope - 2	Unstable	Saddle	Homogeneous	63,9921	0	0,833992231081272	0,166007768918728

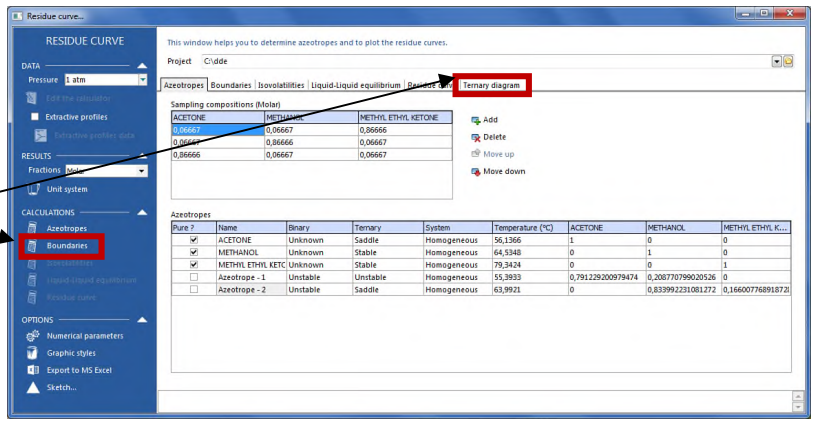
As soon as temperatures are provided, arrows appear between the binaries. It shows the direction of residue composition when increasing the temperature.

You can copy this graph into other applications.



Step 2: Plot the ternary diagram

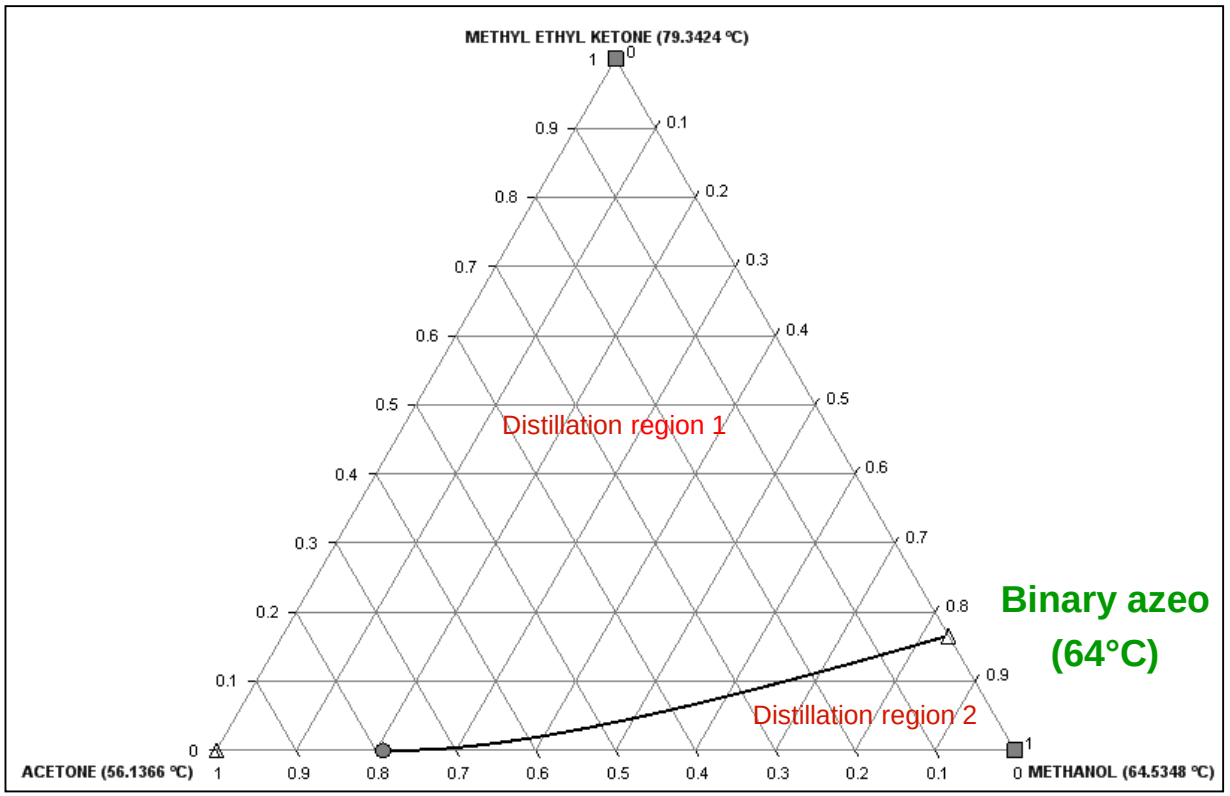
Close the sketch window to go back to the main interface.
Click on "*Boundaries*“ and then on the "*Ternary diagram*" tab.



