1976 words

Real Behaviors of Gases

When working with gases we often simplify our calculations by using the ideal gas law as it is usually relatively accurate when working at low pressures and high temperatures. The ideal gas law equation is:

is $PV=nRT$,

P is the pressure in pascals,
V is the volume in m^3,
n is the number of moles,
R is the gas constant in JK^{-1}mol-1,
T is the temperature in K.

There are several other standard models that exist which are more or less accurate under certain conditions. One is the Van der Waals law considers intermolecular forces and volume taken up by gas molecules

It is defined by:

$$(p + \frac{n^2 a}{V^2})(V - nb) = nRT,$$

a is the measure of the attraction between the molecules in Jm^3/mol^2
b is the volume taken up by the molecules themselves in m^3/mol[1]

Different combination of gases and conditions, result in different intermolecular forces and volume molecules based on their identity.

Research Question

Do specific factors such as temperature, pressure, intermolecular forces, and volume of gas molecules affect a gas' deviation from ideal gas behavior, and if so, in which direction does each one affect it?

---

[1] (Webqc.org).

My hypothesis is that lower temperatures, higher pressures, higher intermolecular forces and higher volume of gas molecules will all result in a greater deviation from ideal gas behavior.

Method

I decided that I was going to change each IV individually and was going to keep all other IVs constant when one is being altered. This means that there would be four separate graphical analyses, one for each of the IVs and each one would have the relevant IV getting manipulated 5 times and all other IVs staying constant. The measured DV for all graphical analyses will be the concept that I call percent deviation.

Percent deviation is defined by the difference between the ideal gas volume and der Waals volume with the given parameters, divided by the van der Waals or "real" gas volume, multiplied by 100. However large or small the volume of the gas is, percent deviation will tell us how far away is the ideal gas volume from the real gas volume as a percentage of the real gas volume. Percent deviation becomes our standard measure for the reliability of the ideal gas law under each condition, given that van der Waals law can be taken as the "real" gas measurement. After having conducted graphical analyses for each IV, the IVs that do affect the deviation can be combined into one graph. This means that in every data point occurs a change in each of the relevant IVs and the percent deviation will be found like above for each data point.

This should model a minimized deviation when all parameters are favorable and a maximized deviation when all parameters are unfavorable. With this, I want to show the possible range of how far or how close the ideal gas law can be from real gas behavior due to the changes in relevant IVs (which are listed below).

Type of Variable	**Variable**	**How is it changed measured or controlled**
IV	**Temperature of gas**	**Is changed by significant values in the range of hundreds of kelvins**
IV	**Pressure of gas**	**Is changed by significant values in the range of hundreds of thousands of pascals**
IV	**a value in Van der Waals (Intermolecular forces)**	**The a value input to Van der Waals is changed by significant values in the range of tenths of tenths Jm^3/mol^2**
IV	**b value in Van der Waals (Volume of gas molecules)**	**The b value input to Van der Waals is changed by significant values in the range of thousandths m^3/mol**
DV	**Percent deviation from real gas volume to ideal gas volume**	**Volume from ideal gas law is obtained, volume from Van der Waals is obtained, the difference is found between real and ideal volumes, this difference is a percentage of the real volume, percent deviation is found**
Controlled	**Moles of gas**	**Moles of gas input is always kept to 1 mole for both equations**
Controlled	**Every other IV than the one which is being focused on**	**The input of all other IVs are kept at a constant value when changing one IV**
Controlled	**Simulation website**	**The same simulation website (Webqc.org) is used for all the calculations and data points so that the data is consistent**

The simulation used is on webqc.org which computes the Van der Waals equation and is therefore used to get the real volume of gas. A graphing method of Van der Waals equation can be used to check the accuracy of the simulation's results[2].

IV Temperature:

1. Choose a constant pressure value and ethanol as the parameter to keep both a and b values constant.

---

[2] No safety or environmental concerns as data collection is fully done using digital means.

