Laboratory 1: Review of Programming User-Defined Function (v. 2.0)

BE 205-002, Winter '06-'07, Drs. Tritt & Richerson

Problem: Estimation of pressures given temperature and molar volume of gas in a container.

Assume we have some containers we wish to fill with certain biologically relevant gasses. It is our job to determine how much volume of gas we can fill the container with while not exceeding the pressure limit of that container.

The van der Waals equation is used to estimate the pressure exerted by a certain gas given the volume of that gas in a container. This equation states $P = \frac{RT}{V-b} - \frac{a}{V^2}$ where b is the correction term for the volume of the molecules and the term a/V^2 is a correction for the molecular attraction. The gas constant R = 0.08206 L-atm/mol-K. T is the absolute temperature in Kelvin. The values of “a” and “b” depends of the type of gas.

Gas	**a (L^2-atm/mol^2)**	**b (L/mol)**
Helium, He	0.0341	0.0237
Hydrogen, H_2	0.244	0.0266
Oxygen, O_2	1.36	0.0318

Write a function to determine the pressure on the basis of the van der Walls equations. Inputs to your function should be volume, temperature, a and b. Outputs should be the pressure.

In another m-file, ask the user to input the type of gas, the volume of gas (in liters/mole) and the temperature (degrees C). Using the table above, pass the correct values of a, b as well as the volume and temperature, to your function. Display the answer returned from your function. Use this answer returned from your function to determine if the pressure exerted exceeds 1 atm. If so, warn the user that the molar volume is too large for the specified conditions.

Laboratory requirements:

Provide (via e-mail, memory stick or CD) the instructor an electronic copy of your code (both your m-file and your function file) so that I can run the program myself. Please remember to comment your code properly. Also include a cover memo with a simple program description and program test results.

This laboratory is due prior to the next laboratory period. Grading rubric and test vectors are attached.

Grading Rubric

The below is the scoring that will be used for Laboratory 1. The scale is a 5 point scale with 5 being superior, 4 being satisfactory, 3 being average, 2 being unsatisfactory and 1 being not undertaken.

Function Requirements

Correct input arguments in function statement	1	2	3	4	5
Correct output arguments in function statement	1	2	3	4	5
Correct calculation of the pressure	1	2	3	4	5
Correct passing of answer back to program	1	2	3	4	5

Program Requirements

Correct assignment of constants	1	2	3	4	5
Accurate and concise input statement to prompt user	1	2	3	4	5
Accurate choices made to select correct “a” and “b”	1	2	3	4	5
Accurate calling and passing of variables to function	1	2	3	4	5
Accurate and concise output of pressure	1	2	3	4	5
Accurate determination if pressure exceeds maximum	1	2	3	4	5
Accurate and concise warning message to user if maximum is exceeded	1	2	3	4	5

Other considerations

Was code adequate tested and the testing document?	1	2	3	4	5
Did comments include student name, course, and description of the problem to be solved?	1	2	3	4	5
Did comments include all variables with units?	1	2	3	4	5
Were meaningful variable names used?	1	2	3	4	5
Was the code generally commented properly?	1	2	3	4	5

Comments:

Total possible points – 100

Points Earned –

Sample Test Vector

Sample Excel spreadsheet for calculating pressures –

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By Dr. C. S. Tritt

	a (l^2-atm/mol^2)	b (l/mol)	p (atm)	Term1	Term2
Helium	0.0341	0.0237	1.002	1.002	0.000
Hydrogen	0.2440	0.0266	1.001	1.002	0.000
Oxygen	1.3600	0.0318	0.999	1.002	0.003
Ideal	0.0000	0.0000	1.001	1.001	0.000

r =	0.08206	L-atm/mol-K
v =	22.40	liters/mole
t (deg. C) =	0.00	deg. C
t (K) =	273.15	K

Sample volumes, temperature and pressures calculated using spreadsheet –

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Volume (liter/mole)	22.4	30.0	3.0	300.0
Temperature (deg. C)	0	20.0	150.0	0.0
Pressures				
Helium	1.0016	0.8025	11.6629	0.0747
Hydrogen	1.0014	0.8023	11.6510	0.0747
Oxygen	0.9994	0.8012	11.5475	0.0747
Ideal	1.0007	0.8019	11.5746	0.0747