

Creation of background screen files for ThermoOptim external mixtures charts

As explained in Volume 3 of the ThermoOptim reference manual, the external classes allow one to define external substances, in particular external mixtures whose calculation is performed by thermodynamic properties servers.

External mixtures not being included in ThermoOptim, the software does not provide their thermodynamic charts. To overcome this limitation, we added to version 2.5 a new chart type, called external mixture chart, which allows the use of simplified entropy and (h,P) charts. This feature is not available in version 1.5.

Using mixture charts

The new charts are simplified compared to the others in that they show only the bubble and dew curves, as well as a single set of isovalues, i.e. the isobars for the entropy chart, and the isotherms for the (h, P) chart.

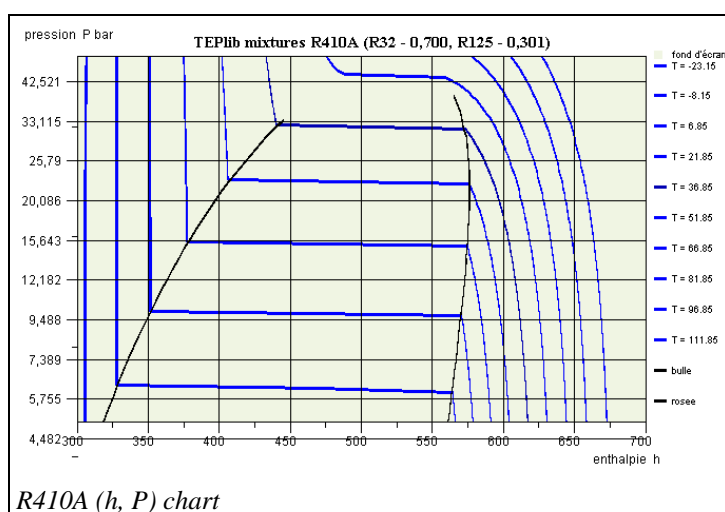
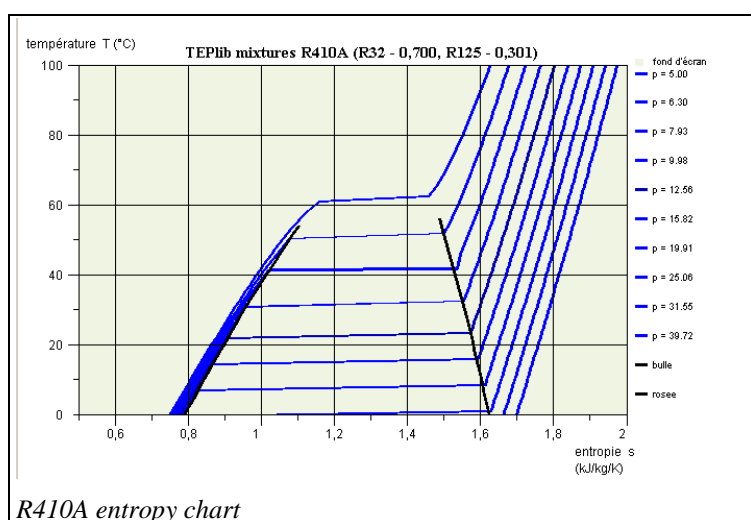
As shown in the entropy chart, the isobars are no longer horizontal segments in the liquid-vapor equilibrium zone, but curves slightly upward.

In the (h, P) chart, the isotherms are no longer horizontal segments in the liquid-vapor equilibrium zone, but curves slightly downward.

Note that the characteristics of the model are recalled in these charts: server properties TEPlib mixtures, name of substance R410A, and molar composition.

For mixture charts to be available, a number of files must be prepared, as described in the documentation of the external CreateMixtureCharts.java class. We assume here that it was done.

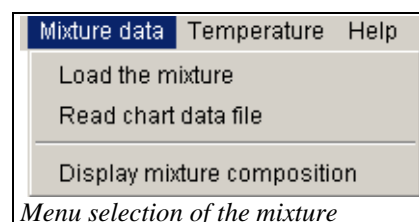
Charts are also loaded from the simulator / interactive chart interface, in which has been added an additional line called "external mixtures", which must be selected.



The chart screen is opened, but without a substance being selected.

The menu "Mixture data" allows you to do it. Select the line "Load the mixture". The list of available charts is displayed. Select the one of interest (here R410A).

Then select the line "Read the chart data file", which allows ThermoOptim to read the two files defining the background. The charts of the previous figures are then available, the behavior of the external mixture chart being similar to that of an internal ThermoOptim vapor chart.