2. Choose 5 temperatures and find the real volume using Van der Waals and ideal volume using PV=nRT for each of them.
3. Find the percent deviation between van der Waals volume and ideal volume for each data point.
4. Plot a graph of temperature on the x-axis and percent deviation on the y-axis.

IV Pressure:

1. Same as IV temperature, just keeping temperature constant, using ethanol and choosing 5 pressures.
2. Plot a graph of pressure on the x-axis and percent deviation on the y-axis.

IV value of a (Intermolecular forces):

1. Same other IVs, but using custom parameters, keeping temperature,pressure,

   and b value constant and choosing 5 a values.
2. Plot a graph of value of a on the x-axis and percent deviation on the y-axis.

IV value of b (Volume of gas molecules):

1. Same method as IVs, using custom parameters, keeping temperature,pressure, and a value constant and choosing 5 b values.
2. Plot a graph of value of b on the x-axis and percent deviation on the y-axis

Second part:

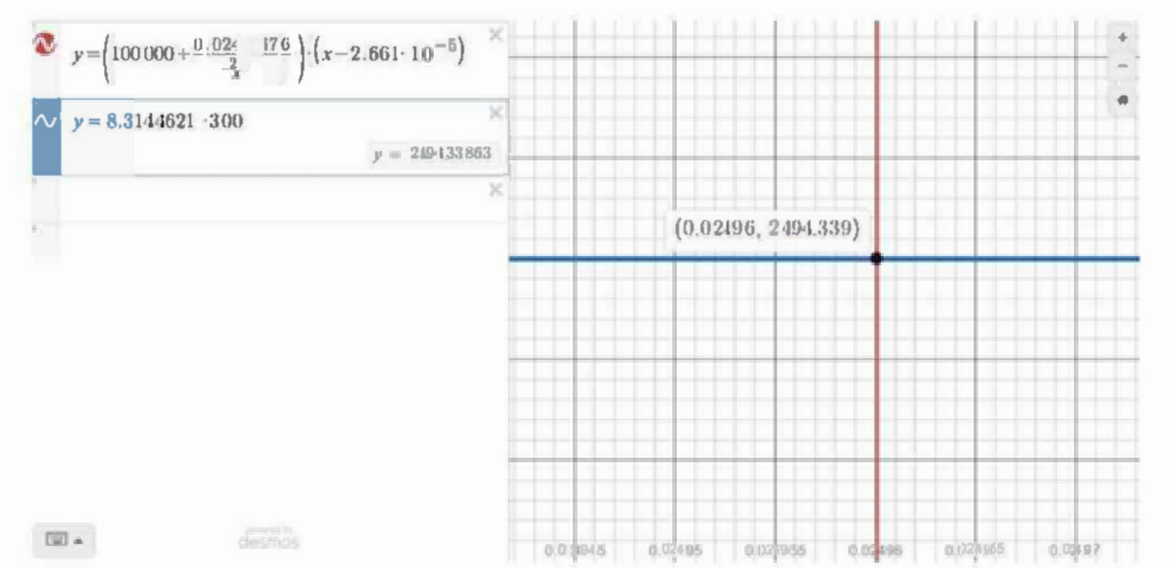
1. Identify the factors affecting percent deviation and direction of effect.
2. Choose 5 values for each relevant IV from least impact on percent deviation to most impact.
3. Combine these values into respective data points so that all relevant IVs are being changed.
4. Plot a graph with changing relevant IVs on the x-axis and percent

deviation on the y-axis; this shows the two extremes of deviation from ideal gas behavior,with minimized deviation on one end and maximized deviation on the other.

Preliminary Calculations

Accuracy of simulation webqc.org:

1 mole of hydrogen at 100000 pascals and 300 K (with a = 0.02476 and b= 2.661*10^{-5} the volume computed is 0.024960087038356 m^3. Using these values in Van der Waals equation and a graphing method:



y = 8.3144621 ·300

y = 2494.33863

(Desmos.com) The volume obtained is 0.02496 m^3 which matches the volume obtained from the simulation.

