Vapour Pressure Tool
User Guide

Introduction to the VP Tool software

The VP Tool software will estimate the vapor pressure at 20 °C of a hydrocarbon mixture, based on the data from a distillation series.

Example of a dis file

A sample distillation data file, in a format suitable for reading by the VP Tool is showed below:

Example 1
Some sample notes…
18.13

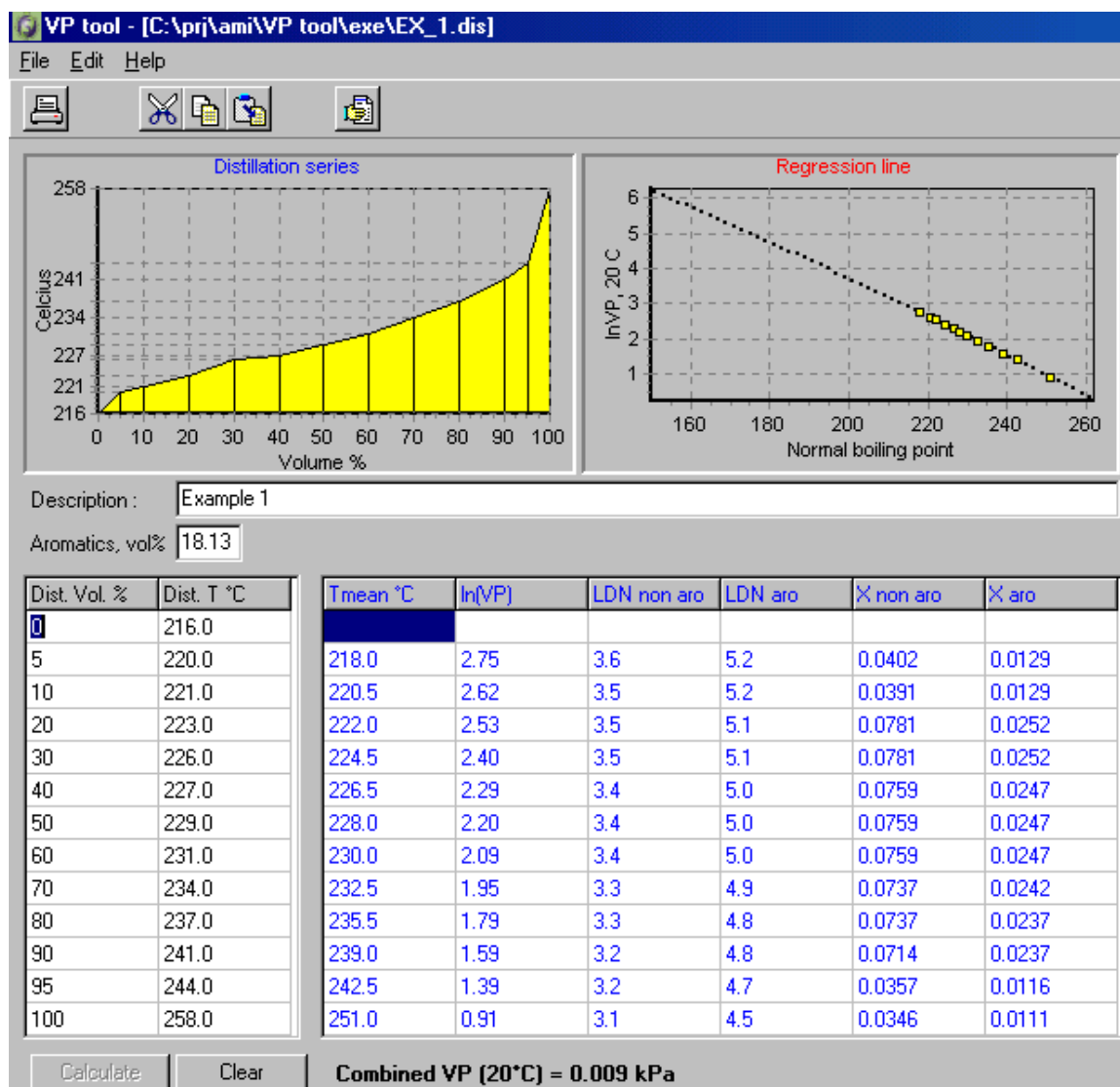| %	°C
0	216.0
5	220.0
10	221.0
20	223.0
30	226.0
40	227.0
50	229.0
60	231.0
70	234.0
80	237.0
90	241.0
95	244.0
100	258.0

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 filextension, dis. Reports of calculated vapour pressures can be save in ascii file, and they can be copied into for instance Word or Excel.

