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Honors Project

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Ideal Gas Law

In this report I will be discussing the Ideal Gas Law – $PV=nRT$ – and the implications of Calculus 3 that are involved. First off, a quick explanation of the law will be essential to understanding the implications mentioned later on.

$$PV=nRT$$

P= pressure of the gas (atm)

V= volume (liters)

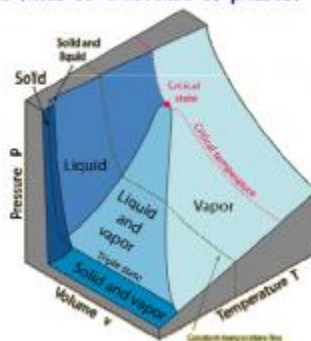
n= number of moles of substance (mol)

T= temperature (Kelvin)

$$R= \text{Universal gas constant} = 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}$$

Below is the graph in 3D of P vs. V vs. T with Pressure graphed on the z-axis, Volume on the x-axis and Temperature on the y-axis.

PVT surface for a real substance
Regions where Van der Waals' PVT surface is multi-valued is where one finds co-existence of phases.



(<http://multivariablecalculus.wordpress.com/4th-quarter-projects/>)

Assuming that the number of moles of a substance is constant, there are many different application of Calculus 3 that can be applied to the equation. First off, solving the equation for each of the remaining variable results in the following equations:

$$P = \frac{nRT}{V}$$

$$V = \frac{nRT}{P}$$

$$T = \frac{PV}{nR}$$

Taking these equations and implicitly differentiating each with respect to time results in the following equations:

Pressure:

$$\frac{\partial P}{dt} = \frac{\partial P}{\partial T} * \frac{\partial T}{dt} + \frac{\partial P}{\partial V} * \frac{\partial V}{dt}$$

From this equation we are able to derive the pressure equation with respect to temperature along with deriving the pressure equation with respect to volume, plugging in for these equations results in:

$$\frac{\partial P}{dt} = \frac{nR}{V} * \frac{\partial T}{dt} + \frac{-nRT}{V^2} * \frac{\partial V}{dt}$$

Volume:

$$\frac{\partial V}{dt} = \frac{\partial V}{\partial T} * \frac{\partial T}{dt} + \frac{\partial V}{\partial P} * \frac{\partial P}{dt}$$

From this equation we are able to derive the volume equation with respect to temperature along with deriving the pressure equation with respect to pressure, plugging in for these equations results in:

$$\frac{\partial V}{dt} = \frac{nR}{P} * \frac{\partial T}{dt} + \frac{-nRT}{P^2} * \frac{\partial P}{dt}$$

Temperature:

$$\frac{\partial T}{dt} = \frac{\partial T}{\partial P} * \frac{\partial P}{dt} + \frac{\partial T}{\partial V} * \frac{\partial V}{dt}$$

From this equation we are able to derive the volume equation with respect to temperature along with deriving the pressure equation with respect to pressure, plugging in for these equations results in:

$$\frac{\partial T}{dt} = \frac{V}{nR} * \frac{\partial P}{dt} + \frac{P}{nR} * \frac{\partial V}{dt}$$

What these equations give us is a way to measure the changes to any particular variable, pressure, volume, or temperature, if the other variables are changing with respect to time.

Using the following spreadsheet, different values for pressure, volume, and temperature can be imputed into the equations listed above with arbitrary changes in each with respect to time to better understand what the formulas present.

	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1	Volume (L)
0.2	0.70	1.39	2.09	2.78	3.48	4.18	4.87	5.57	6.26	6.96		
0.3	1.04	2.09	3.13	4.18	5.22	6.26	7.31	8.35	9.40	10.44		
0.4	1.39	2.78	4.18	5.57	6.96	8.35	9.74	11.14	12.53	13.92		
0.5	1.74	3.48	5.22	6.96	8.70	10.44	12.18	13.92	15.66	17.40		
0.6	2.09	4.18	6.26	8.35	10.44	12.53	14.62	16.70	18.79	20.88		
0.7	2.44	4.87	7.31	9.74	12.18	14.62	17.05	19.49	21.92	24.36		
0.8	2.78	5.57	8.35	11.14	13.92	16.70	19.49	22.27	25.06	27.84		
0.9	3.13	6.26	9.40	12.53	15.66	18.79	21.92	25.06	28.19	31.32		
1	3.48	6.96	10.44	13.92	17.40	20.88	24.36	27.84	31.32	34.80		
1.1	3.83	7.66	11.48	15.31	19.14	22.97	26.80	30.62	34.45	38.28		
1.2	4.18	8.35	12.53	16.70	20.88	25.06	29.23	33.41	37.58	41.76		
1.3	4.52	9.05	13.57	18.10	22.62	27.14	31.67	36.19	40.72	45.24		
1.4	4.87	9.74	14.62	19.49	24.36	29.23	34.10	38.98	43.85	48.72		
1.5	5.22	10.44	15.66	20.88	26.10	31.32	36.54	41.76	46.98	52.20		
1.6	5.57	11.14	16.70	22.27	27.84	33.41	38.98	44.54	50.11	55.68		
1.7	5.92	11.83	17.75	23.66	29.58	35.50	41.41	47.33	53.25	59.16		
1.8	6.26	12.53	18.79	25.06	31.32	37.58	43.85	50.11	56.38	62.64		
1.9	6.61	13.22	19.84	26.45	33.06	39.67	46.29	52.90	59.51	66.12		
2	6.96	13.92	20.88	27.84	34.80	41.76	48.72	55.68	62.64	69.60		
Pressure (atm)	Temperature (K) calculated from $PV = nRT$											

