

CHEG 231 – Chemical Engineering Thermodynamics I

Section 10

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Thermodynamic Analysis of Dimethylamine

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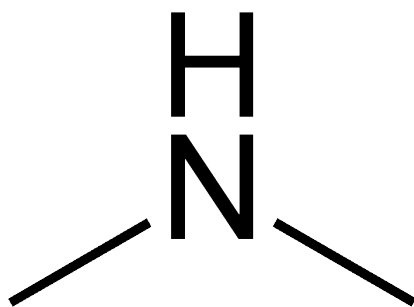


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ABSTRACT

The major aspect of this entire project report is to analyze the thermodynamic properties of dimethylamine compound, which was assigned earlier this semester. There are many different types of equation of states to help describing the behavior of this compound but Peng-Robinson equation of states is used out of the others. The equation is different than the others by its intermolecular forces attraction correction that is temperature dependent, that relates back to its Antoine equation. Although it has its own limit in describing certain types of compound, everyone was assigned to only use that equation. Some thermodynamic properties that were analyzed are the coefficient thermal expansion, constant pressure heat capacity, Joule-Thomson coefficient, compressibility factor, and many more. They were graphed and calculated by using the computer programming MATLAB. Some basic thermodynamic properties can be obtained easily online and are compared with the calculated data. Results of these properties obtained from this MATLAB programming were correctly aligned with their respective theoretical behavior, which makes the analysis right. All the graphs plotted are as attached in the results section and were discussed in detail under the discussion section. In a nutshell, this project report helps to better understand the organic compound behavior from different thermodynamic properties, which can provide the knowledge to the society for their own betterment.

INTRODUCTION

Dimethylamine, C_2H_7N , is an anhydrous compound, which appears to be a colorless gas at low concentrations and ammonia-like at higher concentrations. This fish-like odor, flammable gas is an organic secondary amine, which present abundantly in human urine. Based on the structure of dimethylamine, it consists of 2 $-CH_3$ and one $>NH$ (non-ring) chemical groups. This compound is produced commercially by the exothermic reaction of methanol and ammonia, with the addition of amorphous silica-aluminum catalyst at a temperature within a range of 350 – 450 °C.

This compound has many uses, ranging from agricultural to food industrial uses. It is an important commercial chemical, use greatly by both industries and consumers. Industry wise, it is used as inhibitors for corrosion and acts as anti-scaling agents. Other than that, it is the additives for paint and coating, and as solvents for certain product mixture. Meanwhile, consumers can benefit from the treatment of water and also the plastic and rubber products that can be produced by using this compound. In general, it is used as food additives, in soap manufacturing, growing of crops in agriculture industry, vehicle lubricants, pesticides, and many more. Some manufacturers of this compound include BASF Corporation, The Chemours Company, Eastman Chemical Company, and Allchem Industries Holding Group ^[7].

The concern when handling with this compound is that it is in vapor state in room temperature, and it is a very corrosive gas. It can cause irritation to eyes, nose and throat, also causing a difficulty in breathing when inhaled. It also dissolves readily in water to produce flammable corrosive solutions, which will burn the skin and eyes when come into contact. It has lower (LEL) and upper explosive limit (ULE) of 2.8 % and 14.4 % respectively ^[8].

In a big scale, accidental release of dimethylamine gas to the environment during its production by certain manufacturer can cause massive problems. Prolong exposure to this gas can damage the lungs and lining of the nose. More severe cases are when it also causes drowsiness and damage in the stomach and intestines. Although the release of dimethylamine from manufacturers can be controlled, there are still some aspects of this gas release happened in the environment anyway. This compound is naturally occurring in many foods and some plants. Also, it is volatile from the animal waste, rotting fish, and even from the tobacco smoke ^[7]. In rubber industry, the decomposition product of vulcanizing accelerators produced dimethylamine gas.

METHODS

Peng-Robinson equation of state (PR EOS) is as shown in **Table 1**. It provides the values needed in constructing the equation. Antoine equation (AE) is needed as part of the PR EOS. Pressure, temperature and volume vary depending on any given condition, altogether with any other pressure, temperature and/or volume-dependence thermodynamic data. As part of the analysis, **molar volume is specifically used**, instead of extensive or specific volume.

Antoine Equation	
$P = 10^5 * 10^{A - \frac{B}{T+C}} \text{ (Pascal)}$	
A	4.29371
B	995.445
C	- 47.869
Range of Temperature (K)	201.38 - 280.01
Peng-Robinson Equation of States	
$P = \frac{RT}{v-b} - \frac{a(T)}{v(v+b) + b(v-b)} \text{ (Pascal)}$	
$\omega = -1 - \log_{10}\left(\frac{P_{ant}(Tr=0.7)}{P_{critical}}\right)$	0.2894
$\kappa = 0.37464 + 1.5422\omega - 0.26992\omega^2$	0.7983
$\alpha(T) = \left(1 + \kappa \left(1 - \sqrt{\frac{T}{T_{critical}}}\right)\right)^2$	
$a(T) = \frac{0.45724R^2 * T_{critical}^2 * \alpha(T)}{P_{critical}}$	
$b = 0.0778 * R * \frac{T_{critical}}{P_{critical}}$	5.296E-5

Table 1: Parameters in Peng-Robinson Equation of States

All of the critical properties of dimethylamine are as listed in **Table 2**. The pressure, temperature and compressibility factor were found online, while the critical volume was calculated by using the PR EOS.

Critical Properties	
Pressure (bar)	53.4
Temperature (K)	437.22
Molar volume (m ³ /mol)	2.19E-04
Compressibility factor	0.260

Table 2: Critical Properties of Dimethylamine

There are a few thermodynamic properties generated and plotted through MATLAB. These properties are calculated by using the formula listed below.

1. $a(T)$, the intermolecular attraction forces correction of PR EOS

The equation of $a(T)$ is as listed in **Table 1**.

2. $\alpha(T)$, coefficient of thermal expansion
 $\alpha(T)$ is plotted at the pressure range of $P_r = [0, 0.5, 1]$ and temperature range of $T_{r,tp} \leq T_r \leq 2.5$ by using **Eq.1**.

$$\alpha(T) = \left(\frac{\delta V}{\delta T}\right) \frac{1}{V} \text{ (Eq. 1)}$$

3. $\kappa_T(T)$, isothermal compressibility
 To find $\kappa_T(T)$, **Eq. 2** is used.

$$\kappa_T(T) = \left(\frac{\delta V}{\delta P}\right) \frac{-1}{V} \text{ (Eq. 2)}$$

4. $C_p - C_v$, change in constant pressure and volume heat capacity
 At the temperature range of $T_{r,tp} \leq T_r \leq 2.5$ and at $P_r = 1.0$, $C_p - C_v$ is obtained by **Eq. 3**.

$$C_p - C_v = \frac{TV\alpha(T)}{\kappa_T(T)}, \text{ where } \alpha(T) = \left(\frac{\delta V}{\delta T}\right) \frac{1}{V} \text{ and (Eq. 3)}$$

5. C_p , constant pressure heat capacity
 C_p is obtained by solving for C_v first, at temperature and pressure range of $T_{r,tp} \leq T_r \leq 2.5$ and $P_r = [0, 0.5, 1]$ respectively. Each C_p is found by using **Eq. 4 and 5**.

$$C_v(V, T) = C_v^*(T) + T \int_{V=\infty, T}^{V, T} \frac{\delta^2 P}{\delta T^2} dV \text{ (Eq. 4)}$$

$$C_p(P, T) = [C_p(P, T) - C_v(V, T)] \text{ (Eq. 3)} + C_v(V, T) \text{ (Eq. 5)}$$

$C_v^*(T)$ is the constant volume heat capacity at lower pressure limit, where it only depends on temperature. $C_v^*(T) = C_p^*(T) - R$, and $C_p^*(T)$ equation with its parameters are tabulated in **Table 3**. On the same plot, C_p estimated by Joback method is also plotted, with its parameters in the same **Table 3**.

Equation of $C_p^*(T)$ experimentally	
$C_p^*(T) = A + BT + CT^2 + DT^3$	
$C_v^*(T) = C_p^*(T) - R$	
A	-1.15E+00
B	2.7679E-01
C	-1.4572E-04
D	2.9921E-08
Equation of $C_p^*(T)$ by Joback Method	
$C_p^*(T) = a + bT + cT^2 + dT^3$	
a	-1.4E-01
b	2.7E-01
c	-1.336E-04
d	2.31E-08

Table 3: Parameters of $C_p^*(T)$ of both experimental and Joback method's data ^{[2] [6]}

6. Z, compressibility factor

A bunch of Z curves are plotted by using the reduced temperature and pressure range of $T_r = [1, 1.1, 1.25, 1.5, 1.75, 2]$ and $0 \leq P_r \leq 8$ respectively, by using **Eq. 6**. On a separate graph, Z is plotted at reduced temperature of 1.00 by using PR EOS, van der Waals equation of states (vdW EOS), with its parameters listed in **Table 4**, and the data obtained from the textbook, Figure 6.6-3, by reading off the values from the chart manually.

$$Z = \frac{PV}{RT} \text{ (Eq. 6)}$$

van der Waals Equation of States	
$P = \frac{RT}{v-b} - \frac{a}{v^2}$	
a	$\frac{27R^2T_{\text{Critical}}^2}{64P_{\text{Critical}}}$
b	$\frac{RT_{\text{Critical}}}{8P_{\text{Critical}}}$

Table 4: van der Waals equation of state's parameters

7. μ_{JT} , Joule-Thomson coefficient
 μ_{JT} is determined by using **Eq. 7**.

$$\mu_{JT} = \left. \frac{\delta T}{\delta P} \right|_H = \frac{-[V - T(\frac{\delta V}{\delta T})]}{C_p} \text{ (Eq. 7)}$$

The equation is further simplified to accommodate with the calculated data in the previous part as shown by **Eq. 8**.

$$\mu_{JT} = \frac{V}{C_p} * (T\alpha(T) - 1) \text{ (Eq. 8)}$$

8. Pressure-Volume (PV) curve of dimethylamine

PV curve is plotted for a reduced temperature range of $T_r = [0.7, 0.8, 0.9, 1.0, 1.25, 1.5]$. The curves are all plotted together with the spinodal and binodal curve.

The spinodal curve are obtained by plotting a set of pressure values against the corresponding molar volume with a temperature range of $0 \leq T \leq T_{\text{critical}}$.

$$\frac{\delta P}{\delta V} = 0, \text{ in order to find the pressure values (Eq. 9)}$$

By using **Eq. 9**, there will be two points that satisfy the equation for each isotherm, within the temperature range. All of these points are plotted to form the spinodal curve.

