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AIM - The first objective is to estimate the parameters of Antoine equation using regression. While several functional forms are proposed to predict vapor pressure (p vap) as a function of temperature, the Antoine equation is often preferred. The form of the equation is:

$$\ln(p^{vap}) = A - \frac{B}{T}$$

where A and B are parameters that vary with compounds, and T is temperature. The data of p vap for different temperature is given for CH_3OH and H_2O.

1. Determine A and B for CH_3OH and H_2O using linear regression on the training dataset.

2. Report the training and test dataset's root mean squared error.

3. Make plots for CH_3OH and H_2O to show the predicted ln (p vap) and the actual ln (p vap) as a function of temperature (T).

The second objective is to compute the molar volume of CO_2 and H_2 in mol/m3 at 78 bar and 210 °C using ideal gas, Redlich-Kwong (RK), and Peng-Robinson (PR) equations of state. RK and PR belong to a class of cubic equation of state. The generic form of the equation can be stated as follows:

$$V = \frac{RT}{P} + b - \frac{a(T)}{P}\frac{V-b}{(V+\epsilon b)(V+\sigma b)}$$

METHOD -

1. Load the data for both components given in the Excel sheet using the readmatrix function.

2. Use the fitlm function with the training dataset to estimate A and B for CH3OH and H2O.

3. Using the computed parameters, estimate $p\ vap$ for the testing set and compute the root mean squared error.

The above equation is nonlinear in V and may be solved using the fsolve function. It is often convenient to define the following dimensionless quantities:

$$\beta = \frac{bP}{RT}, q = \frac{a(T)}{bRT}, \Omega = \frac{\beta T_r}{P_r}, \Psi = \frac{q\Omega T_r}{\alpha(T_r,\omega)}, T_r = \frac{T}{T_c}, P_r = \frac{P}{P_c}$$

Table 1. Parameters for equations of state.

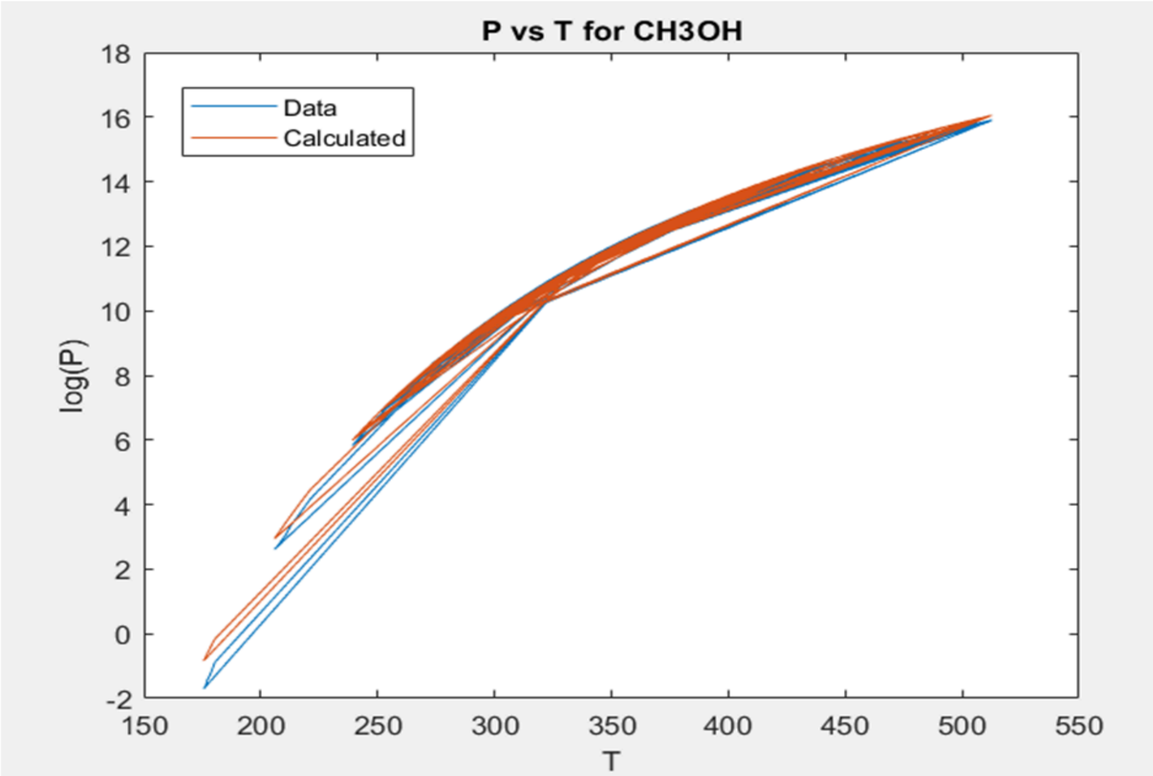
Eq. of state	$\alpha(T_r)$	σ	ϵ	Ω	Ψ
RK	$T_r^{-0.5}$	1	0	0.08664	0.42748
PR	$[1 + (0.37464 + 1.54226\omega - 0.26992\omega^2)(1 - T_r^{0.5})]^2$	$1+\sqrt{2}$	$1-\sqrt{2}$	0.0778	0.45724

