Engineering 14100
Flowcharting Post-Activity

Individual Assignment: See the course syllabus for a definition of this term.

Task 1 (of 1)

Objective: To demonstrate the individual ability to create flowcharts for complex algorithms

You are a chemical engineering co-op student working at the NASA Goddard Space Flight Center in the Earth Observing System (EOS) Program Office. You have been assigned to work with the Solar Radiation and Climate Experiment (SORCE) mission team. It's your first day on the job and you go to your new boss's office to introduce yourself. After she makes a brief "welcome aboard" statement, she invites you to a meeting with the planning team of engineers looking into the next generation of instrumentation they will be putting on a future satellite.

Upon your arrival, you are surprised to see a whole team of engineers seated at the conference table in your boss's office. She introduces you and a discussion ensues. After lengthy discourses by several engineers, dealing with things you have never heard about, you boss turns to you and says "Let's have our new intern work on designing two of the gas pressure vessels that will be used aboard the satellite. I will assist in getting things started."

After the meeting is over and everyone has left the office, she begins explaining that oxygen and carbon dioxide are needed to operate various instruments aboard the satellite. She tells you that in order to design the pressure vessels, you will need to estimate the molal volume (v) of carbon dioxide and oxygen for a number of different temperature and pressure combinations. You think for a moment and then blurt out that this is simply an application of the *ideal gas law*. On a piece of paper you write

$$\mathrm{pV} = \mathrm{nRT} \tag{1}$$

where p is the absolute pressure, V is the volume, n is the number of moles, R is the universal gas constant, and T is the absolute temperature. She says, "While the *ideal gas law* is widely used, it is only accurate over a limited range of pressures and temperatures. In addition, it is more appropriate for some gases than for others." She goes on to explain that an alternative equation of state for gases is given by the *van der Waals equation* and writes

$$\left(\mathrm{p} + \frac{\mathrm{a}}{\mathrm{v}^2}\right)(\mathrm{v} - \mathrm{b}) = \mathrm{RT} \tag{2}$$

where $v = V/n$ is the molal volume and a and b are empirical constants that depend on the particular gas. She explains that, for all of the various gasses to be stored on the satellite, the significant changes in temperature and pressure that are expected during operation of the satellite could produce wide fluctuations in the molal volume of the gas, which in turn could impact the performance of the instruments that depend on that gas for proper operation. **She explains one of the first things the team will need to know is how v will change, for a given gas, over a specified pressure range at a constant temperature. Therefore, she recommends you write a program (for which you should first write a**

flowchart) to compute *v* for a given gas and illustrate how it changes with pressure at a constant temperature. Some of the current operating specifications for the vessel include:

She then proceeds to rewrite eq. (2) such that

$$f(v) = \left(p + \frac{a}{v^2}\right)(v - b) - RT = 0 \tag{3}$$

She says finding a value for *v* that satisfies eq. (3), solves the problem, but also notes that solving explicitly for *v* is not possible. You also reason that it has to be a positive, real number or else the answer does not make much sense. Since this is nothing more than finding the root of an equation, you look up all the different methods that are available to do this and decide to use a method called the *Newton-Raphson method*. An excerpt from a book you found in the library describes the *Newton-Raphson method* as follows:

> Perhaps the most widely used of all root-locating formulas is the Newton-Raphson equation. If the initial guess of the root is x_i, a tangent can be extended from the point $[x_i, f(x_i)]$. The point where this tangent crosses the *x*-axis usually represents an improved estimate of the root.
>
> The Newton-Raphson method can be derived on the basis of this geometrical interpretation. As shown in the fig. 1, the first derivative at x_i is equivalent to the slope:
>
> $$f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$$
>
> which can be rearranged to yield
>
> $$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$
>
> and is commonly called the *Newton-Raphson formula*. This equation can be used in an iterative procedure until a converged solution (a root) is obtained. Convergences is determined by comparing a previous estimate to the root to the current estimate of the root, such that
>
> $$|\varepsilon| = \left|\frac{x_{i+1} - x_i}{x_{i+1}}\right| \leq \text{tolerance}$$
>
> where the tolerance is some small number.

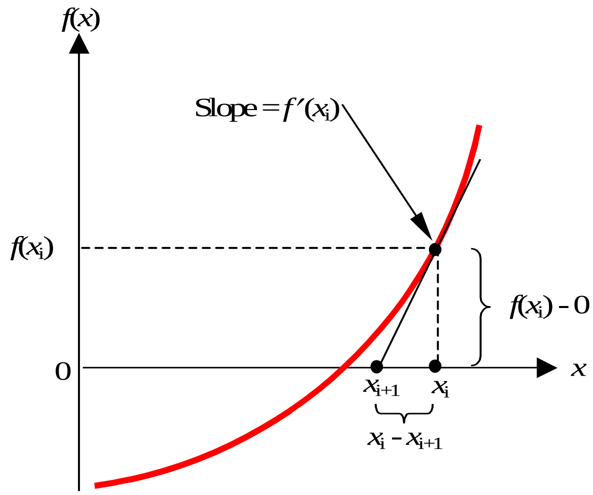

Fig. 1 Graphical depiction of the Newton-Raphson method.

