System - Cumene

Critical Temperature - 631K
Critical Pressure - 32.09 bar
Acentric factor (w) - 0.3274
Source - Perry's Chemical Engineers Handbook.

Equation of State - Peng Robinson

$$P = \frac{RT}{V_m - b} - \frac{a\alpha}{V_m^2 + 2bV_m - b^2}$$

$$a = \frac{0.45724 R^2 T_c^2}{P_c}$$

$$b = \frac{0.07780 R T_c}{P_c}$$

$$\alpha = \left(1 + \left(0.37464 + 1.54226\omega - 0.26992\omega^2\right)\left(1 - T_r^{0.5}\right)\right)^2$$

$$T_r = \frac{T}{T_c}$$

Here, Tc is the critical temperature in Kelvin.

V_m is the molar volume.

T_r is the reduced temperature.

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Antoine Coefficients
  log(P) = A-B/(T+C) where P is in mmHg and T is in Celsius
Source of data: Yaws and Yang (Yaws, C.  L.  and Yang, H.  C.
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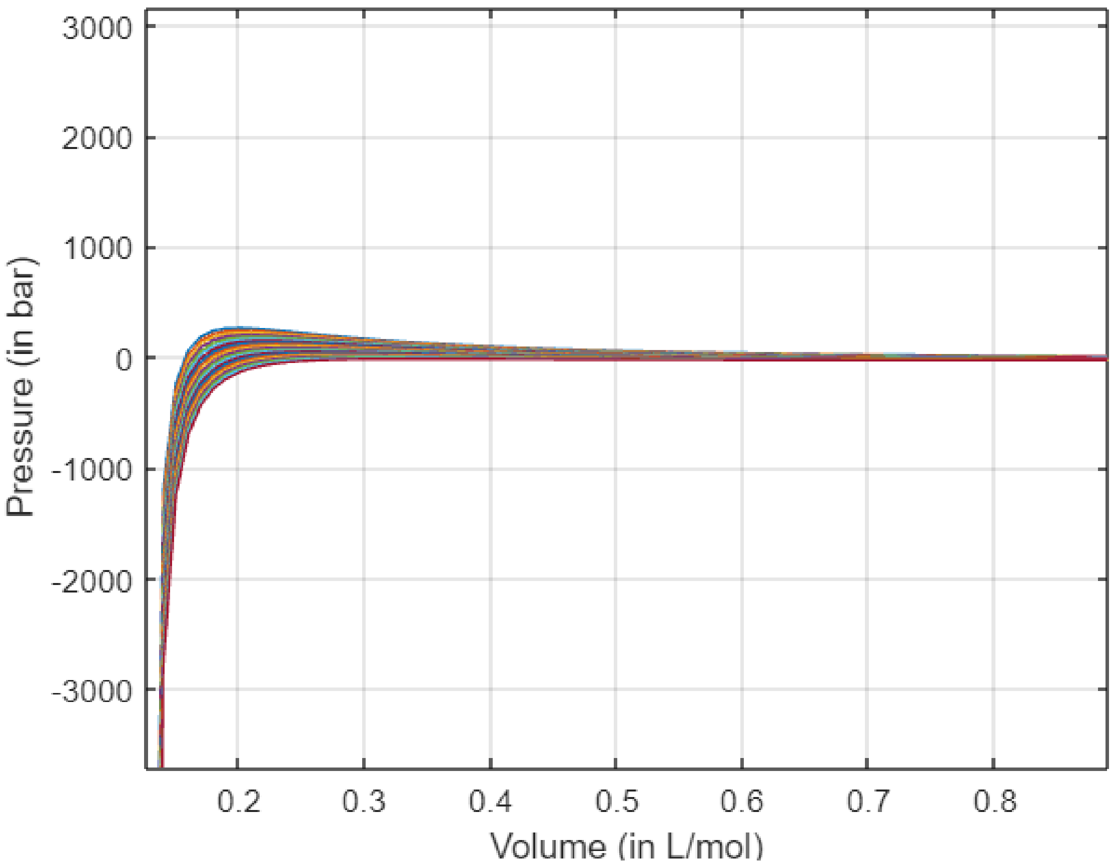
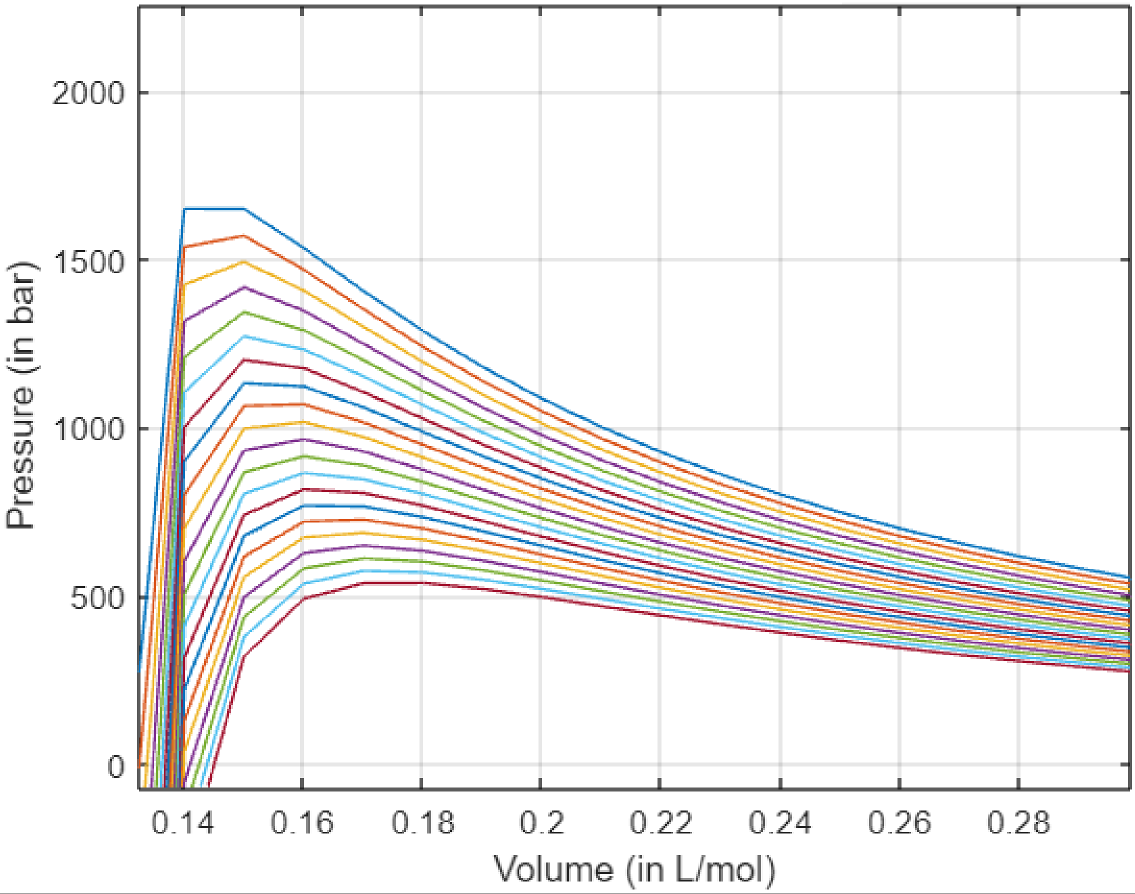
compound name	A	B	C	Tmin	Tmax	??	?
cumene	6.93666	1460.793	207.777	38	181	Y3	0