VP tool - [C:\prj\ami\VP tool\exe\EX_1.dis]

File Edit Help

Distillation series

Regression line

Description : Example 1

Aromatics, vol% 18.13

Dist. Vol. %	Dist. T °C	Tmean °C	ln(VP)	LDN non aro	LDN aro	X non aro	X aro
0	216.0						
5	220.0	218.0	2.75	3.6	5.2	0.0402	0.0129
10	221.0	220.5	2.62	3.5	5.2	0.0391	0.0129
20	223.0	222.0	2.53	3.5	5.1	0.0781	0.0252
30	226.0	224.5	2.40	3.5	5.1	0.0781	0.0252
40	227.0	226.5	2.29	3.4	5.0	0.0759	0.0247
50	229.0	228.0	2.20	3.4	5.0	0.0759	0.0247
60	231.0	230.0	2.09	3.4	5.0	0.0759	0.0247
70	234.0	232.5	1.95	3.3	4.9	0.0737	0.0242
80	237.0	235.5	1.79	3.3	4.8	0.0737	0.0237
90	241.0	239.0	1.59	3.2	4.8	0.0714	0.0237
95	244.0	242.5	1.39	3.2	4.7	0.0357	0.0116
100	258.0	251.0	0.91	3.1	4.5	0.0346	0.0111

Calculate   Clear   **Combined VP (20°C) = 0.009 kPa**

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% [18.13]	**Fraction of aromatics** The aromatic fraction in vol% (estimated) of the whole sample is entered. Possible range: 0-100%. Aromatics% will have an effect on the estimated mole fractions of both aromatics and not aromatics, because aromatics and non-aromatics are expected to have a different density (mol/volume) in the density/normal boiling point plot used.
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 Vol% and temperatures in Celcius of the distillation series are entered into the grid. The fractions must cover all the way from the initial (0%) to the final (100%) fraction of the sample. The number of fractions, (13) in the grid is fixed. The volume fractions should always be: 0, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 95, and 100 according to the standard. The temperatures must never decrease.
Dist. Vol. % / Dist. T °C / Tmean °C 0 / 216.0 / 5 / 220.0 / 218.0 10 / 221.0 / 220.5 20 / 223.0 / 222.0 30 / 226.0 / 224.5 40 / 227.0 / 226.5	**Tmean** The mean temperature of each distillation fraction is calculated automatically (TMean column)

Calculation results

Click the **Calculate** button to recalculate whenever you modify any of the distillation series data.
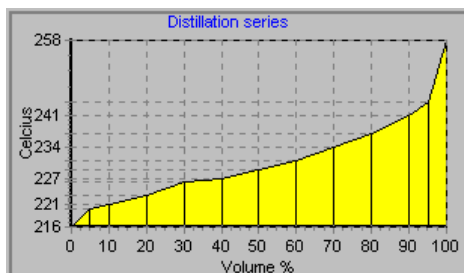
A graphical presentation of the distillation series is created
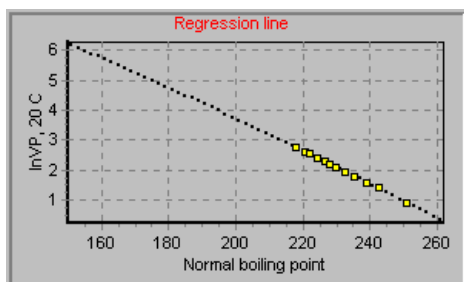
Plot of lnVP(20C) / NBP
This relation is used to estimate the vapour pressure of all fractions of the distillation series. Using the lnVP(20C) / NBP plot, the lnVP(20C) is calculated for each distillation fraction.

LDN non.aro	LDN aro
5.1	7.5
4.9	7.2
4.7	6.9

Liquid density
LDN columns showing liquid density of all fractions. Based on plots of density versus 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 aromatics and nonaromatics of each distillation fraction.

Combined VP (20°C) = 0.009 kPa

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