The gas constant that will be used for the ideal gas law component will be the same as the one used in the simulation. When comparing the gas constant value found in the simulation to the exact value of gas constant: 8.314462618 J/mol/K[3], the difference in both values can give a %uncertainty for the value of percent deviation from ideal gas behavior in each calculation. 8.314462618 - 8.3144621 = 0.000000518 = Absolute uncertainty of gas constant. (0.000000518/8.3144621)*100 =6.23*10^{-6} = Percentage uncertainty of gas constant and percent deviation. The uncertainty for percent deviation is so small that is considered negligible. The uncertainty would result in error bars that

---

[3] (Nist.gov)

would be too small to see. This means that the max and min lines will also be very close together and that is why they will be excluded as well.

Raw Data

Table 1: Separate IVs With Their Manipulations

	Temperature (K)	**Pressure (Pa)**	**Gas Type (choosing a gas to keep a and b values constant)**
Manipulation of IV Temperature	**450**	**100000**	**Ethanol**
	550	**100000**	**Ethanol**
	650	**100000**	**Ethanol**
	750	**100000**	**Ethanol**
	850	**100000**	**Ethanol**
Manipulation of IV Pressure	**850**	**100000**	**Ethanol**
	850	**200000**	**Ethanol**
	850	**300000**	**Ethanol**
	850	**400000**	**Ethanol**
	850	**500000**	**Ethanol**
	Temperature (K)	**Value of a (J m$^{3/}$mol^{2}) Intermolecular Forces**	**Value of b (m^{3}/mol) Volume of molecules**
Manipulation of value of a (Intermolecular force)	**450**	**0.3**	**0.001**
	550	**0.4**	**0.002**
	650	**0.5**	**0.002**
	750	**0.6**	**0.002**
	850	**0.7**	**0.002**
Manipulation of value of b (Volume of molecules)	**850**	**0.03**	**3 x 10^{-5}**
	850	**0.03**	**3 x 10^{-5}**
	850	**0.03**	**3 x 10^{-5}**
	850	**0.03**	**3 x 10^{-5}**
	850	**0.03**	**3 x 10^{-5}**

Processed Data

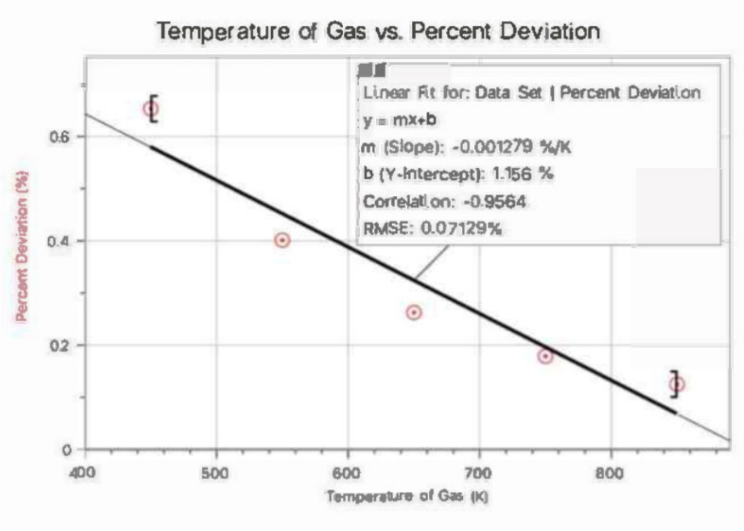
Table 2: Ideal gas and Van Der Waals Volume with Percent Deviation from Real Gas for each Manipulation

