

van der Waals Gas Law for Real Gases Course Project Proposal

Background: The ideal gas law states that $PV = nRT$ where P is pressure, V is volume, n is the amount of gas, R is the ideal gas constant, and T is the temperature. Like many things in life, gases are rarely ideal. van der Waals developed a similar equation for real gases that takes into account two correction factors: the van der Waals correction, a , and a correction for the volume of individual gas molecules, b .

$$\left[P + \frac{an^2}{V^2} \right] (V - nb) = nRT$$

In 1976, DeSantis derived a relationship for the compressibility factor, z , of real gases:

$$z = \frac{1 + y + y^2 - y^3}{(1 - y)^3}$$

where $y = a/(4b)$.

Project: Develop a numerical software package that will approximate the missing value from (z, a, b) given the other two. You do not need to have a single function for all cases (although this will score a nontrivial bonus). This software must allow the user the option of at least three different numerical techniques. In addition, there should be one function that has at least quadratic convergence.

Paper: Write a paper detailing the mathematics behind your software including any mathematical preprocessing included in your algorithms. The paper should also include necessary background to state the problem, a concise statement of the problem being addressed, a description of the software package including an error analysis, tests on known data, and a performance comparison of the various functions in the package. A brief users guide (i.e. instructions on how to run your software) should be included as an appendix.

Presentation: At the end of the semester, your group will give a 7-10 minute presentation on this project.

Peer Evaluations: Peer evaluations will be emailed to me by the individuals. Each student will numerically rank the participation of the group members and provide a written account of who did what during the project. Each group member must write at least one routine in the project to receive any credit for the project.