The binodal curve are then obtained by plotting a set of pressure values against the corresponding molar volume with a temperature range of $0 \leq T \leq T_{\text{critical}}$. Binodal curve consists of data points at which the liquid and vapor coexist at the same temperature and pressure. The Gibb's free energy (G) of liquid and vapor should be equivalent when in equilibrium. The change in G between these two states of matter should be zero (**Eq. 10**). **Eq. 10** can be simplified further into **Eq. 11 and 12**.

$$dG|_T = V dP, \text{ since } T \text{ is constant at each isotherm curve (Eq. 10)}$$

$$\int_{Pa1}^{Pa2} V dP + \int_{Pa2}^{Pa3} V dP + \int_{Pa3}^{Pa1} V dP = 0 \text{ (Eq. 11)}$$

$$\int_{V1}^{V3} [P(T, V) - P_{guess}] dV = 0 \text{ (Eq. 12)}$$

P_{guess} in Eq. 12 is an arbitrary number, in order to plot for the binodal curve. The range of P_{guess} that was used is set to be $-30E+6 \leq P_{guess} \leq P_{critical}$. The V and corresponding P values that can result the integration of Eq. 12 to be 0 are recorded and plotted to form the binodal curve. The integration corresponds to the area under the curve, which implicitly defined Eq. 10 to be equal to 0.

9. Pressure-Temperature (PT) curve of dimethylamine

P-T curve are plotted as shown in the figure. Three different curves are plotted on the same graph, which are the fusion, sublimation and vaporization curves. The sublimation curve is plotted by using the Clausius-Clapeyron (CC) EOS at the sublimation point, by referring to Eq. 13.

$$\log_{10}[P(T)] = A - \frac{B}{T}, \text{ where } B = \Delta H_{sublimation}/R, \text{ and } A = 28.2147 \text{ (constant) (Eq. 13)}$$

The fusion curve is plotted by connecting two known points. The two points are the triple and normal melting points. It is expected to have a straight line with an equation of $P = mT + c$, where m is the slope, and c is the y-intercept. m is $-1.2187E+5$ Pa/K and $c = 2.2055E+7$.

For the vaporization curve, three different curves are plotted by using three different equation of states (CC EOS, vdW EOS, and PR EOS). For CC EOS, Eq. 14 is used.

$$\ln \frac{P1}{P_{triple}} = \frac{1}{R} \left(\frac{1}{T_{triple}} - \frac{1}{T1} \right) * \Delta H_{vaporization} \text{ (Eq. 14)}$$

The data used to plot the vaporization curve of PR EOS are obtained from the binodal curve in the previous section.

RESULTS

By referring to **Table 5**, the corresponding temperature, pressure and molar volume of each three different type of conditions are listed. The molar volume for each data point is obtained by using the PR EOS. For normal melting and triple point, the minimum and maximum volume obtained numerically correspond to the liquid and vapor volume respectively.

Type of data	Temperature (K)	Pressure (bar)	Molar volume (m ³ /mol)	
			Liquid Volume	Vapor Volume
Normal melting point	180.15	1.00E+00	No vapor exists. Liquid volume couldn't be obtained numerically and online	
Triple point	180.97	6.53E-04	5.84E-05	2.30E+01
Critical point	437.22	5.34E+01	No liquid exists	2.19E-04

Table 5: Thermodynamic properties at three different interest points

In **Table 6**, there are three vaporization enthalpies and one of each for fusion and sublimation enthalpies, that could be obtained and calculated. The sublimation enthalpy was calculated by using **Eq. 15**, making sure all enthalpies recorded/calculated are from the same conditions (same P, T and V). The ΔH_{fusion} and $\Delta H_{\text{sublimation}}$ in the table above are recorded/calculated at the triple point, while the $\Delta H_{\text{vaporization}}$ in the exact order tabulated above, are obtained at normal room condition, boiling and triple point respectively.

$$\Delta H_{\text{sublimation}} = \Delta H_{\text{vaporization}} + \Delta H_{\text{fusion}} \text{ (Eq. 15)}$$

Enthalpies			
Type of enthalpy	Enthalpy (kJ/mol)	Pressure (bar)	Temperature (°C)
$\Delta H_{\text{vaporization}}$	25.05	1.00E+00	25.00
	26.40	4.37E-01	6.88
	33.78	6.53E-03	-92.18
ΔH_{fusion}	5.94	6.53E-03	-92.18
$\Delta H_{\text{sublimation}}$	39.72	6.53E-03	-92.18

Table 6: Different type of enthalpy change ^{[3] [5]}

In **Table 7**, the acentric and critical compressibility factor were found from an experimental data and also calculated by using the PR EOS.

Data	Calculated values	Experimental values
Acentric factor, ω	0.2894	0.293
Critical compressibility factor, Z_c	0.3214	0.260

Table 7: Comparison of calculated and experimental data for acentric and critical compressibility factor ^[4]

The following **Figure 1 – 11** are the graph plotted in MATLAB of the thermodynamic properties in interest. **Table 8 – 14** in the **Appendices** tabulate some of the data used to plot **Figure 1 – 7**.