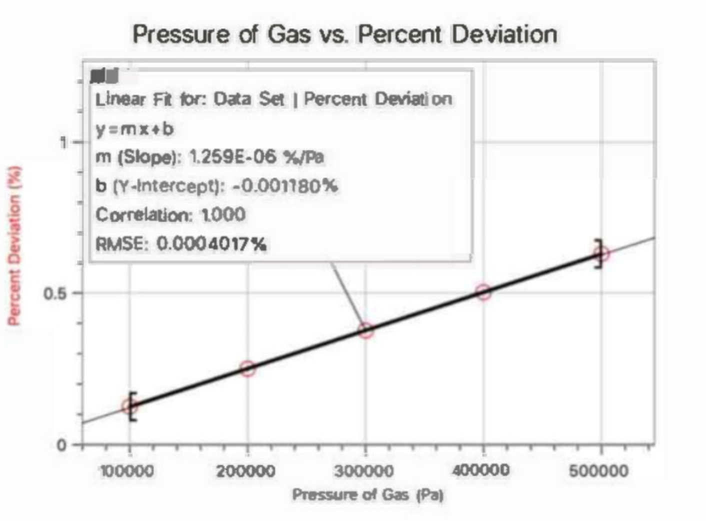
Ideal Gas Volume (m^3)	Van Der Waals Volume (m^3)	Percent Deviation (%)
0.03742	0.03717	0.6533
0.04573	0.04555	0.4015
0.05404	0.05390	0.2626
0.06236	0.06225	0.1789
0.07067	0.07058	0.1251
0.03534	0.03525	0.2505
0.02356	0.02347	0.3762
0.01767	0.01758	0.5023
0.01413	0.01405	0.6288
0.07067	0.07066	0.01760
0.07067	0.07065	0.03765
0.07067	0.07063	0.05771
0.07067	0.07062	0.07778
0.07067	0.07060	0.09787
0.07067	0.07167	1.390
0.07067	0.07267	2.747
0.07067	0.07367	4.067
0.07067	0.07467	5.352
0.07067	0.07567	6.603

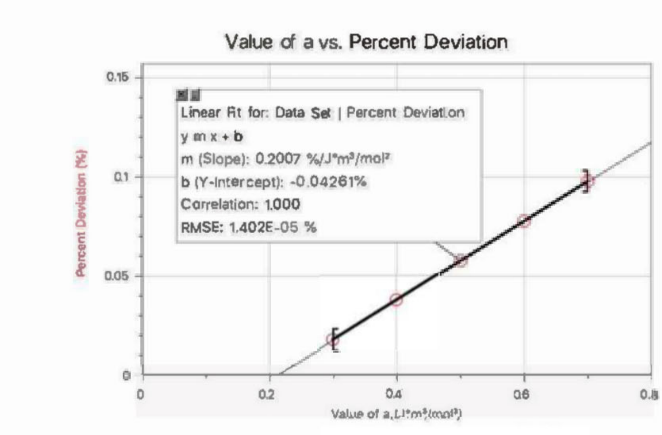
Sample Calculation

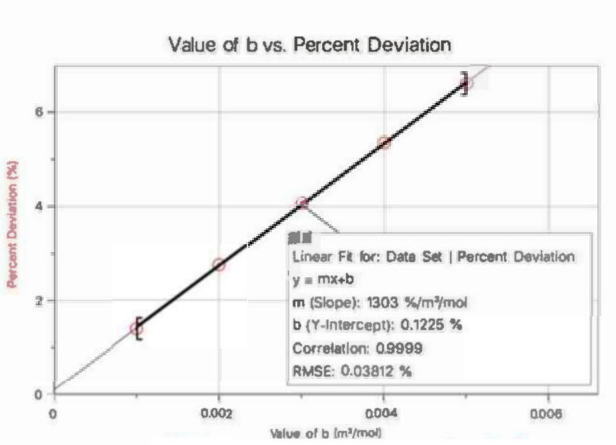
Ideal Gas Volume (m^3) = (Moles (mol)* Gas Constant (J /mol/K) * T emperature (K)) I Pressure(Pa) $((1 mol)*(8.3144621 J/mol/K)*(450K))$ $/(100000 Pa)$ $= 0.03742\ m^3$	Van der Waals Volume = From Simulation $= 0.03717\ m^3$	Percent Deviation (%) = (Ideal gas Volume (m^3) − Van Der Waals Volume (m^3)) /Van Der Waals Volume (m^3) * 100 $((0.03742\ m^3 - 0.03717\ m^3)/$ $0.03717\ m^3) * 100$ $= 0.6533\%$

Graphs 1-4: Each predetermined IV versus the Percent Deviation from Ideal Gas behaviour for each manipulation









Error bars, max and min lines are excluded due to prior examination of the uncertainties in the Preliminary Calculations).