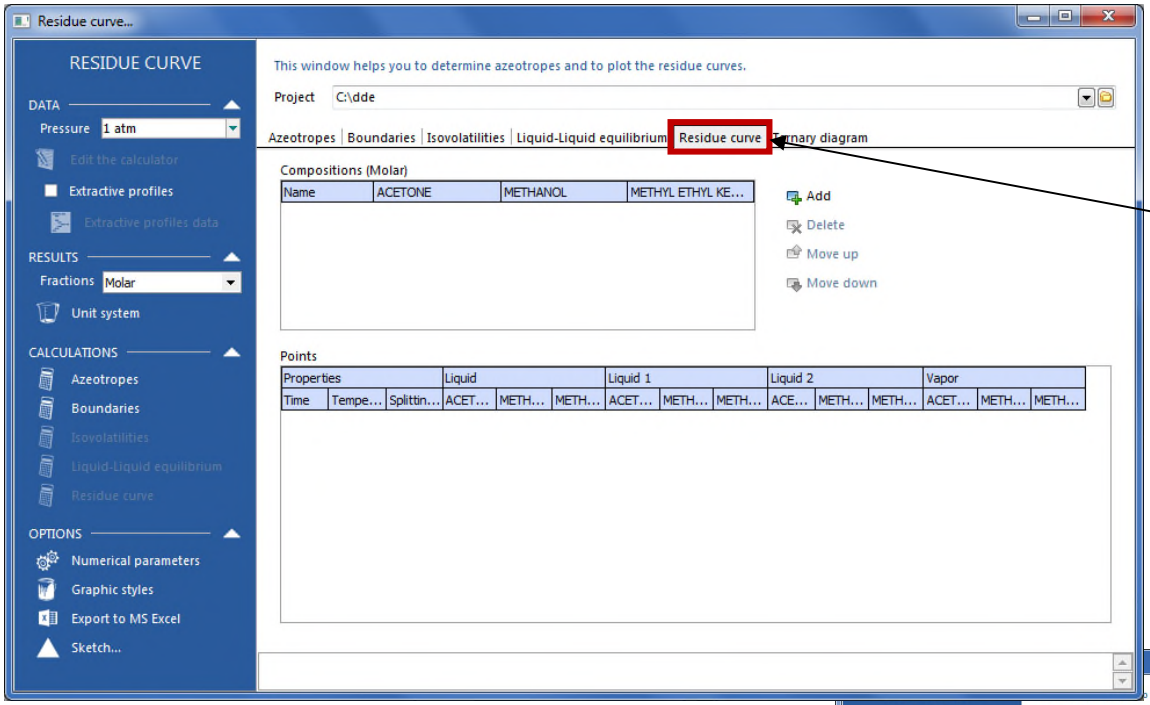
This diagram shows the distillation dividing curve which is called *distillation boundary*.

A *distillation boundary* corresponds to a frontier that can not be crossed by distillation.

The presence, location and structure of the distillation boundaries are crucial to evaluate the distillation feasibility. For each distillation column, the distillate and the bottom products must be in the same distillation region.