(<http://multivariablecalculus.wordpress.com/4th-quarter-projects/>)

From these values, taking 1 atm for the pressure and .5 L for volume results in 17.40 K for temperature from the PV=nRT when n=.35 and R= Universal gas constant= $8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}$. If the volume of the gas was increasing .05 L per second and the temperature was increasing 1 K per second, the change of the pressure could be calculated using the equation listed previously. The calculations are as follows:

$$\frac{\partial P}{dt} = \frac{nR}{V} * \frac{\partial T}{dt} + \frac{-nRT}{V^2} * \frac{\partial V}{dt}$$

$$\frac{\partial P}{dt} = \frac{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} * 1 \text{ K}}{.5 \text{ L}} + \frac{-.35 * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} * 17.40 \text{ K}}{(.5 \text{ L})^2} * \frac{.05 \text{ L}}{\text{sec}}$$

$$\frac{\partial P}{dt} = \frac{-4.306911 \text{ atm}}{\text{sec}}$$

With the same values from the previous calculations (1 atm for the pressure and .5 L for volume results in 17.40 K for temperature from the PV=nRT when n=.35 and R= Universal gas constant= $8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}$), If the pressure of the gas was increasing .05 atm per second and the temperature was increasing 1 K per second, the change of the volume could be calculated using the equation listed previously. The calculations are as follows:

$$\frac{\partial V}{dt} = \frac{nR}{P} * \frac{\partial T}{dt} + \frac{-nRT}{P^2} * \frac{\partial P}{dt}$$

$$\frac{\partial V}{dt} = \frac{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} * 1 \text{ K}}{1 \text{ atm}} + \frac{-.35 * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}} * 17.40 \text{ K}}{(1 \text{ atm})^2} * \frac{.05 \text{ atm}}{\text{sec}}$$

$$\frac{\partial V}{dt} = \frac{.37830975 \text{ L}}{\text{sec}}$$

With the same values from the previous calculations (1 atm for the pressure and .5 L for volume results in 17.40 K for temperature from the PV=nRT when n=.35 and R= Universal gas constant= $8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}$), If the pressure of the gas was increasing .05 atm per second and the volume was increasing .05 L per second, the change of the temperature could be calculated using the equation listed previously. The calculations are as follows:

$$\frac{\partial T}{dt} = \frac{V}{nR} * \frac{\partial P}{dt} + \frac{P}{nR} * \frac{\partial V}{dt}$$

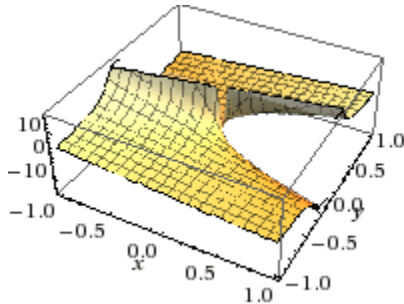
$$\frac{\partial T}{dt} = \frac{.5 \text{ L}}{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}} * \frac{.05 \text{ atm}}{\text{sec}} + \frac{1 \text{ atm}}{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} \cdot \text{K}}} * \frac{.05 \text{ L}}{\text{sec}}$$

$$\frac{\partial T}{dt} = \frac{.0257725316 \text{ K}}{\text{sec}}$$

Assuming the equations listed earlier and using the Pressure equation, if you were to assume $n=.35$ and $R=$ Universal gas constant $= 8.3145 \frac{\text{J}}{\text{mol} * \text{K}}$ and substitute $T=x$ along with $V=y$ for the purpose of graphing on a 3D plot, the equation would end up as follows:

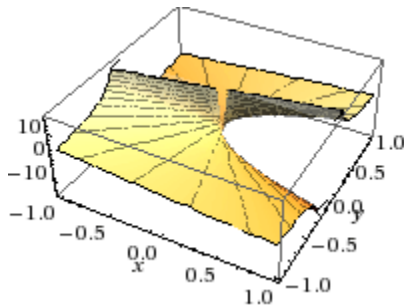
$$P = \frac{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} * \text{K}} x}{y}$$