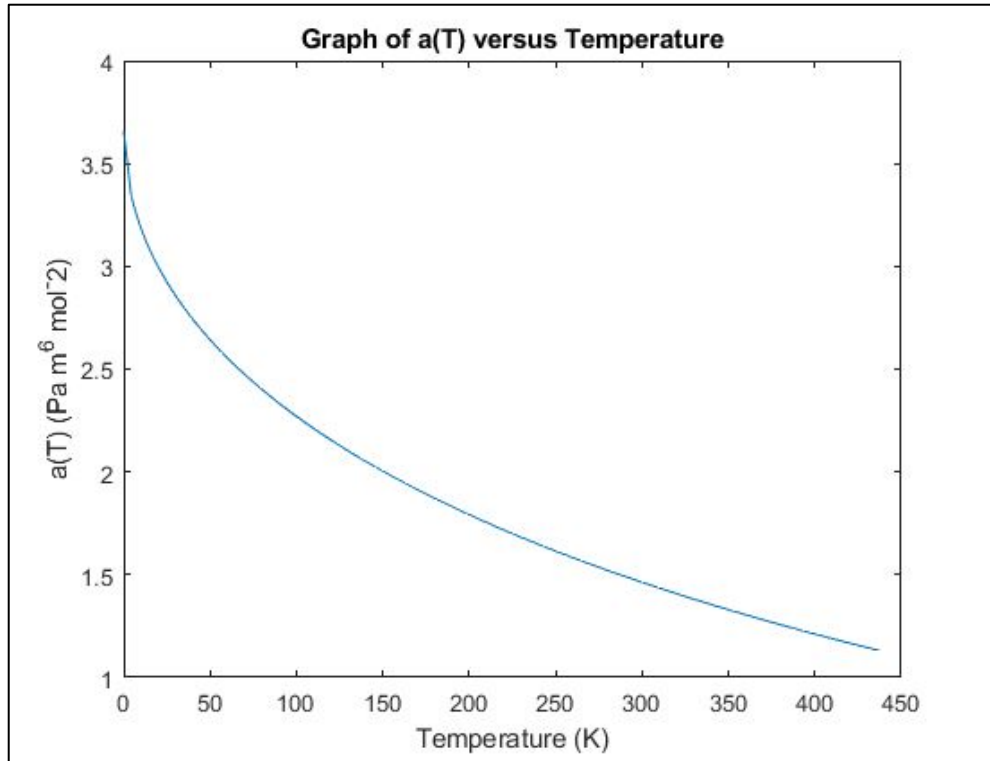


Figure 1: Graph of $a(T)$ of PR EOS versus temperature

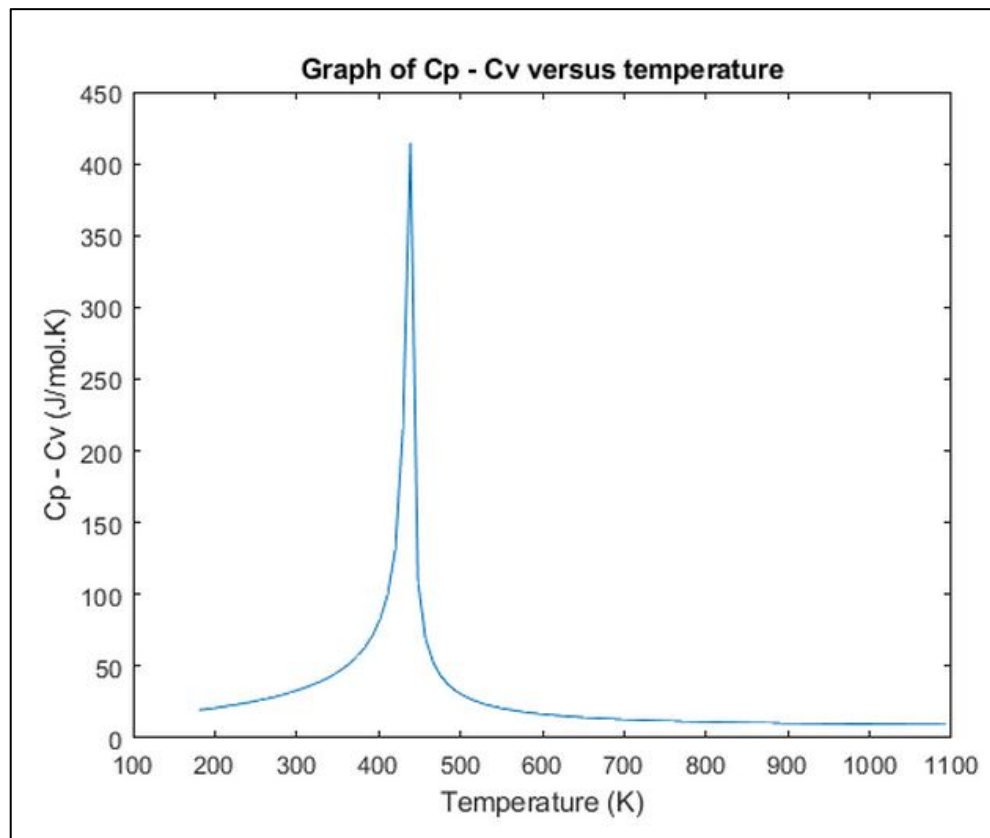


Figure 2: Graph of $C_p - C_v$ versus temperature

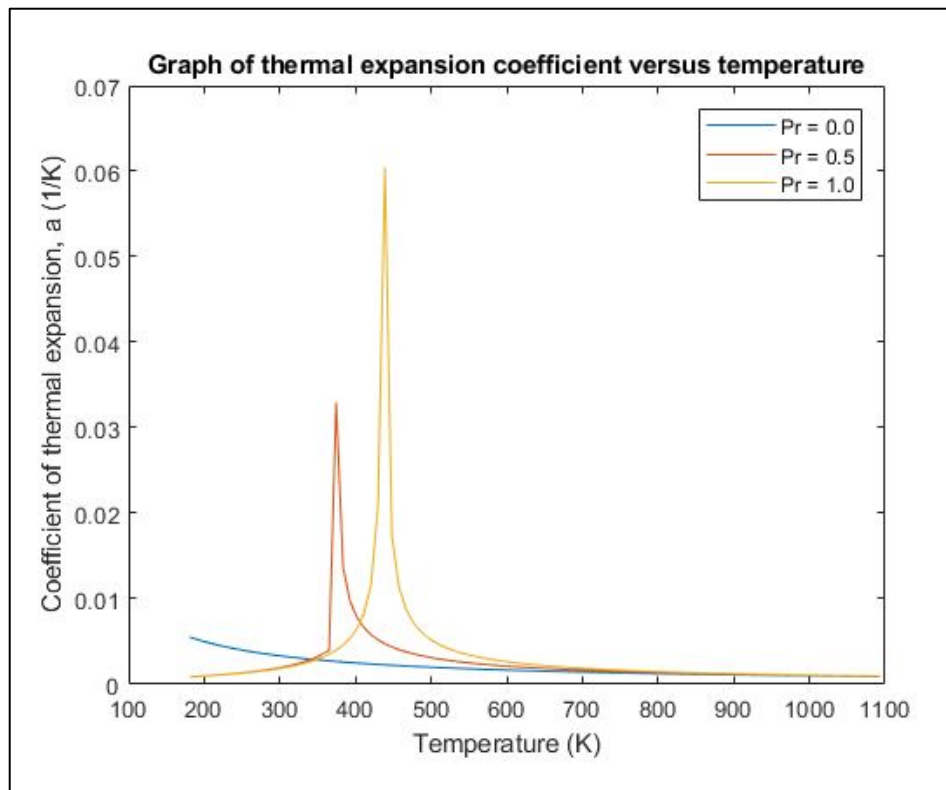


Figure 3: Graph of $\alpha(T)$ versus temperature

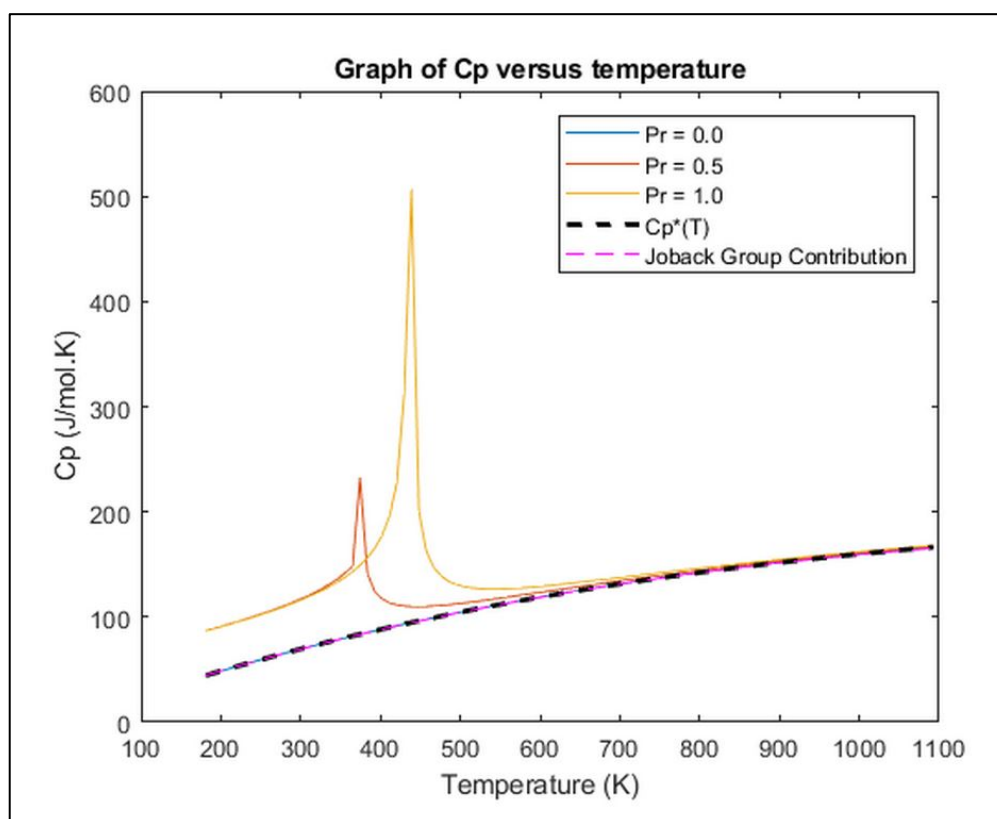


Figure 4: Graph of C_p versus temperature

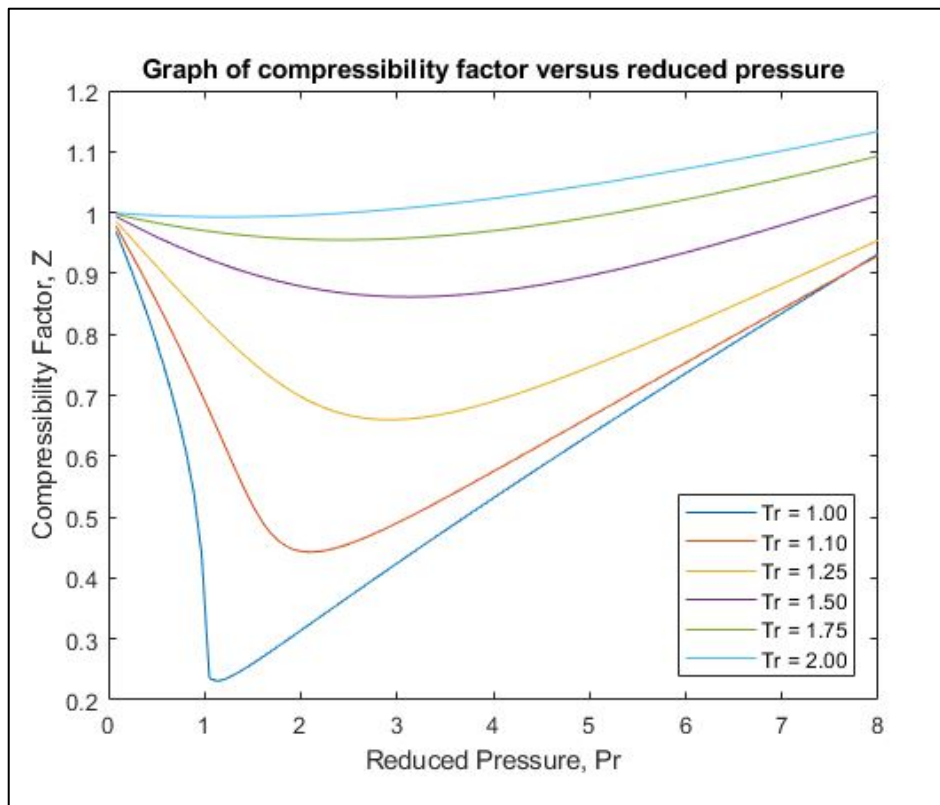


Figure 5: Z at different temperature versus reduced pressure

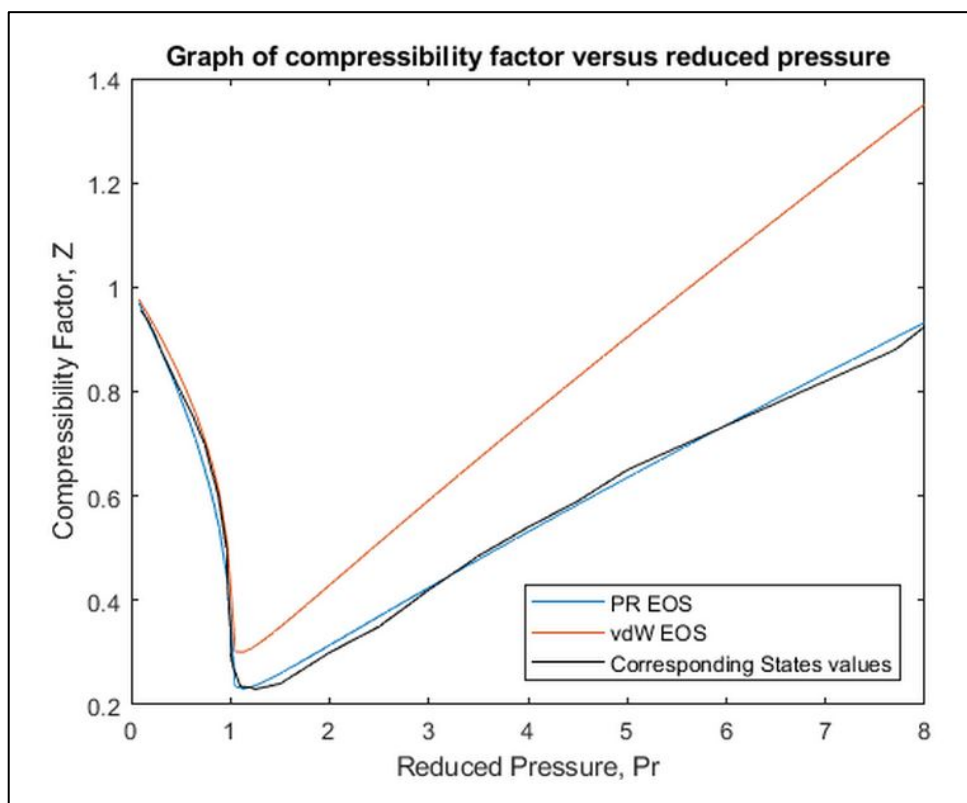


Figure 6: Graph of Z versus reduced pressure by using different equation of states

