



Introduction to the VP Tool software

The VP Tool software will estimate the vapour pressure (VP) at 20 °C of a hydrocarbon solvent, based on readily available physical data: the distillation profile (obtained by ASTM D86) and the aromatics content (e.g. by using ASTM D1319). Aromatic contents below 1 vol % have no effect on the VP calculation result and can thus be omitted.

Two software versions are available:

- VP Pressure Tool with installer for users who have full administrative rights on their computers and can install software.
- VP Pressure Tool without installer for users who do not have full administrative rights on their computer.

To install the programme, you can click on one of the links on the website and save it to a directory of your choice. Once the file has downloaded, double click on it and "unzip" the file. Once the file is unzipped, double click on the button *setup.exe* or *VPTool.exe* and follow the on-screen instructions, using the password "esig" when prompted.

Example of a '.dis file'

A sample distillation data file, in a format that can be read by the VP Tool is shown below:

Example*:

Product x

Sample notes...

18.1

%	°C
0	216.0
5	220.0
10	221.0
20	223.0
30	226.0
40	227.0
50	229.0
60	231.0
70	234.0
80	237.0
90	241.0
95	244.0
100	258.0

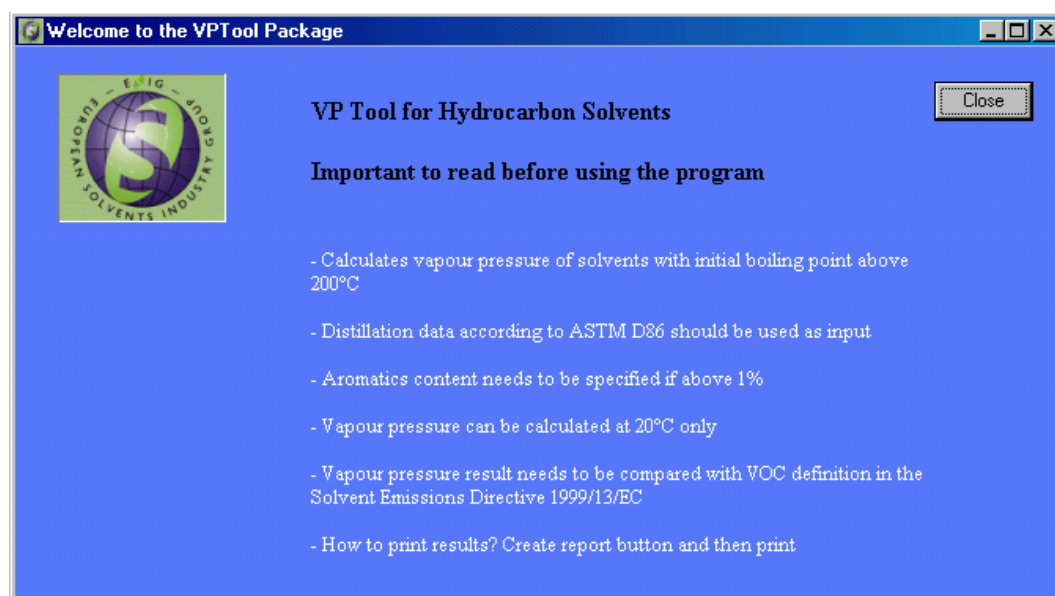
* First line: sample name.

Second line: Description/sample notes.

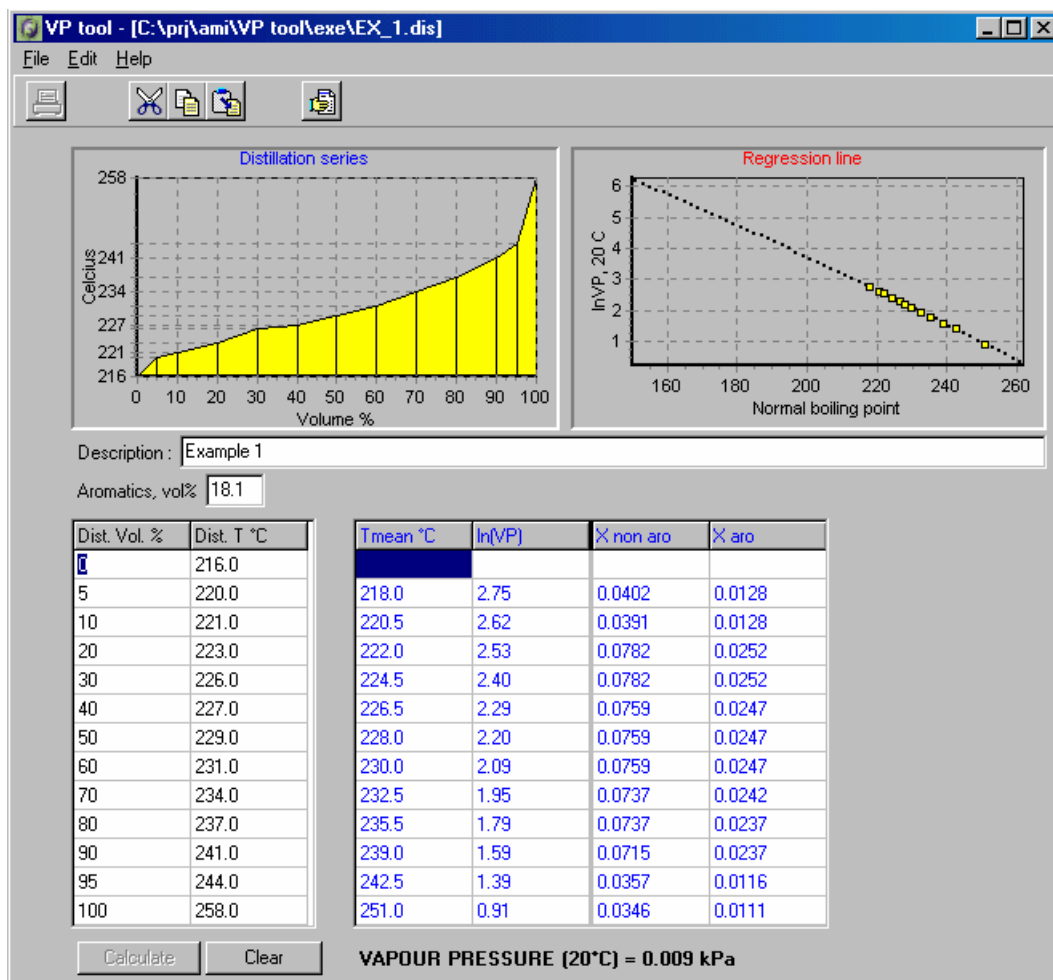
Third line: Aromatic content.