For the particular problem at hand, you reason that application of the Newton-Raphson formula will yield something like the following

$$\text{for i} = 1: \quad v_2 = v_1 - \frac{f(v_1)}{f'(v_1)} \quad \rightarrow \quad |\varepsilon| = \left|\frac{v_2 - v_1}{v_2}\right| > \text{tolerance}$$

$$\text{for i} = 2: \quad v_3 = v_2 - \frac{f(v_2)}{f'(v_2)} \quad \rightarrow \quad |\varepsilon| = \left|\frac{v_3 - v_2}{v_3}\right| > \text{tolerance}$$

$$\text{for i} = 3: \quad v_4 = v_3 - \frac{f(v_3)}{f'(v_3)} \quad \rightarrow \quad |\varepsilon| = \left|\frac{v_4 - v_3}{v_4}\right| > \text{tolerance}$$

$$\vdots$$

$$\text{for i} = n - 1: \quad v_n = v_{n-1} - \frac{f(v_{n-1})}{f'(v_{n-1})} \quad \rightarrow \quad |\varepsilon| = \left|\frac{v_n - v_{n-1}}{v_n}\right| \leq \text{tolerance}$$

where the initial value v_1 is found using the Ideal Gas Law, and $f(v_1)$ and $f'(v_1)$ are the van der Waals equation and its derivative evaluated for molal volume v_1.

Now that you have the *Newton-Raphson method* figured out, you go to another reference book and find the empirical constants *a* and *b* (for both carbon dioxide and oxygen), as well as the universal gas constant. The values you found are the following:

$$R = 0.082054 \frac{L \cdot atm}{mol \cdot K}$$

Carbon Dioxide
a = 3.59200
b = 0.04267

Oxygen
a = 1.36000
b = 0.03183

You are now ready to design your algorithm. You first determine the required inputs for your algorithm:

Table 1. Input Data
Temperature (K)
initial pressure (atm)
final pressure (atm)
number of pressure increments
gas type
a (for a gas, if **not** carbon dioxide or oxygen)
b (for a gas, if **not** carbon dioxide or oxygen)
maximum number of iterations
convergence criteria/tolerance
Output file name

In addition, on a piece of engineering paper you write out what the output should look like. For example:

Temperature (K): 300.000
Pressure (atm): 100.000
Molal Volume (L/mol) (vdW): 0.0795108
Iterations: 10
Molal Volume (L/mol) (IGL): 0.2461620

Temperature (K): 300.000
Pressure (atm): 110.000
Molal Volume (L/mol) (vdW): 0.0772383
Iterations: 7
Molal Volume (L/mol) (IGL): 0.2237836
.
.
.
Temperature (K): 300.000
Pressure (atm): 200.000
Molal Volume (L/mol) (vdW): 0.0676846
Iterations: 7
Molal Volume (L/mol) (IGL): 0.1230810

If the Newton-Raphson method fails to converge after the maximum number of iterations, a value of 0.0 should be returned as the root along with the maximum number of iterations performed.

Specific Requirements:

Individually, develop an appropriate overall algorithm and several sub-algorithms (as specified) in the form of flowcharts to estimate the molal volume (*v*) of gas for a number of different temperature and pressure combinations based on the input data described in Table 1 using the *van der Waals equation* (eq. 2). If the gas type is not carbon dioxide or oxygen, the algorithm should indicate the constants *a* and *b* are also to be input. Lastly, from an input perspective, the algorithm should allow for input of the maximum number of allowable iterations and specification of a convergence criterion (see above). All other sub-algorithms that will allow for the calculation of the molal volume should be included.

Specifically, you must do the following:

1. Create a written problem statement describing the problem to be solved in your own words
2. Create a high-level flowchart (low detail) laying out the overall process to be used
3. Create a detailed flowchart of the overall process, using subroutines for each separate sub-algorithm
4. Create separate flowcharts for sub-algorithms that do the following:
    1) collect the input data
    2) compute the function $f(v_i)$
    2) compute the derivative $f'(v_i)$
    3) perform the Newton-Raphson method (including the convergence check)

    Finally, you recall that a high level of detail is appropriate for flowcharts to be used to structure the implementation of an algorithm in a computer program. You know that the logic to be included should be quite specific unless otherwise specified, as this will make the actual programming simpler.

Submit your work to the appropriate BlackBoard dropbox
Problem Statement and all flowcharts: `Flowcharting_PA_`*`login`*`.pdf`.