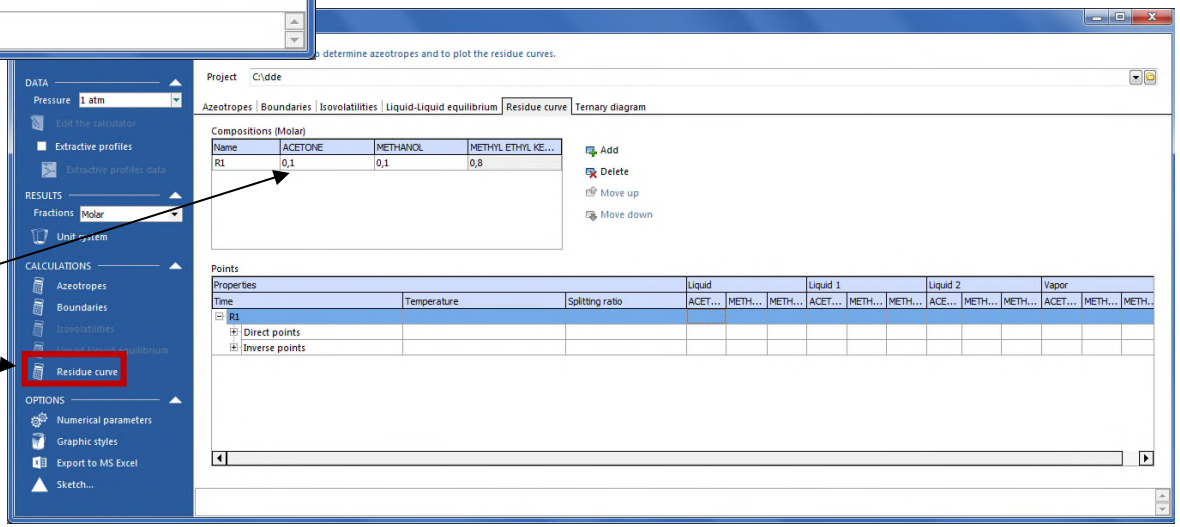
Step 3: Plot the residue curves



Click on the "*Residue curve*" tab.

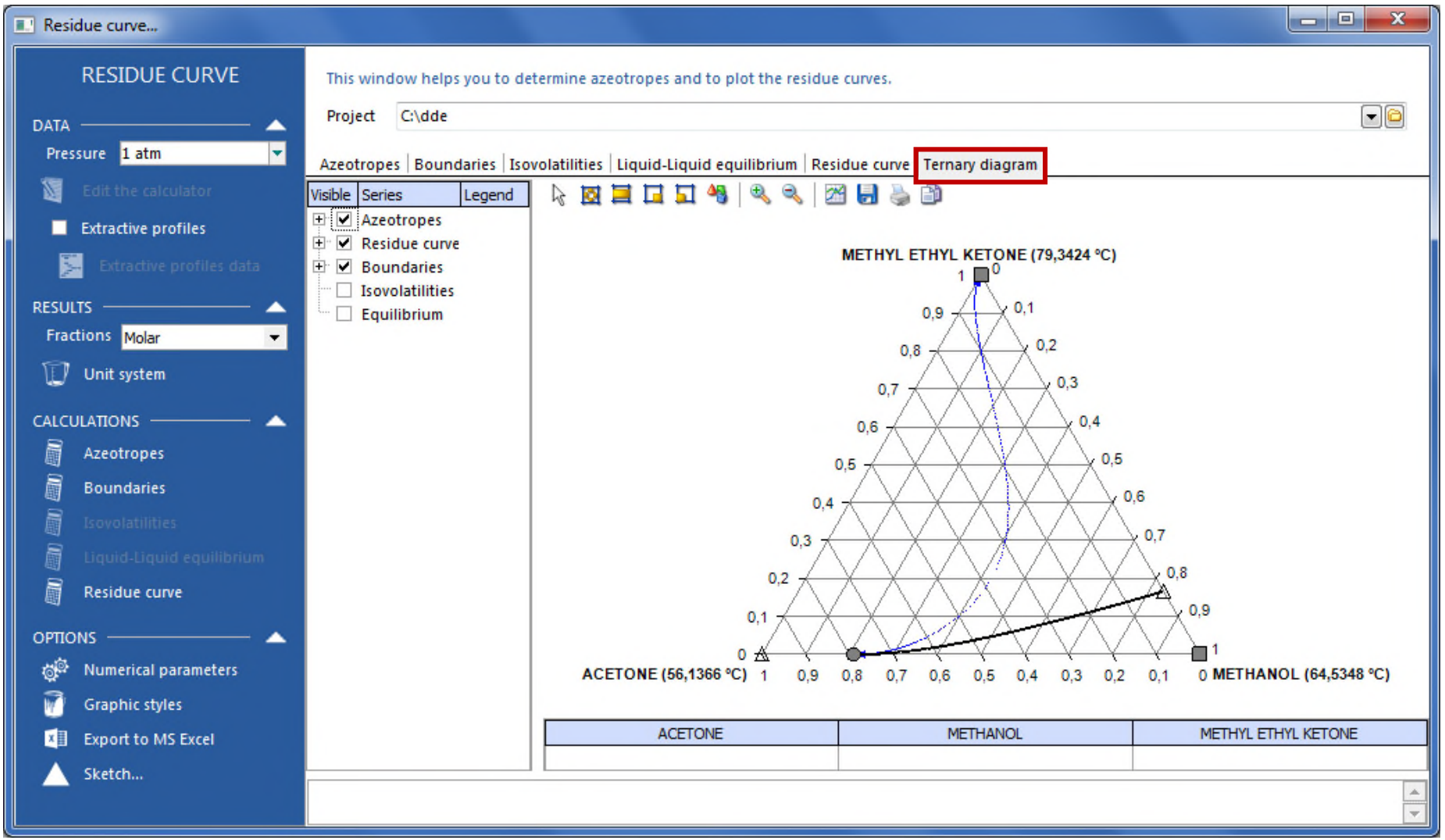
Create a table with one line in which you will enter a mixture composition.