Data file format

The distillation series entered into VP Tool are stored as ascii files. Consequently, they can be edited in any text editor, for example Notepad. They can be identified by their file extension, .dis. Reports of calculated vapour pressures can be saved as ascii files, and they can be copied into Word or Excel, for example.



Splash screen of the VP Tool Program



Main screen of the VP Tool program.

The following is a summary of the calculations in VP Tool

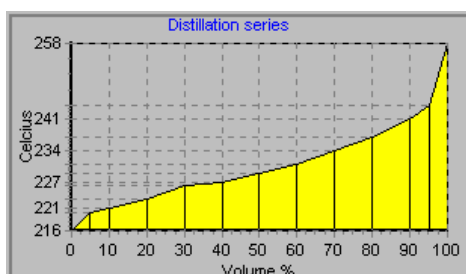
Input of a distillation series data set

Aromatics, vol% <input type="text" value="18.1"/>	Fraction of aromatics The aromatic fraction in vol% (estimated) of the whole sample is entered. Possible range: 0-100%. The aromatics % will have an effect on the estimated mole fractions of both the aromatics and the nonaromatics, because these are expected to have different molar densities (mol/volume) in the density/normal boiling point plot used.																						
<table border="1"> <thead> <tr> <th>Dist. Vol. %</th> <th>Dist. T °C</th> </tr> </thead> <tbody> <tr><td>0</td><td>216.0</td></tr> <tr><td>5</td><td>220.0</td></tr> <tr><td>10</td><td>221.0</td></tr> <tr><td>20</td><td>223.0</td></tr> <tr><td>30</td><td>226.0</td></tr> </tbody> </table>	Dist. Vol. %	Dist. T °C	0	216.0	5	220.0	10	221.0	20	223.0	30	226.0	Fraction size (vol%) and temperature The Dist. Vol% and temperatures in degrees Celsius of the distillation test results are entered into the grid. Temperatures should be entered with an accuracy of 0.1°C. The fractions must cover the entire distillation range, from the initial (0% = IBP) to the final (100% = FBP/DP) fraction of the sample*. The number of fractions in the grid has been fixed at thirteen: 0, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 95, and 100. The temperatures must never decrease.										
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* For the purpose of the calculation, the "100" Dist. Vol.% corresponds to the experimental Final Boiling Point or Dry Point.

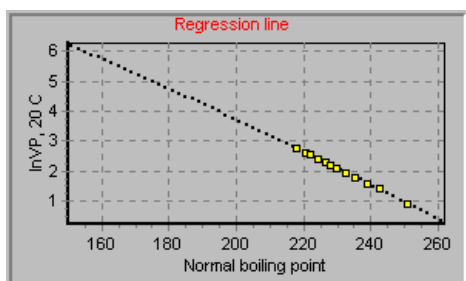
Calculation results

Click the **Calculate** button to recalculate whenever you modify any of the distillation series data.



Distillation curve

A graphical presentation of the distillation curve (boiling point distribution of the sample) is shown.



Plot of lnVP(20°C) / NBP

The lnVP(20°C) / NBP plot is used to estimate the vapour pressure for each of the fractions of the distillation curve: For each Tmean, there is a corresponding vapour pressure for the given fraction.

NBP = Normal Boiling Point

X non aro	X aro
0.0402	0.0129
0.0391	0.0129
0.0781	0.0252
0.0781	0.0252

X non aro, X aro (mole fractions)

Using regression plots of density / NBP, volume fractions are converted to mole fractions for both the aromatics and the nonaromatics of each distillation fraction.

VAPOUR PRESSURE (20°C) = 0.009 kPa

VP result

The final result is presented as a single number. The unit used is kPa.