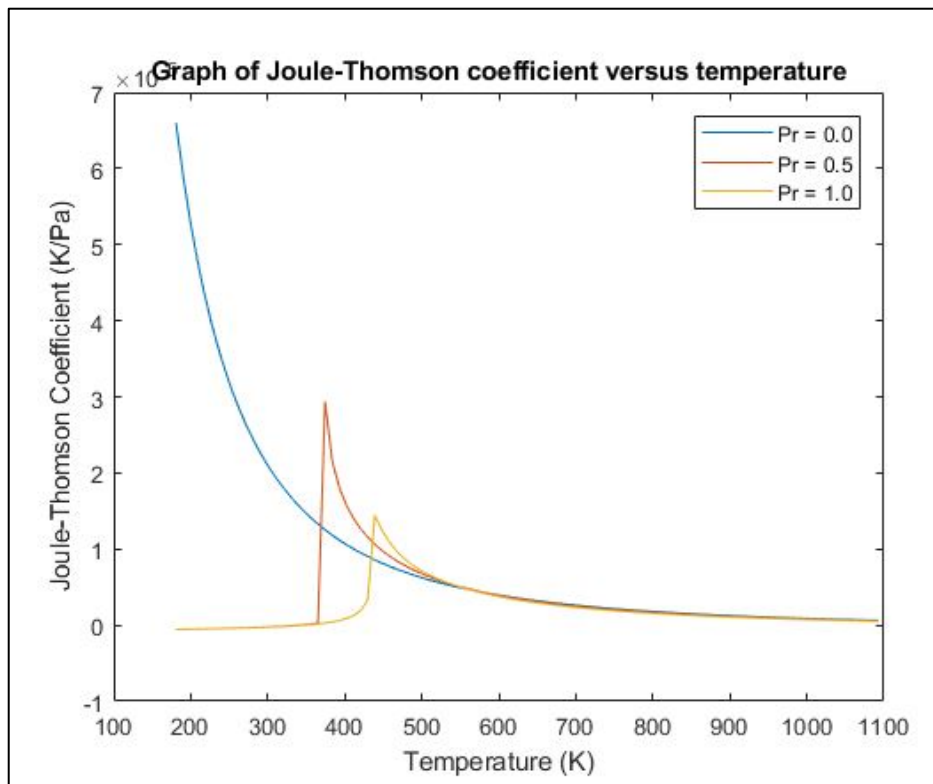


Figure 7: Graph of μ_{JT} versus temperature

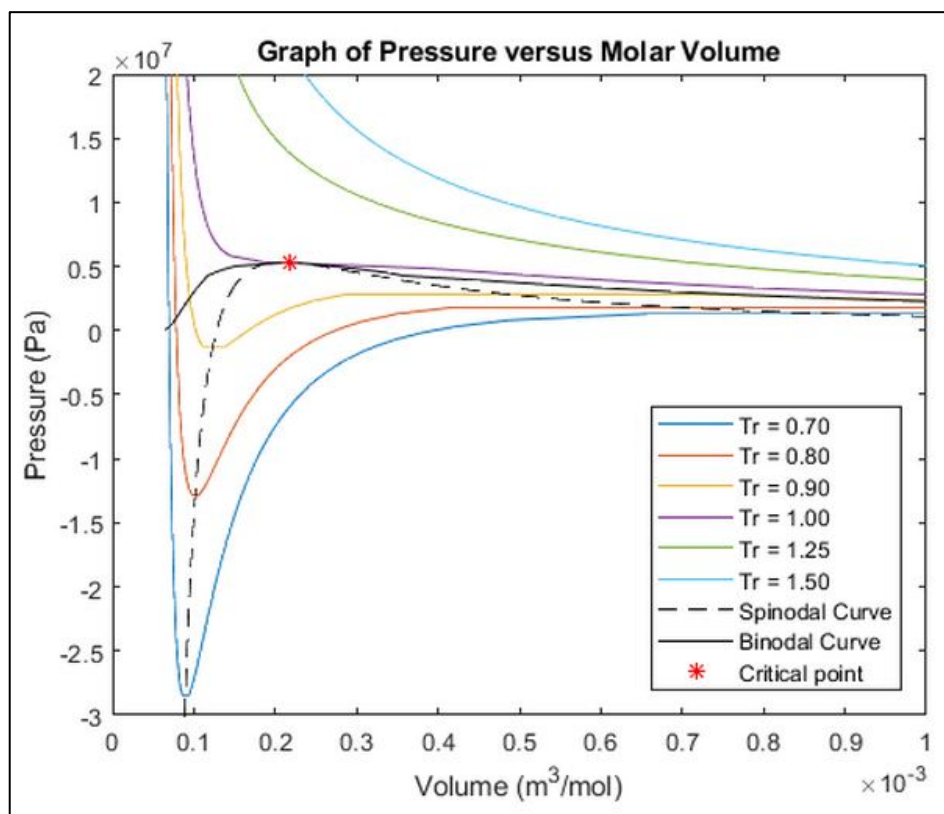


Figure 8: PV diagram of dimethylamine, with binodal and spinodal curves

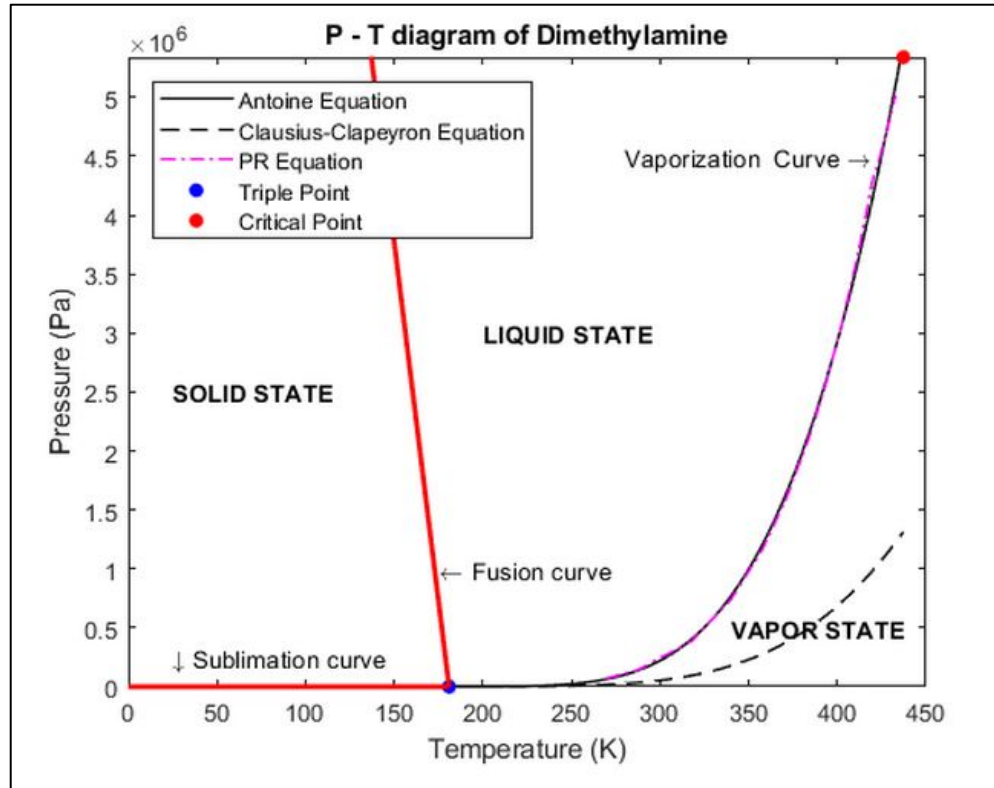


Figure 9: PT diagram of dimethylamine

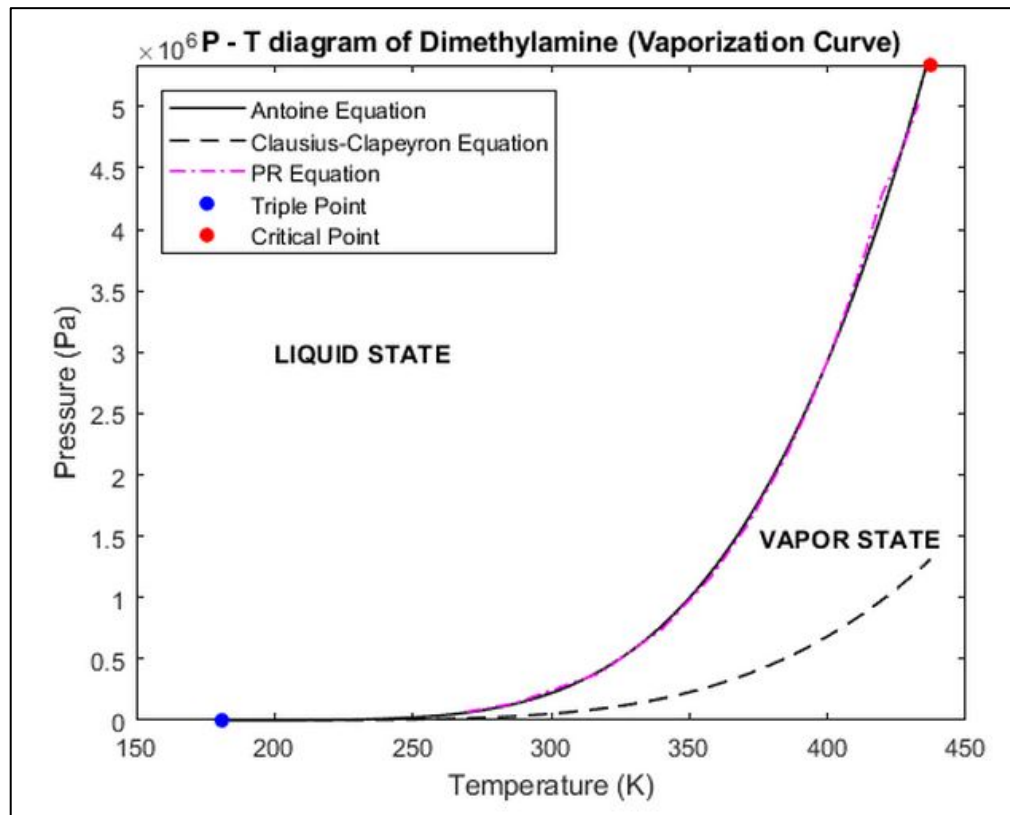


Figure 10: Vaporization curve with three different equation of states

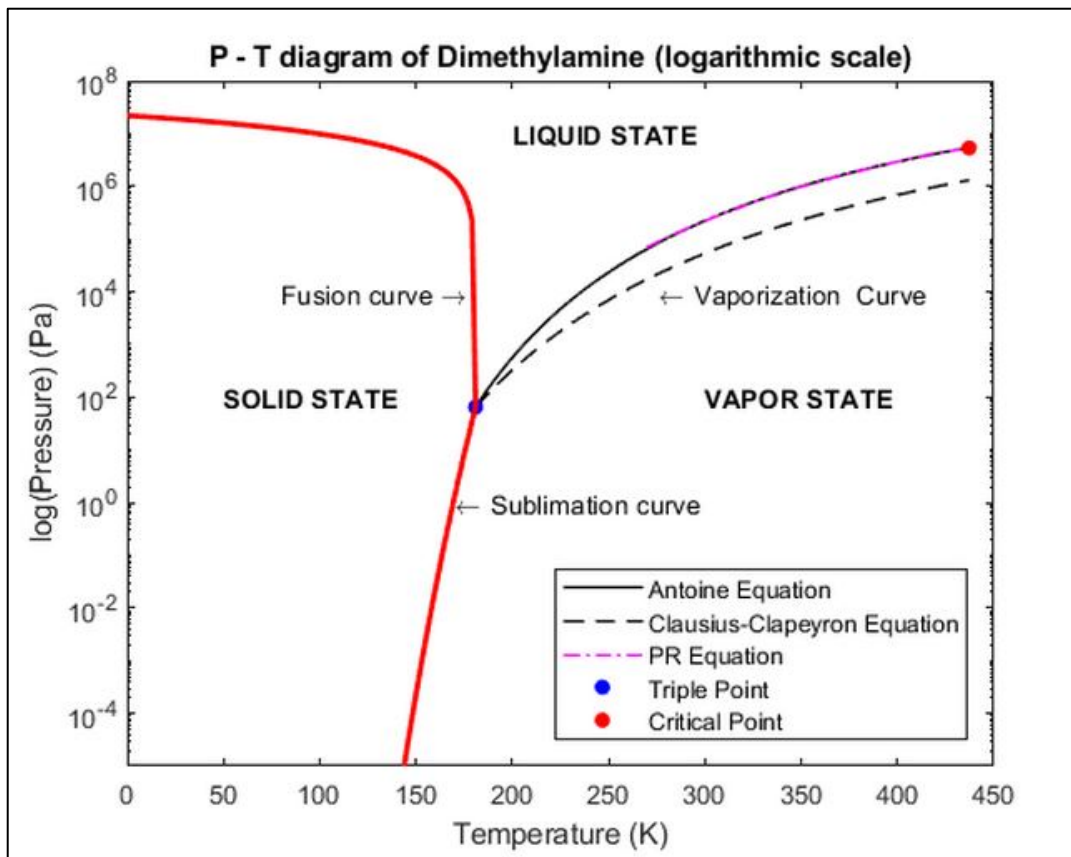


Figure 11: Graph of logarithmic pressure versus temperature of dimethylamine

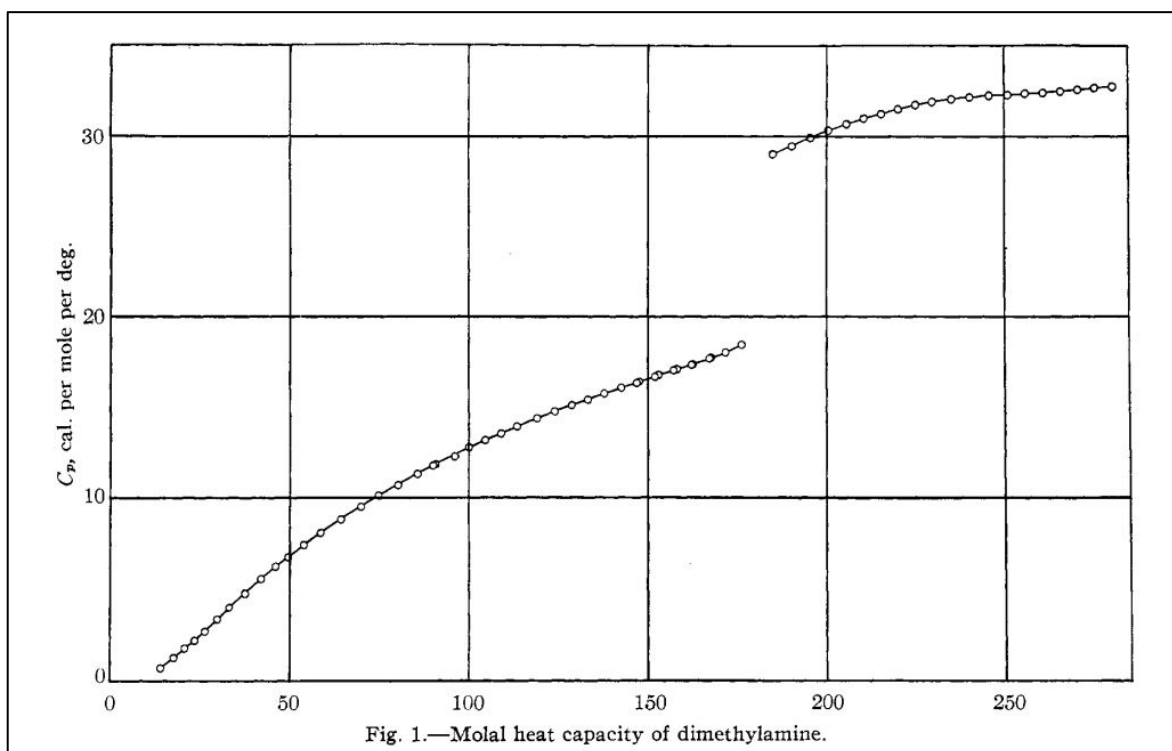


Figure 12: Heat capacity of dimethylamine obtained experimentally ^[1]

DISCUSSION

In **Figure 1**, the graph is downward sloping as temperature increases. The particles have less average kinetic energy and cannot break weak intermolecular attractions as easily as at higher temperature. For this compound, PR EOS is only suitable to predict the behavior of non-polar compound, but dimethylamine is polar, which will mistakenly predict its thermodynamic behavior.

From **Figure 2**, the peak of $C_p - C_v$ curve is at the critical temperature, because it is plotted at critical pressure. For each curve of C_p in **Figure 4** also shows a peak at the respective temperature at which the pressure is used to plot. C_p increases with temperature and deviates from ideal gas behavior as pressure increases. The curve of C_p estimated by Joback method and $C_p^*(T)$ overlaps with the curve measure at zero pressure, because they all show the ideal gas behavior. By comparing the obtained results with the experiment conducted based on **Figure 12**, within the temperature range of 0 and 250 °C, it shows an upward sloping trend, increasing with temperature, which has no significant difference in trend than **Figure 4**.

In **Figure 3 and 7**, by looking at the peak of each pressure, the $\alpha(T)$ increases with temperature, as pressure increases. However, it shows an inverse relationship in the μ_{JT} . As the temperature increases, μ_{JT} decreases with increasing pressure. By looking at **Eq. 7**, μ_{JT} is directly and inversely proportional to temperature and pressure respectively, and vice versa for $\alpha(T)$ based on **Eq. 1**.

In **Figure 5**, all plot converges to $Z = 1$ as the reduced pressure decreases. It converges to the ideal gas behavior at low pressure limit, as stated in ideal gas law ($PV = RT$), and based on **Eq. 6**. By comparing different EOS (PR and vdW) with the **corresponding states (CS) values from the textbook (Figure 6)**, it is observed that PR EOS provides the closest predictions to the CS values.

Figure 8 shows the PV diagram while **Figure 9 – 11** shows the PT diagram of the compound. **Figure 10** shows a clear distinction between three different vaporization curves plotted with different EOS. CC-EOS has a lower gradient of vaporization curve in comparison with the PR and Antoine EOS. It will differ in gradient based on which $\Delta H_{\text{vaporization}}$ is used in **Eq. 14**. In this case, $\Delta H_{\text{vaporization}}$ used is at triple point condition. **Figure 11** is obtained with logarithmic y-axis, to have a better representation in sublimation curve.

One of the environmental significances of dimethylamine is that it exists as vapor at room temperature, which makes it easily compressed to be commercially used. From this advantage, dimethylamine can be used as pesticides for the agricultural uses^[9]. Aside from that, with its easy-to-dissolve property in a liquid solvent, it makes itself useful to be used as additives in paint and coating^[9].

CONCLUSION