Click on "*Residue curve*" to run the calculation.



Step 3: Plot the residue curves

Click on the "*Ternary diagram*" tab to view the graph.



Step 3: Plot the residue curves

Compositions (Molar)

Name	ACETONE	METHANOL	METHYL ETHYL KE...
R1	0,1	0,1	0,8
R2	0,1	0,8	0,1
R3	0,8	0,1	0,1
R4	0,2	0,2	0,6
R5	0,2	0,6	0,2
R6	0,6	0,2	0,2

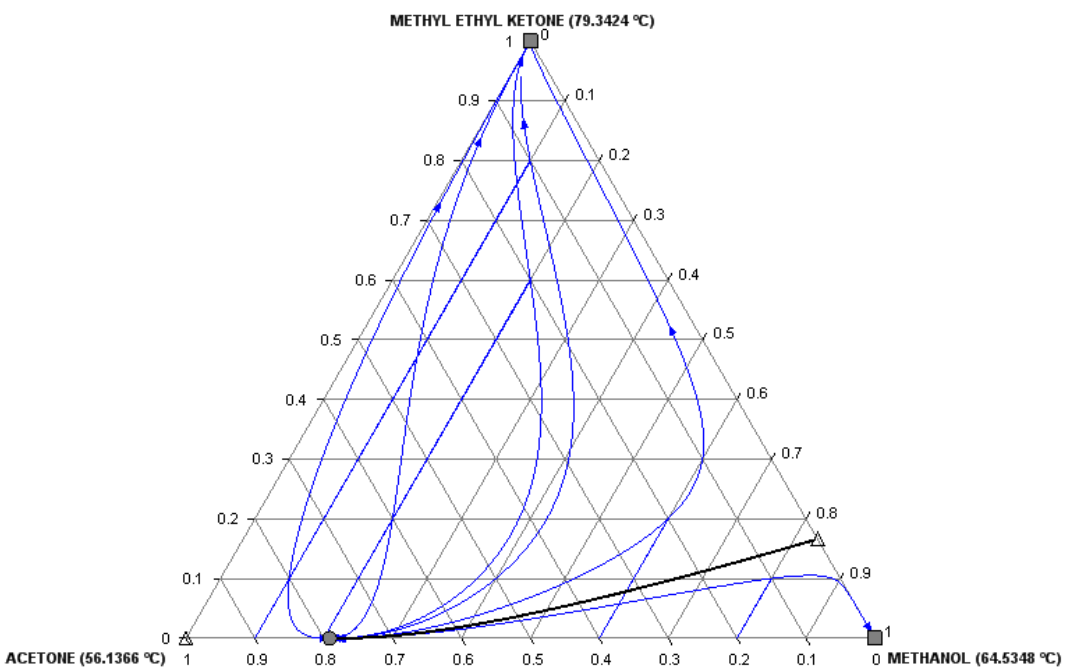
Add
Delete
Move up
Move down

You can add more composition samples in order to have additional residue curves and a more comprehensive analysis of the system.