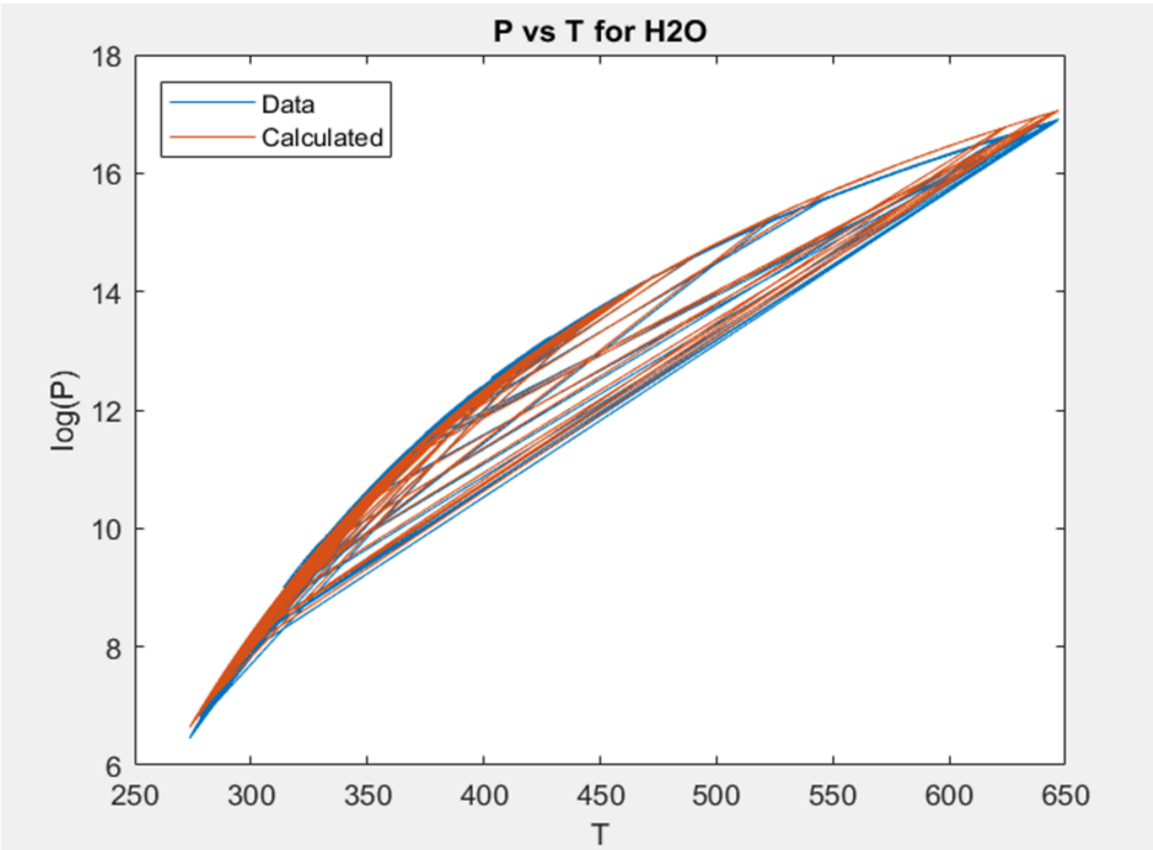
Table 2. Parameters for CO_2 and H_2.

Substance	P_c (bar)	T_c (K)	ω
CO_2	7.38	304.15	0.225
H_2	12.93	33.18	-0.22

RESULT -

- A_CH3OH = 24.850034739689832
- A_H2O = 24.695726929983188
- B_CH3OH = 4.510372064085043e+03
- B_H2O = 4.940460460481752e+03
- rms_test_CH3OH = 0.073576299704207
- rms_train_CH3OH = 0.073996352008509
- rms_test_H20 = 0.075949087194976
- rms_train_H2O = 0.078482677132507
- V_CO2_PR = 5.845814056333681e-04
- V_CO2_RK = 5.881422791853185e-04
- V_H2_PR = 5.128264014540197e-04
- V_H2_RK = 5.184023916415067e-04


P vs T for CH3OH
Data
Calculated
log(P)
T
18
16
14
12
10
8
6
4
2
0
-2
150
200
250
300
350
400
450
500
550


P vs T for H2O
Data
Calculated
log(P)
T
18
16
14
12
10
8
6
250
300
350
400
450
500
550
600
650