In conclusion, the thermodynamic analysis of dimethylamine is conducted in order to increase the awareness of this uncommon compound on its effect on the environment and human to the society. It is an uncommon compound that people might not have done the analysis computationally yet in order to better understand its properties. The analysis was conducted and measured by using the computer programming MATLAB, to have a better representation graphically. To recap, some of the thermodynamic properties analyzed are the constant pressure heat capacity, coefficient of thermal expansion, Joule-Thomson coefficient, change in constant pressure and volume heat capacity, compressibility factor with different equation of states, and pressure-temperature and pressure-volume diagram of dimethylamine. In order to make sure that the analysis of these properties was done correctly, they were compared with theoretical behavior or/and with the graphical experimental data conducted in the past. It is ensured to be approximately equivalent to have a clear judgment when explaining the trend of each properties. The trends of each properties were aligned with the expected trend, which translates to having a normal-behaving compound with a predictable manner.

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APPENDICES

a) Coding for Figure 1

```
syms V T
R = 8.314;
Ttriple = 180.97;
Tcrit = 437.22;
Pcrit = 5.34e+6;
antA = 4.29371;
antB = 995.445;
antC = -47.869;
Pant = @(T) (10^5)*10^(antA - (antB/(T + antC)));
Ptriple = Pant(Ttriple)
syms T V
omega = -1 - log10(Pant(0.7*Tcrit)/Pcrit)
k_small = 0.37464 + 1.5422*omega - 0.26992*omega^2
alpha_T = @(T) (1 + k_small*(1 - sqrt(T./Tcrit)))^2;
a_T = @(T) (0.45724*(R^2)*(Tcrit^2)/Pcrit) * alpha_T(T);
Trange_a = linspace(0,Tcrit,100);
a_array = [];
for i = 1:length(Trange_a)
    val = a_T(Trange_a(i));
    a_array(i) = val;
end
plot(Trange_a,a_array)
xlabel('Temperature (K)')
ylabel('a(T) (Pa m^6 mol^-2)')
title('Graph of a(T) versus Temperature')
b = 0.0778*R*Tcrit/Pcrit
Prb = @(T,V) R*T./(V - b) - a_T(T)/(V.*(V + b) + b*(V - b));
Vcrit = vpasolve(Prb(Tcrit,V) == Pcrit,V,[0 Inf]);
acentric = omega
Zc = Pcrit*Vcrit/(R*Tcrit)
% FOR REPORT PURPOSES
% CLAUSIUS CLAPEYRON EQUATION
C = log(Pcrit) + (33.78e+3)/(R*Tcrit)
P_unknown = exp(C - (26.4e+3)/(R*(6.88+273.15)))
P_norm = exp(C - (25.05e+3)/(R*(298)))/10^5
Vtriple = vpasolve(Prb(Ttriple,V) == Ptriple,V,[0 Inf])
Vcrit = vpasolve(Prb(Tcrit,V) == Pcrit,V,[0 Inf])
Vnormal = vpasolve(Prb(180.15,V) == 1*10^5,V,[0 Inf])
```

b) Coding for Figure 2 – 4 and 7.

```

syms T V
R = 8.314;
Ttriple = 180.97;
Tcrit = 437.22;
Pcrit = 5.34e+6;
antA = 4.29371;
antB = 995.445;
antC = -47.869;
Pant = @(T) (10^5)*10^(antA - (antB/(T + antC)));
b = 0.0778*R*Tcrit/Pcrit;
omega = -1 - log10(Pant(0.7*Tcrit)/Pcrit);
k_small = 0.37464 + 1.5422*omega - 0.26992*omega^2;
alpha_T = @(T) (1 + k_small*(1 - sqrt(T./Tcrit)))^2;
a_T = @(T) (0.45724*(R^2)*(Tcrit^2)/Pcrit) * alpha_T(T);
Prb = @(T,V) R*T./(V - b) - a_T(T)/(V.*(V + b) + b*(V - b));
Trange = linspace(Ttriple,2.5*Tcrit,100);
Prange = Pcrit*[0.00000001,0.5,1];
% NO 4 - Cp - Cv vs. T graph
alpha = zeros(1,length(Trange));
% doing approximation method in dvdt instead of actual diff dvdt
for i = 1:length(Trange)

    t_up = Trange(i) + 0.1;
    t_down = Trange(i) - 0.1;
    v1 = max(vpasolve(Prb(t_up,V) == Pcrit, V, [0 Inf]));
    v2 = max(vpasolve(Prb(t_down,V) == Pcrit, V, [0 Inf]));
    dvdt = (v1 - v2)/(t_up - t_down);
    Vreal = max(vpasolve(Prb(Trange(i),V) == Pcrit, V, [0 Inf]));
    alpha(i) = dvdt/Vreal;
end
Varray = zeros(1,length(Trange));
kappa = zeros(1,length(Trange));
dvdp = matlabFunction(1/diff(Prb,V));
for i = 1:length(Trange)
    Vreal = max(vpasolve(Prb(Trange(i),V) == Pcrit, V, [0 Inf]));
    Varray(i) = Vreal;
    kappa(i) = (-1/Vreal)*dvdp(Trange(i),Vreal);
end
cp_cv_array = zeros(1,length(Trange));
for i = 1:length(Trange)
    cp_cv_array(i) = Trange(i)*Varray(i)*alpha(i)^2/kappa(i);
end
plot(Trange,cp_cv_array)
xlabel('Temperature (K)')
ylabel('Cp - Cv (J/mol.K)')
title('Graph of Cp - Cv versus temperature')
% NO 7 - thermal expansion vs. T graph
% setting up three sets of alpha w.r.t 3 diff pressure