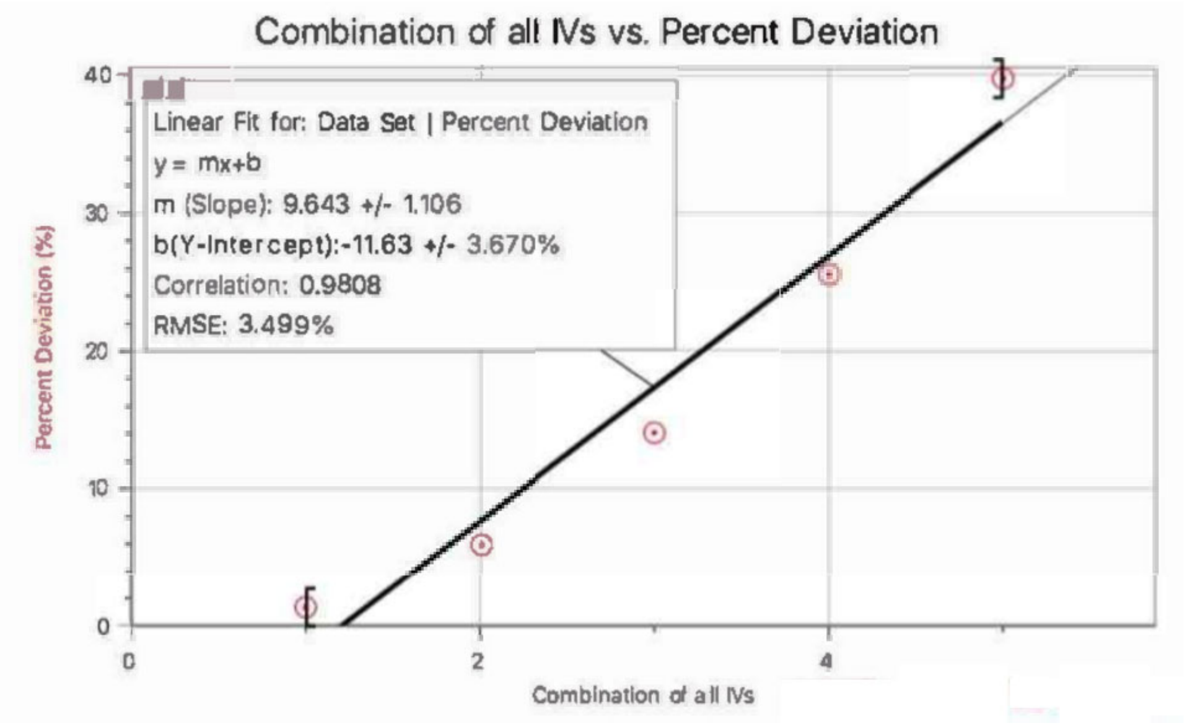
Table 3: Manipulation of all IVs at the Same Time from Least to Greatest Impact on Percent Deviation from Ideal Gas Behavior

Temperature (K)	**Pressure (Pa)**	**Value of a (Jm^3/mol^2) Intermolecular Forces**	**Value of b (m^3/mol) Volume of Molecules**
850	**100000**	**0.3**	**0.001**
750	**200000**	**0.4**	**0.002**
650	**300000**	**0.5**	**0.003**
550	**400000**	**0.6**	**0.004**
450	**500000**	**0.7**	**0.005**

Table 4: Ideal gas and Van Der Waals Volume with Percent Deviation after combiningall IVs

Ideal Gas Volume (m^3)	Van Der Waals Volume (m^3)	Percent Deviation (%)
0.07067	0.07163	1.338
0.03118	0.03312	5.867
0.01801	0.02095	14.00
0.01143	0.01536	25.57
0.00748	0.01242	39.7