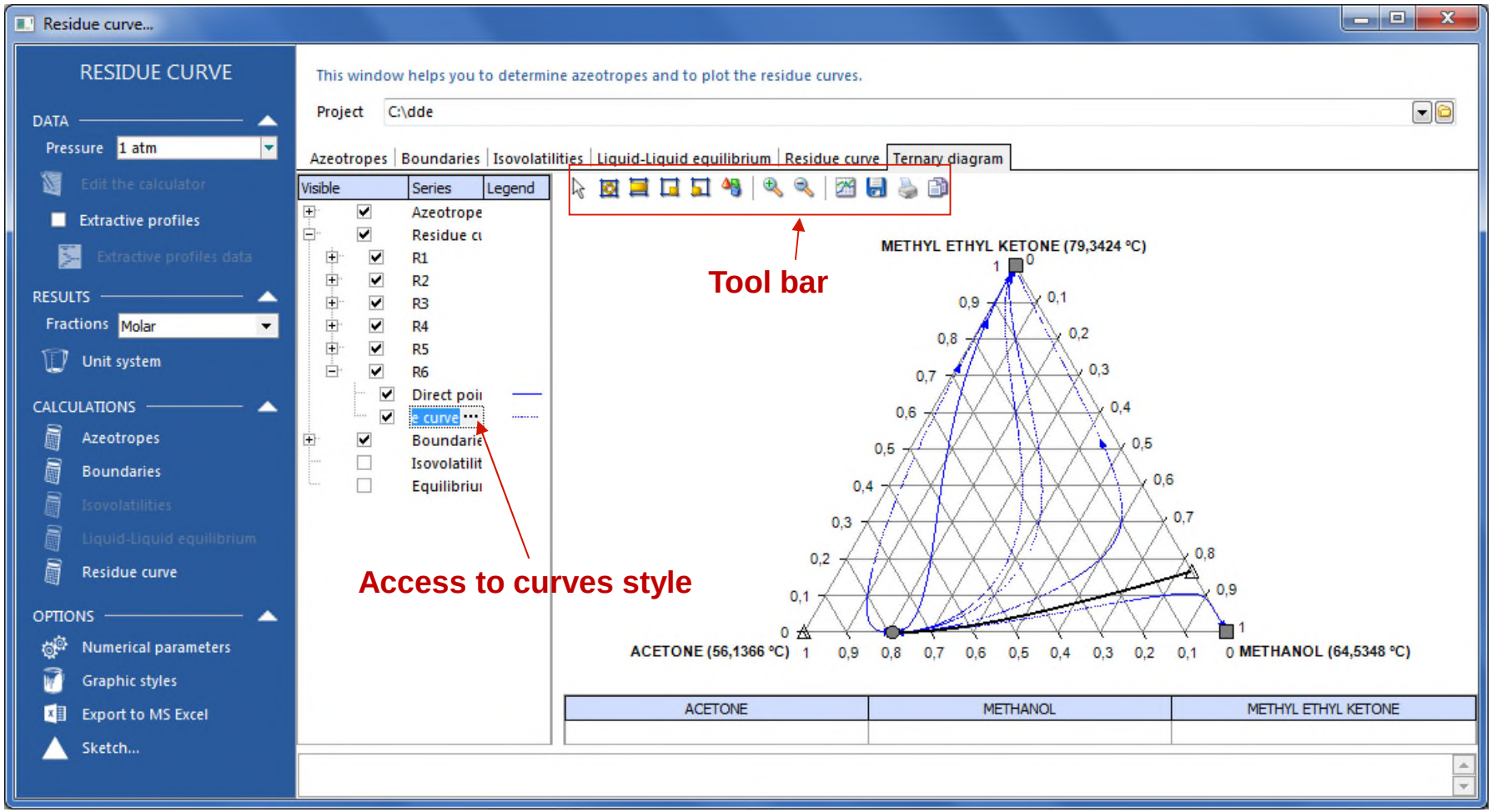
Here, we enter 6 different compositions corresponding to 6 different residue curves R1 to R6.

The direction of the residue curves goes from the lightest boiling point (acetone-methanol azeotrope) toward MEK or methanol, depending on the initial composition.

The location of the feed point determines the distillation region of the potential distillate and product.



Step 3: Plot the residue curves



You can switch the diagram summits, and modify the graphical properties of the diagram and the curves. You can also copy the diagram into other documents or save it as a picture.

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