Use of mixture charts

The preparation of chart background screens uses a special external class called CreateMixtureCharts.java that we present here, after explaining how the charts are represented.

Representation of the charts

A chart is represented simply as a set of curves, defined by a number of points and as many pairs (abscissa, ordinate) as there are points. In the example below, the first line is a simple comment, the second one defines the properties of the external mixture (system name, properties server, name of substance, composition and mole fractions). The third line specifies the number of curves (12).

Then there are 12 sets of 4 lines including firstly a label ($p = 5.00$), secondly the number of values per line (99) and two lines with 99 values of on the one hand the entropy and on the other hand the temperature (only 6 values are shown).

mixture data file

```
R410A TEPlib mixtures R410A 2      R32    0.6993 R125   0.3007
```

```
12
```

```
p = 5.00
```

```
99
```

```
0.667254819    0.675894465    0.684531769    0.693168267    0.701805551    0.710445271
```

```
250    251.5    253    254.5    256    257.5
```

```
p = 6.30
```

```
100
```

```
0.662810251    0.671441872    0.680070819    0.688698607    0.697326806    0.705957039
```

```
250    251.5    253    254.5    256    257.5
```

Build the chart background is to generate such a file. This is what the class CreateMixtureCharts.java does.

Use of the class CreateMixtureCharts

The interface of the class is shown in the figure below. This is an external driver, of type "mixture chart creator."

You must first open a project in Thermoptim using the external substance for which you wish to draw the chart, and then load the driver.

The button "Initialize" displays, in the dropdown menu which shows here R410A, the list of substances found in the project loaded.

Select the substance you want. Its name is copied in the "Chart name" field, which can be edited. It plays a fundamental role, because it is used to identify the four files that define charts and their settings. Their names are in fact obtained by concatenating the name (chartName) with other strings:

Mixture chart creation interface

initialize

R410A Chart name R410A

Tmin 150 Tmax 435

Pmin 0.1 Pmax 50

number of points 100

Calculate (T,s) chart Save (T,s) chart

Calculate (h,P) chart Save (h,P) chart

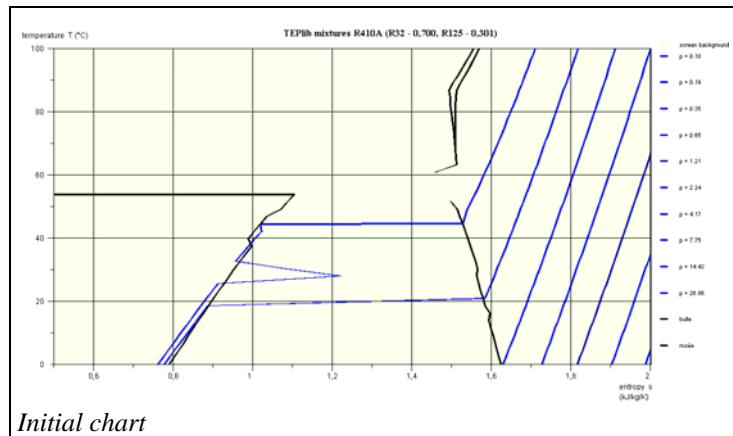
Class interface

chartNameTs.txt is the background screen of the entropy chart, chartNameHp.txt the background screen of the (h,P) chart and paramchartNameTs.txt and paramchartNameHp.txt the files defining the charts settings for the axes and colors.

Then select the upper and lower temperatures and pressures and the number of points (100 by default), then click "Calculate (T, s) chart" to calculate the entropy chart and "Calculate (h, P) chart" to calculate the (h, P) chart.

Once the calculation is complete, you can save the values generated by clicking the buttons "Save (T, s) chart" and "Save (h, P) chart".

The problem is that usually miscalculations occur, so that the resulting files must be reworked by hand.



This task a bit tedious can be performed with the help of a spreadsheet like Excel, where you can easily view different sets of isovalues, to identify errors and remove them. It is then necessary to amend the number of points that appears in the file.

Once the chart refined, the four files that define the charts and their settings must be placed in the directory "data" and the name chartName added in a new line in the file "extMixtCharts.ini" which lists the charts available.

Presentation of the class CreateMixtureCharts

Class CreateMixtureCharts. Java contains methods for performing calculations and backups outlined in the previous section. The code is very simple to understand and directly translates these features.

External mixture is instantiated by the method setupExtMixture() as selectedSubstance. The method lect_data_mel() provides access to its characteristics available in the file mel_ext.txt.

The calculated values are stored in tables tS_Values and hP_Values, and labeled in tS_ref and hP_ref then saved in background screen files whose names are generated as explained above