Graph 5: All IV are being manipulated to conceptualize a minimized and maximized deviation



Linear Fit for: Data Set | Percent Deviation
y = mx+b
m (Slope): 9.643 +/- 1.106
b(Y-Intercept):-11.63 +/- 3.670%
Correlation: 0.9808
RMSE: 3.499%

Conclusion

The main assumptions that are made when taking a look at ideal gases are:

- The molecules of the gas themselves don't take up any volume.
- All the collisions of the molecules are elastic (there are no intermolecular forces present or attraction between molecules)

These are the two concepts that the Van der Waals equation takes into account and therefore, the gas will deviate more from ideal gas behavior when the a and b values are higher.

As pressure increases, the molecules of gas are closer together and are therefore more prone to colliding inelastically because the intermolecular forces can have more effect.

The attraction between the molecules also has a greater effect when the temperature ofthe gas is lower. At low temperatures the average kinetic energy of the molecules is smaller and they are more likely to attract one another.

Due to the lack of a and b values in the ideal gas law, gases deviate more when placed in low temperatures and high pressures[4].

Results Supporting Theory:

The results show that the percent deviation increases at lower temperatures and is directly proportional to the pressure, a, and b values of a gas. The graphs all have very strong correlations, all being above 0.95, with the pressure and a value graph correlation being

1.00 and the b value graph correlation being 0.99. Thus, all the independent variables have a very strong relationship with the dependent variable, percent deviation. When combining all

of them into one, again, there is a strong correlation of 0.98 and the percent deviation is shown to be only around 1% on one end and reach nearly 40% on the other end of the spectrum. It shows that certain gases under certain conditions can strongly .

deviate from ideal gas behaviour and the ideal gas model would become useless in those situations.

For this whole process, two equations were used, one of which was computed by a simulation. The simulation results were checked against

---

[4] (Lumenlearning.com)

a graphing method and were found to give very accurate data values. Since the data was purely found using predetermined equations and the simulation had only a $6.23*10^{-6}$ percent uncertainty for gas constant, the resulting trend lines were accurate for the set of controlled parameters of the equations. This process is also a reliable one, because even if other simulations or methods were used to compute Van der Waals equation, the volumes and percent deviations should be the same.
This is true because the ideal gas and Van der Waals laws have standard well-known equations which are the same, whichever source is being used.

Weaknesses

The data processing was fully done using digital means and carried through using the standard equations, there really isn't much possible error that could have affected the data. It could be said that there is no random error involved because random error usually occurs when experimental trials are carried out in lab conditions.
The lack of random error is also reflected in the correlations of some of the graphs where the values were 0.99 or even 1.00. There might have been very small amounts of systematic error due to the fact that the gas constant value used was not exact all the way to a large number of decimal places. This error, is very minimal and that is also why the uncertainties were neglected in this IA. However, no real gas model is a perfect representation of real gases. There are other models which could have been used instead of Van der Waals which are generally a more accurate representation of real gases such as the Redlich-Kwong model [5]Overall, such an alternative would help to find more accurate real gas volumes and percent deviations but still would never be exact

---

[5] (Chemistry LibreTexts).

Works Cited

"16.2: Van Der Waals and Redlich-Kwong Equations of State." *Chemistry LibreTexts*, 18 June 2014, chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Map%3A_Physical_Chemistry_(McQuarrie_and_Simon)/16%3A_The_Properties_of_Gases/16.02%3A_van_der_Waals_and_Redlich-Kwong_Equations_of_State. Accessed 29 Nov. 2020.

"CODATA Value: Molar Gas Constant." *Nist.Gov*, 2018, physics.nist.gov/cgi-bin/cuu/Value?r. Accessed 29 Nov. 2020.

"Desmos | Graphing Calculator." *Desmos*, 2020, www.desmos.com/calculator/eo0taie6p9. Accessed 29 Nov. 2020.