```

```

for j = 1:length(Prange)
    alpha = zeros(1,length(Trange));
    for i = 1:length(Trange)
        t_up = Trange(i) + 0.1;
        t_down = Trange(i) - 0.1;
        v1 = max(vpasolve(Prb(t_up,V) == Prange(j), V, [0 Inf]));
        v2 = max(vpasolve(Prb(t_down,V) == Prange(j), V, [0 Inf]));
        dvdt = (v1 - v2)/(t_up - t_down);
        Vreal = max(vpasolve(Prb(Trange(i),V) == Prange(j), V, [0 Inf]));

        alpha(i) = dvdt/Vreal;
    end
    plot(Trange,alpha)
    hold on
    if j == 1
        alpha_P1 = alpha;
    elseif j == 2
        alpha_P2 = alpha;
    elseif j == 3
        alpha_P3 = alpha;
    end
end
xlabel('Temperature (K)')
ylabel('Coefficient of thermal expansion, a (1/K)')
title('Graph of thermal expansion coefficient versus temperature')
legend('Pr = 0.0', 'Pr = 0.5', 'Pr = 1.0')
hold off
% setting up three sets of kappa and volume w.r.t 3 diff pressure
for j = 1:length(Prange)
    kappa = zeros(1,length(Trange));
    Varray = zeros(1,length(Trange));
    for i = 1:length(Trange)
        Vreal = max(vpasolve(Prb(Trange(i),V) == Prange(j), V, [0 Inf]));
        Varray(i) = Vreal;
        kappa(i) = (-1/Vreal)*dvdp(Trange(i),Vreal);
    end
    if j == 1
        kappa_P1 = kappa;
        Vol1 = Varray;
    elseif j == 2
        kappa_P2 = kappa;
        Vol2 = Varray;
    elseif j == 3
        kappa_P3 = kappa;
        Vol3 = Varray;
    end
end
end
for j = 1:length(Prange)
    cp_cv_array = zeros(1,length(Trange));

```

```

for i = 1:length(Trange)
    if j == 1
        cp_cv_array(i) = Trange(i)*Vol1(i)*alpha_P1(i)^2/kappa_P1(i);
    elseif j == 2
        cp_cv_array(i) = Trange(i)*Vol2(i)*alpha_P2(i)^2/kappa_P2(i);
    elseif j == 3
        cp_cv_array(i) = Trange(i)*Vol3(i)*alpha_P3(i)^2/kappa_P3(i);
    end
    if j == 1
        cp_cv1 = cp_cv_array;
    elseif j == 2
        cp_cv2 = cp_cv_array;
    elseif j == 3
        cp_cv3 = cp_cv_array;
    end
end
end

% NO 5 - Cp vs. T graph
a_cp = -1.151;
b_cp = 27.679e-2;
c_cp = -14.572e-5;
d_cp = 29.921e-9;
cp_star = @(T) a_cp + b_cp*T + c_cp*T.^2 + d_cp*T.^3;
cv_star = @(T) cp_star(T) - R;
dpdt = diff(Prb,T);
dpdt_secdiff = matlabFunction(diff(dpdt,T));
for j = 1:length(Prange)
    cv = zeros(1,length(Trange));
    for i = 1:length(Trange)
        if j == 1
            intgr1 = @(T)- int(dpdt_secdiff(T,V),V,Vol1(i),Inf);
            cv(i) = cv_star(Trange(i)) + Trange(i)*intgr1(Trange(i));
        elseif j == 2
            intgr1 = @(T)- int(dpdt_secdiff(T,V),V,Vol2(i),Inf);
            cv(i) = cv_star(Trange(i)) + Trange(i)*intgr1(Trange(i));
        elseif j == 3
            intgr1 = @(T)- int(dpdt_secdiff(T,V),V,Vol3(i),Inf);
            cv(i) = cv_star(Trange(i)) + Trange(i)*intgr1(Trange(i));
        end
    end
end
if j == 1
    cp = cp_cv1 + cv;
    cp_P1 = cp;
elseif j == 2
    cp = cp_cv2 + cv;
    cp_P2 = cp;
elseif j == 3
    cp = cp_cv3 + cv;
    cp_P3 = cp;
end

```

```

    end
    plot(Trange,cp)
    hold on
end
cp_star_array = zeros(1,length(Trange));
for i = 1:length(Trange)
    cp_star_array(i) = cp_star(Trange(i));
end
plot(Trange,cp_star_array,'k--','LineWidth',2)
A_job = -0.14;
B_job = 0.27;
C_job = -1.336e-4;
D_job = 2.31e-8;
cp_star_job = @(T) A_job + B_job*T + C_job*T.^2 + D_job*T.^3;
cp_job = zeros(1,length(Trange));
for i = 1:length(Trange)
    cp_job(i) = cp_star_job(Trange(i));
end
plot(Trange,cp_job,'m--')
xlabel('Temperature (K)')
ylabel('Cp (J/mol.K)')
title('Graph of Cp versus temperature')
legend('Pr = 0.0','Pr = 0.5','Pr = 1.0','Cp*(T)','Joback Group Contribution')
hold off
% NO 7 - JT-coefficient vs. T graph
for j = 1:length(Prange)
    u_jt = zeros(1,length(Trange));
    for i = 1:length(Trange)
        Vreal = max(vpasolve(Prb(Trange(i),V) == Prange(j), V, [0 Inf]));
        if j == 1
            u_jt(i) = (Vreal/cp_P1(i)).*(Trange(i).*alpha_P1(i)-1);
        elseif j == 2
            u_jt(i) = (Vreal/cp_P2(i)).*(Trange(i).*alpha_P2(i) - 1);
        elseif j == 3
            u_jt(i) = (Vreal/cp_P3(i)).*(Trange(i).*alpha_P3(i) - 1);
        end
    end
    end
    if j == 1
        u_jt1 = u_jt;
    elseif j == 2
        u_jt2 = u_jt;
    elseif j == 3
        u_jt3 = u_jt;
    end
end
plot(Trange,u_jt1)
hold on
plot(Trange,u_jt2)
plot(Trange,u_jt3)

```

```
xlabel('Temperature (K)')
ylabel('Joule-Thomson Coefficient (K/Pa)')
title('Graph of Joule-Thomson coefficient versus temperature')
legend('Pr = 0.0', 'Pr = 0.5', 'Pr = 1.0')
hold off
```


c) Coding for Figure 5 and 6

```

syms T V
R = 8.314;
Ttriple = 180.97;
Tcrit = 437.22;
Pcrit = 5.34e+6;
antA = 4.29371;
antB = 995.445;
antC = -47.869;
Pant = @(T) (10^5)*10^(antA - (antB/(T + antC)));
b = 0.0778*R*Tcrit/Pcrit;
omega = -1 - log10(Pant(0.7*Tcrit)/Pcrit);
k_small = 0.37464 + 1.5422*omega - 0.26992*omega^2;
alpha_T = @(T) (1 + k_small*(1 - sqrt(T./Tcrit)))^2;
a_T = @(T) (0.45724*(R^2)*(Tcrit^2)/Pcrit) * alpha_T(T);
Prb = @(T,V) R*T./(V - b) - a_T(T)/(V.*(V + b) + b*(V - b));
Trange = Tcrit*[1,1.1,1.25,1.5,1.75,2];
Prange = linspace(0,8*Pcrit,100);
for i = 1:length(Trange)
    Zarray = [];
    P_newarray = [];
    for j = 1:length(Prange)
        Vreal = vpasolve(Prb(Trange(i),V) == Prange(j),V,[0 Inf]);

        if numel(Vreal) == 1
            Zarray = [Zarray Prange(j)*Vreal(1)/(R*Trange(i))];
            P_newarray = [P_newarray Prange(j)];
        elseif numel(Vreal) == 2
            Zarray = [Zarray Prange(j)*Vreal(1)/(R*Trange(i))
            Prange(j)*Vreal(2)/(R*Trange(i))];
            P_newarray = [P_newarray Prange(j) Prange(j)];
        end
    end
    if i == 1
        Z1 = double(Zarray');
    elseif i == 2
        Z2 = double(Zarray');
    elseif i == 3
        Z3 = double(Zarray');
    elseif i == 4
        Z4 = double(Zarray');
    elseif i == 5
        Z5 = double(Zarray');
    elseif i == 6
        Z6 = double(Zarray');
    end

    [P_newarray,sortIdx] = sort(P_newarray);
    Zarray = Zarray(sortIdx);