For 400<T<600



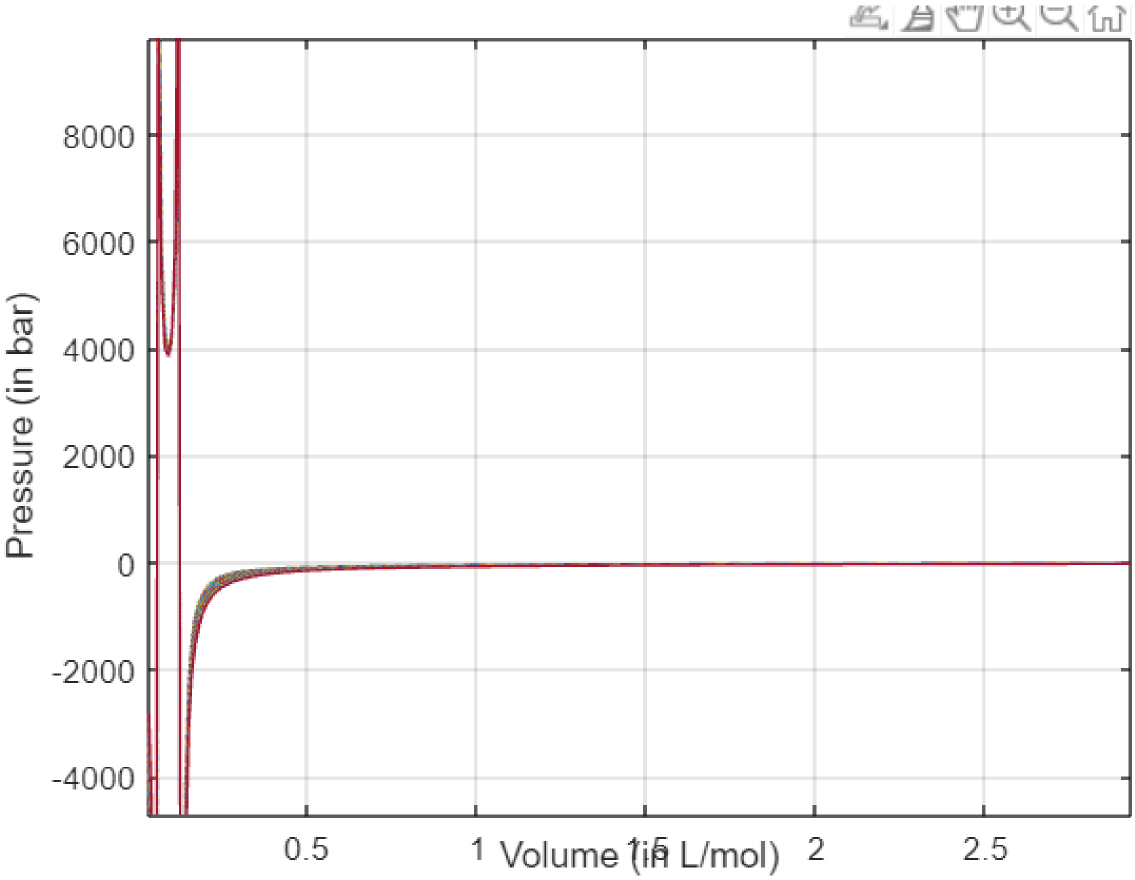
3000
2000
1000
0
-1000
-2000
-3000
Pressure (in bar)
0.2
0.3
0.4
0.5
0.6
0.7
0.8
Volume (in L/mol)

For 100<T<300



2000
1500
1000
500
0
Pressure (in bar)
0.14
0.16
0.18
0.2
0.22
0.24
0.26
0.28
Volume (in L/mol)

For 800<T<1000



Algorithm:-

First estimate saturation pressure using antoine equation.
Then substitute values in Peng Robinson EOS to find minimum and maximum values. Store in an array.

Use eqn 1 to find the roots.

$Pv^3 + (Pb - RT)v^2 + (-3Pb^2 - 2bRT + a\alpha)v + (Pb^3 - a\alpha b + RTb^2) = 0$ ---- Eqn 1

Using $\mu g - \mu l = 0$, we get

$log(vmin/(vmin - b)) - a\alpha/(bRT * (\sigma - \varepsilon))log((b\sigma + vmin)/(b\varepsilon + vmin)) + log(1/vmin) + Pvmin/R$

-[

$log(vmax/(vmax - b)) - a\alpha/(bRT * (\sigma - \varepsilon))log((b\sigma + vmax)/(b\varepsilon + vmax)) + log(1/vmax) + Pvmax$

] = 0

------- Eqn 2

Substituting vmin,vmax in Eqn 1 and solving simultaneously with eqn 2 using fsolve, gives 3 values corresponding to saturation pressure, maximum volume and minimum volume

Using spline to fit the curve.