3D Graph:



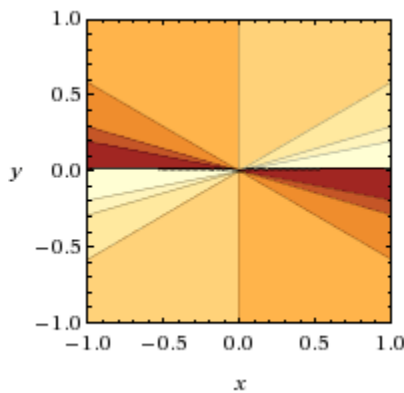
(<http://www.wolframalpha.com>)

3D Graph with Contour Lines Shown:



(<http://www.wolframalpha.com>)

Contour Plot:

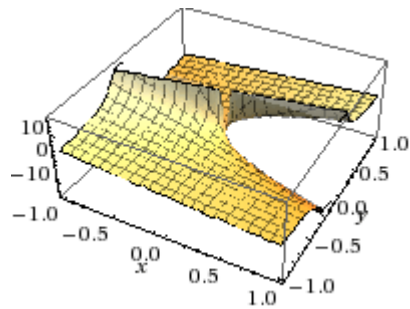


(<http://www.wolframalpha.com>)

Assuming the equations listed earlier and using the Volume equation, if you were to assume $n=.35$ and $R=$ Universal gas constant $= 8.3145 \frac{\text{J}}{\text{mol} * \text{K}}$ and substitute $T=x$ along with $P=y$ for the purpose of graphing on a 3D plot, the equation would end up as follows:

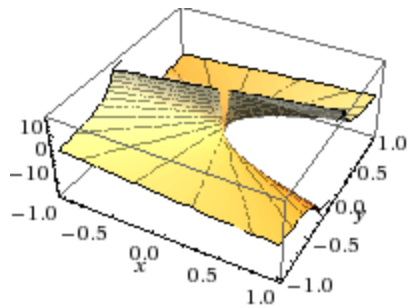
$$V = \frac{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} * \text{K}} x}{y}$$

3D Graph:



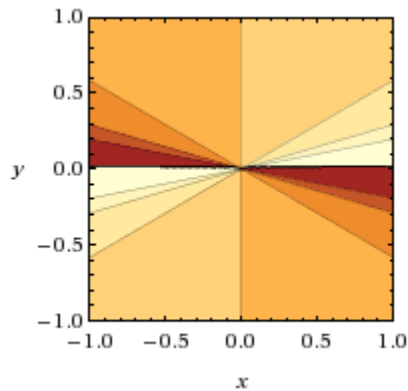
(<http://www.wolframalpha.com>)

3D Graph with Contour Lines Shown:



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Contour Plot:

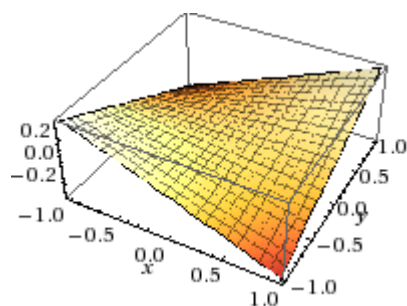


(<http://www.wolframalpha.com>)

Assuming the equations listed earlier and using the Temperature equation, if you were to assume $n=.35$ and $R=$ Universal gas constant $= 8.3245 \frac{\text{J}}{\text{mol} * \text{K}}$ and substitute $V=x$ along with $P=y$ for the purpose of graphing on a 3D plot, the equation would end up as follows:

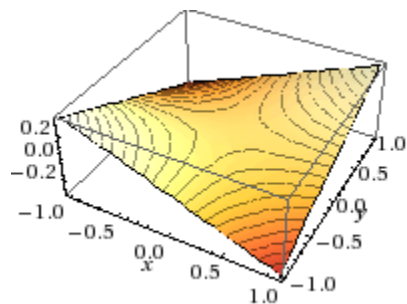
$$V = \frac{xy}{.35 \text{ mol} * 8.3145 \frac{\text{J}}{\text{mol} * \text{K}}}$$

3D Graph:



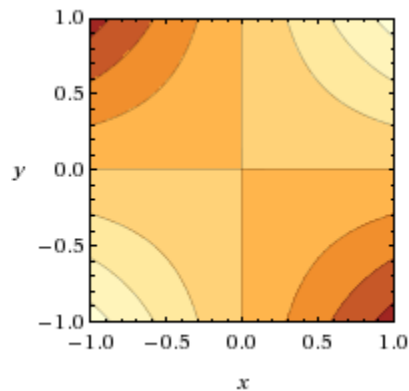
(<http://www.wolframalpha.com>)

3D Graph with Contour Lines Shown:



(<http://www.wolframalpha.com>)

Contour Plot:



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