```

```

    plot(P_newarray/Pcrit,Zarray)
    hold on

end
legend({'Tr = 1.00','Tr = 1.10','Tr = 1.25','Tr = 1.50','Tr = 1.75','Tr = 2.00'},'Location','southeast')
xlabel('Reduced Pressure, Pr')
ylabel('Compressibility Factor, Z')
title('Graph of compressibility factor versus reduced pressure')
hold off
Zarray = [];
P_newarray = [];
for i = 1:length(Prange)
    Vreal = vpasolve(Prb(Tcrit,V) == Prange(i),V,[0 Inf]);
    if numel(Vreal) == 1
        Zarray = [Zarray Prange(i)*Vreal(1)/(R*Tcrit)];
        P_newarray = [P_newarray Prange(i)];
    elseif numel(Vreal) == 2
        Zarray = [Zarray Prange(i)*Vreal(1)/(R*Tcrit)
Prange(i)*Vreal(2)/(R*Tcrit)];
        P_newarray = [P_newarray Prange(i) Prange(i)];
    end
end
[P_newarray,sortIdx] = sort(P_newarray);
Zarray = Zarray(sortIdx);
plot(P_newarray/Pcrit,Zarray)
hold on
a_vdW = 27*R^2*Tcrit^2/(64*Pcrit);
b_vdW = R*Tcrit/(8*Pcrit);
PvdW = @(T,V) R*T./(V - b_vdW) - a_vdW/V.^2;
Zarray = [];
P_newarray = [];
for i = 1:length(Prange)
    Vreal = vpasolve(PvdW(Tcrit,V) == Prange(i),V,[0 Inf]);
    if numel(Vreal) == 1
        Zarray = [Zarray Prange(i)*Vreal(1)/(R*Tcrit)];
        P_newarray = [P_newarray Prange(i)];
    elseif numel(Vreal) == 2
        Zarray = [Zarray Prange(i)*Vreal(1)/(R*Tcrit)
Prange(i)*Vreal(2)/(R*Tcrit)];
        P_newarray = [P_newarray Prange(i) Prange(i)];
    elseif numel(Vreal) == 3
        Zarray = [Zarray Prange(i)*Vreal(1)/(R*Tcrit)
Prange(i)*Vreal(2)/(R*Tcrit) Prange(i)*Vreal(3)/(R*Tcrit)];
        P_newarray = [P_newarray Prange(i) Prange(i) Prange(i)];
    end
end
[P_newarray,sortIdx] = sort(P_newarray);
Zarray = Zarray(sortIdx);

```

```

plot(P_newarray/Pcrit,Zarray)
Z_book = [0.955 0.942 0.925 0.905 0.88 0.86 0.84 0.82 0.8 0.75 0.7 0.6 0.5 0.4
0.35 0.3 0.278 0.235 0.233 0.23 0.24 0.3 0.35 0.42 0.485 0.54 0.59 0.65 0.88
0.925];
P_book = [0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.63 0.74 0.88 0.96 0.98 1 1
1.02 1.1 1.2 1.25 1.5 2 2.5 3 3.5 4 4.5 5 7.7 8];
plot(P_book,Z_book,'k-')
xlabel('Reduced Pressure, Pr')
ylabel('Compressibility Factor, Z')
title('Graph of compressibility factor versus reduced pressure')
legend({'PR EOS','vdW EOS','Corresponding States values'},'Location','southeast')

```

d) Coding for Figure 8

```
syms T V
R = 8.314;
Ttriple = 180.97;
Tcrit = 437.22;
Pcrit = 5.34e+6;
antA = 4.29371;
antB = 995.445;
antC = -47.869;
Pant = @(T) (10^5)*10^(antA - (antB/(T + antC)));
b = 0.0778*R*Tcrit/Pcrit;
omega = -1 - log10(Pant(0.7*Tcrit)/Pcrit);
k_small = 0.37464 + 1.5422*omega - 0.26992*omega^2;
alpha_T = @(T) (1 + k_small*(1 - sqrt(T./Tcrit)))^2;
a_T = @(T) (0.45724*(R^2)*(Tcrit^2)/Pcrit) * alpha_T(T);
Prb = @(T,V) R*T./(V - b) - a_T(T)/(V.*(V + b) + b*(V - b));
dpdv = matlabFunction(diff(Prb,V));
Trange = Tcrit*[0.7,0.8,0.9,1,1.25,1.5];
Prange = linspace(-30e+6,20e+6,100);

for j = 1:length(Trange)
    P_rangenew = [];
    Varray = [];
    for i = 1:length(Prange)
        Vval = vpasolve(Prb(Trange(j),V) == Prange(i),V,[0 Inf]);

        n = numel(Vval);

        if n == 1
            P_rangenew = [P_rangenew Prange(i)];
            Varray = [Varray Vval(1)];
        elseif n == 2
            P_rangenew = [P_rangenew Prange(i) Prange(i)];
            Varray = [Varray Vval(1) Vval(2)];
        elseif n == 3
            P_rangenew = [P_rangenew Prange(i) Prange(i) Prange(i)];
            Varray = [Varray Vval(1) Vval(2) Vval(3)];
        end
    end

    [Varray,sortIdx] = sort(Varray);
    P_rangenew = P_rangenew(sortIdx);
    plot(Varray,P_rangenew,'-')
    hold on
end

P_spin = [];
V_spin = [];
Tnew = linspace(0,Tcrit,1000);
for k = 1:length(Tnew)
```

```

Vval2 = vpasolve(dpdv(Tnew(k),V) == 0,V,[0 Inf])';
m = numel(Vval2);
if m == 2
    P_spin = [P_spin Prb(Tnew(k),Vval2(1)) Prb(Tnew(k),Vval2(2))];
    V_spin = [V_spin Vval2(1) Vval2(2)];

elseif m == 1
    P_spin = [P_spin Prb(Tnew(k),Vval2(1))];
    V_spin = [V_spin Vval2(1)];
elseif m == 3
    P_spin = [P_spin Prb(Tnew(k),Vval2(1)) Prb(Tnew(k),Vval2(2))
Prb(Tnew(k),Vval2(3))];
    V_spin = [V_spin Vval2(1) Vval2(2) Vval2(3)];
end
end
[V_spin,sortIdx] = sort(V_spin);
P_spin = P_spin(sortIdx);
plot(V_spin,P_spin,'k--')
Trange = linspace(0,Tcrit,100);
Prange = linspace(Pcrit,-30e+6,1000);
V_bin = [];
P_bin = [];
P_bin_nine = [];
T_bin_nine = [];
for j = 1:length(Trange)
    for i = 1:length(Prange)
        Vval3 = sort(vpasolve(Prb(Trange(j),V) == Prange(i),V,[0 Inf])');
        m = numel(Vval3);
        n = 1;
        if m == 3
            area = int(Prb(Trange(j),V) - Prange(i),V,Vval3(1),Vval3(3));
            if abs(area) <= 100
                V_bin = [V_bin Vval3(1) Vval3(3)];
                P_bin = [P_bin Prange(i) Prange(i)];
                P_bin_nine = [P_bin_nine Prange(i)];
                T_bin_nine = [T_bin_nine Trange(j)];
                n = n + 1;
                break
            end
        end
    end
    if n ~= 1
        break
        break
    end
end
end
Vcrit = vpasolve(Prb(Tcrit,V) == Pcrit,V,[0 Inf]);
V_bin = [V_bin Vcrit];
P_bin = [P_bin Pcrit];

```

```

[V_bin,sortidx] = sort(V_bin);
P_bin = P_bin(sortidx);
plot(V_bin,P_bin,'k-','linewidth',2)
plot(Vcrit,Pcrit,'r*')
xlim([0 0.001])
ylim([-30e6 20e6])
xlabel('Volume (m^3/mol)')
ylabel('Pressure (Pa)')
title('Graph of Pressure versus Molar Volume')
legend({'Tr = 0.70','Tr = 0.80','Tr = 0.90','Tr = 1.00','Tr = 1.25','Tr = 1.50','Spinodal Curve','Binodal Curve','Critical point'},'Location','southeast')
hold off

```

e) Coding for Figure 9

```

syms T V
R = 8.314;
Ttriple = 180.97;
Tcrit = 437.22;
Tfus = 180.15;
Proom = 10^5;
Pcrit = 5.34e+6;
antA = 4.29371;
antB = 995.445;
antC = -47.869;
Pant = @(T) (10^5)*10^(antA - (antB/(T + antC)));
b = 0.0778*R*Tcrit/Pcrit;
Ptriple = Pant(Ttriple);
H_vap = 33780;
omega = -1 - log10(Pant(0.7*Tcrit)/Pcrit);
k_small = 0.37464 + 1.5422*omega - 0.26992*omega^2;
alpha_T = @(T) (1 + k_small*(1 - sqrt(T./Tcrit)))^2;
a_T = @(T) (0.45724*(R^2)*(Tcrit^2)/Pcrit) * alpha_T(T);
Prb = @(T,V) R*T./(V - b) - a_T(T)/(V.*(V + b) + b*(V - b));
Vcrit = vpasolve(Prb(Tcrit,V) == Pcrit,V,[0 Inf]);
Trange_vap = linspace(Ttriple,Tcrit,100);
% VAP CURVE - if antoine equation
Pvap_ant = zeros(1,length(Trange_vap));
for i = 1:length(Trange_vap)
    Pvap_ant(i) = Pant(Trange_vap(i));
end
plot(Trange_vap,Pvap_ant,'k-','linewidth',1)
hold on
% VAP CURVE - if clausius clayperon eqn
Pclaus = @(T) Ptriple*exp(H_vap/R*(1/Ttriple - 1/T));
Pvap_claus = zeros(1,length(Trange_vap));
for i = 1:length(Trange_vap)
    Pvap_claus(i) = Pclaus(Trange_vap(i));
end
plot(Trange_vap,Pvap_claus,'k--','linewidth',1)
% VAP CURVE - PR EOS
plot(T_bin_nine,P_bin_nine,'m-.','linewidth',1)
% TRIPLE AND CRITICAL POINT
plot(Ttriple,Ptriple,'b.','MarkerSize',20)
plot(Tcrit,Pcrit,'r.','MarkerSize',20)
% Setup of sublimation curve
syms A T
deltaHsub = 39.72086e+3;
B = deltaHsub/R;
Psub = @(A,T) 10^(A - B/T);
Trange_sub = linspace(0,Ttriple,100);
Aact = vpasolve(Psub(A,Ttriple) == Ptriple,A)
Psublim = zeros(1,length(Trange_sub));

```

```

for i = 1:length(Trange_sub)
    Psublim(i) = Psub(Aact,Trange_sub(i));
end
plot(Trange_sub,Psublim,'r-','linewidth',2)
% Setup of fusion curve
m = (Proom - Ptriple)/(Tfus - Ttriple)
c = Ptriple - m*Ttriple
Trange_fus = linspace(0,Ttriple,100);
Pfus = @(T) m*T + c;
Pfusion = zeros(1,length(Trange_fus));
for i = 1:length(Trange_fus)
    Pfusion(i) = Pfus(Trange_fus(i));
end
plot(Trange_fus,Pfusion,'r-','linewidth',2)
txt1 = 'Vaporization Curve \rightarrow';
text(420,4.5e+6,txt1,'HorizontalAlignment','right')
txt2 = '\leftarrow Fusion curve';
text(175,1e+6,txt2)
txt3 = '\downarrow Sublimation curve';
text(25,0.25e+6,txt3)
txt4 = 'SOLID STATE';
text(25,2.5e6,txt4,'fontweight','bold')
txt5 = 'LIQUID STATE';
text(200,3e6,txt5,'fontweight','bold')
txt6 = 'VAPOR STATE';
text(340,0.5e6,txt6,'fontweight','bold')
txt7 = 'STATE';
text()
title('P - T diagram of Dimethylamine')
xlabel('Temperature (K)')
ylabel('Pressure (Pa)')
ylim([0 Pcrit])
legend({'Antoine Equation','Clausius-Clapeyron Equation','PR Equation','Triple Point','Critical Point'},'Location','northwest')
hold off
% PLOTTING VAP CURVE TO HAVE A BETTER VIEW
plot(Trange_vap,Pvap_ant,'k-','linewidth',1)
hold on
plot(Trange_vap,Pvap_claus,'k--','linewidth',1)
plot(T_bin_nine,P_bin_nine,'m-.','linewidth',1)
plot(Ttriple,Ptriple,'b.','MarkerSize',20)
plot(Tcrit,Pcrit,'r.','MarkerSize',20)
txt5 = 'LIQUID STATE';
text(200,3e6,txt5,'fontweight','bold')
txt6 = 'VAPOR STATE';
text(375,1.5e6,txt6,'fontweight','bold')
title('P - T diagram of Dimethylamine (Vaporization Curve)')
xlabel('Temperature (K)')
ylabel('Pressure (Pa)')

```



```

ylim([0 Pcrit])
legend({'Antoine Equation','Clausius-Clapeyron Equation','PR Equation','Triple
Point','Critical Point'},'Location','northwest')
hold off
% PLOTTING LOG SCALE
plot(Trange_vap,Pvap_ant,'k-','linewidth',1)
hold on
plot(Trange_vap,Pvap_claus,'k--','linewidth',1)
plot(T_bin_nine,P_bin_nine,'m-.','linewidth',1)
plot(Ttriple,Ptriple,'b.','MarkerSize',20)
plot(Tcrit,Pcrit,'r.','MarkerSize',20)
plot(Trange_fus,Pfusion,'r-','linewidth',2)
plot(Trange_sub,Psublim,'r-','linewidth',2)
set(gca,'YScale','log')
txt1 = '\leftarrow Vaporization Curve ';
text(420,1e4,txt1,'HorizontalAlignment','right')
txt2 = 'Fusion curve \rightarrow';
text(80,1e+4,txt2)
txt3 = '\leftarrow Sublimation curve';
text(170,1,txt3)
txt4 = 'SOLID STATE';
text(50,1e2,txt4,'fontweight','bold')
txt5 = 'LIQUID STATE';
text(200,1e7,txt5,'fontweight','bold')
txt6 = 'VAPOR STATE';
text(300,1e2,txt6,'fontweight','bold')
title('P - T diagram of Dimethylamine (logarithmic scale)')
xlabel('Temperature (K)')
ylabel('log(Pressure) (Pa)')
ylim([1e-5 1e8])
legend({'Antoine Equation','Clausius-Clapeyron Equation','PR Equation','Triple
Point','Critical Point'},'Location','southeast')
hold off

```

f) Table of Values (8 – 14)

Table 8: Intermolecular attraction correction for Peng-Robinson Equation of States (FIGURE 1)	
Temperature (K)	a(T) (Pa.m⁶.mol²)
0.000	3.659
4.416	3.340
8.833	3.212
13.249	3.115
35.331	2.794
66.245	2.504
97.160	2.288
141.324	2.045
216.402	1.730
220.818	1.714
340.060	1.355
344.476	1.344
375.391	1.268
393.056	1.227
432.804	1.141
437.220	1.131

Table 9: C_P – C_V (FIGURE 2)	
Temperature (K)	C_P - C_V (J/mol.K)
180.97	19.47
190.18	20.18
254.67	26.39
263.89	27.54
346.80	44.75
356.02	48.18
429.72	215.25
438.93	414.26
540.27	22.06
549.49	20.88
641.62	14.71
770.60	11.68
862.73	10.65
871.94	10.58
945.64	10.06
954.86	10.01
1037.77	9.61
1083.84	9.44
1093.05	9.41

Table 10: Coefficient thermal expansion (FIGURE 3)			
Temperature (K)	alpha (P _r = 0) (1/K)	alpha (P _r = 0.5) (1/K)	alpha (P _r = 1) (1/K)
180.97	0.00553	0.00087	0.00085
190.18	0.00526	0.00092	0.00090
273.10	0.00366	0.00157	0.00152
282.31	0.00354	0.00169	0.00162
365.23	0.00274	0.00401	0.00352
374.44	0.00267	0.03298	0.00398
438.93	0.00228	0.00474	0.06047
448.14	0.00223	0.00437	0.01737
531.06	0.00188	0.00270	0.00391
540.27	0.00185	0.00260	0.00366
623.19	0.00160	0.00199	0.00240
632.40	0.00158	0.00194	0.00232
770.60	0.00130	0.00144	0.00158
779.81	0.00128	0.00142	0.00155
853.51	0.00117	0.00126	0.00134
862.73	0.00116	0.00125	0.00132
918.00	0.00109	0.00115	0.00121
927.22	0.00108	0.00114	0.00119
1000.92	0.00100	0.00104	0.00107
1093.05	0.00091	0.00094	0.00096

Table 11: Cp (FIGURE 4)					
Temperature (K)	C _p (P _r = 0) (J/mol.K)	C _p (P _r = 0.5) (J/mol.K)	C _p (P _r = 1) (J/mol.K)	C _p (Joback) (J/mol.K)	C _p * (J/mol.K)
180.97	44.34	87.14	86.98	44.48	44.34
190.18	46.42	88.97	88.79	46.54	46.42
236.25	56.50	99.23	98.87	56.49	56.50
346.80	78.56	136.60	133.59	78.39	78.56
402.08	88.53	117.22	177.67	88.32	88.53
595.55	118.33	122.96	128.79	118.15	118.33
650.83	125.52	129.08	133.12	125.36	125.52
761.38	138.32	140.64	143.00	138.18	138.32
844.30	146.68	148.44	150.17	146.49	146.68
853.51	147.54	149.26	150.94	147.35	147.54
918.00	153.29	154.71	156.08	153.00	153.29
927.22	154.07	155.45	156.78	153.76	154.07
1083.84	165.76	166.69	167.56	164.97	165.76
1093.05	166.37	167.27	168.13	165.53	166.37

Table 12: Joule-Thomson coefficient (FIGURE 7)			
Temperature (K)	μ_{JT} ($P_r = 0$) (K/Pa)	μ_{JT} ($P_r = 0.5$) (K/Pa)	μ_{JT} ($P_r = 1$) (K/Pa)
180.97	6.60E-05	-5.65E-07	-5.67E-07
282.31	2.41E-05	-3.10E-07	-3.22E-07
356.02	1.41E-05	1.38E-07	6.77E-08
466.57	7.39E-06	8.50E-06	9.81E-06
540.27	5.14E-06	5.32E-06	5.33E-06
641.62	3.30E-06	3.21E-06	3.05E-06
752.17	2.14E-06	2.02E-06	1.88E-06
761.38	2.06E-06	1.94E-06	1.81E-06
844.30	1.52E-06	1.42E-06	1.31E-06
853.51	1.48E-06	1.37E-06	1.26E-06
964.07	9.89E-07	9.13E-07	8.38E-07
973.28	9.57E-07	8.83E-07	8.10E-07
1010.13	8.38E-07	7.71E-07	7.06E-07
1093.05	6.28E-07	5.64E-07	5.14E-07

Table 13: Compressibility factor (FIGURE 5)						
Reduced Pressure	Z ($T_r = 1$)	Z ($T_r = 1.1$)	Z ($T_r = 1.25$)	Z ($T_r = 1.5$)	Z ($T_r = 1.75$)	Z ($T_r = 2$)
0.0808	0.9689	0.9774	0.9856	0.9932	0.9970	0.9990
0.1616	0.9368	0.9544	0.9713	0.9865	0.9941	0.9981
1.0505	0.2353	0.6735	0.8199	0.9230	0.9691	0.9928
1.1313	0.2306	0.6451	0.8072	0.9182	0.9675	0.9927
2.4242	0.3610	0.4520	0.6700	0.8682	0.9551	0.9989
2.5051	0.3700	0.4563	0.6669	0.8667	0.9551	0.9998
3.4747	0.4755	0.5293	0.6690	0.8630	0.9619	1.0133
3.5556	0.4841	0.5362	0.6716	0.8637	0.9630	1.0147
4.4444	0.5777	0.6144	0.7131	0.8800	0.9789	1.0325
4.5253	0.5861	0.6216	0.7177	0.8822	0.9807	1.0343
5.4141	0.6772	0.7011	0.7730	0.9111	1.0035	1.0560
5.4949	0.6854	0.7084	0.7783	0.9141	1.0058	1.0581
6.2222	0.7583	0.7732	0.8279	0.9439	1.0284	1.0782
6.3030	0.7663	0.7804	0.8335	0.9474	1.0311	1.0805
7.0303	0.8380	0.8446	0.8848	0.9808	1.0563	1.1023
7.1111	0.8459	0.8517	0.8906	0.9847	1.0592	1.1048
7.9192	0.9244	0.9224	0.9486	1.0246	1.0896	1.1306
8.0000	0.9322	0.9295	0.9545	1.0287	1.0928	1.1333

Table 14: Compressibility factor with different equation of states (FIGURE 6)				
Reduced Pressure	Z (PR EOS)	Z (vdW EOS)	Reduced Pressure	Z (Corresponding States)
0.0808	0.9689	0.9755	0.1000	0.9550
0.1616	0.9368	0.9500	0.1500	0.9420
0.2424	0.9035	0.9232	0.2000	0.9250
0.3232	0.8689	0.8949	0.2500	0.9050
1.1313	0.2306	0.3006	0.3000	0.8800
1.2121	0.2340	0.3080	0.3500	0.8600
1.6162	0.2719	0.3669	0.4000	0.8400
1.6970	0.2806	0.3799	0.4500	0.8200
2.5051	0.3700	0.5117	0.5000	0.8000
2.5859	0.3789	0.5248	0.6300	0.7500
3.4747	0.4755	0.6674	0.7400	0.7000
3.5556	0.4841	0.6802	0.8800	0.6000
4.0404	0.5355	0.7563	0.9600	0.5000
4.1212	0.5440	0.7689	0.9800	0.4000
4.2020	0.5525	0.7815	1.0000	0.3500
4.8485	0.6195	0.8813	1.0000	0.3000
4.9293	0.6278	0.8936	1.0200	0.2780
5.2525	0.6608	0.9429	1.1000	0.2350
5.3333	0.6690	0.9552	1.2000	0.2330
5.4141	0.6772	0.9674	1.2500	0.2300
5.5758	0.6935	0.9919	1.5000	0.2400
5.6566	0.7017	1.0041	2.0000	0.3000
6.3030	0.7663	1.1010	2.5000	0.3500
6.3838	0.7743	1.1131	3.0000	0.4200
6.7879	0.8142	1.1730	3.5000	0.4850
6.8687	0.8222	1.1850	4.0000	0.5400
7.0303	0.8380	1.2089	4.5000	0.5900
7.1111	0.8459	1.2208	5.0000	0.6500
7.9192	0.9244	1.3392	7.7000	0.8800
8.0000	0.9322	1.3510	8.0000	0.9250