Advanced Calculator Skills: Solver

Concepts

- Determining the volume of a van der Waal's gas

Materials

- TI-84 Plus

Overview

The Solver function on the TI-84 Plus is a powerful tool for solving complex equations. In this activity, the Solver will be demonstrated in determining the volume of a van der Waal's gas.

Introduction

The relationship between pressure, volume, and temperature of gases can in many cases be described by the ideal gas equation,

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

where P = pressure, n = number of moles,
R = 0.0821 L-atm/K-mol, T = temperature in Kelvin, and V = volume.

The ideal gas equation assumes that gas particles do not attract or repel one another and that gas particles themselves occupy no volume.

Under conditions of high pressure and/or low temperatures, these assumptions break down, and the behavior of real gases deviates from that given by the "ideal gas" equation.

The van der Waal's equation

$$P = \frac{nRT}{V - nb} - \frac{n^2a}{V^2}$$

is an improvement of the ideal gas equation. The parameter *a* gives an indication of the strength of attraction between gas particles, and *b* represents the volume occupied by a mole of gas particles.

With the van der Waal's equation, it is easy to calculate P if you know n, V, and T (and the van der Waal's parameters a and b), but much more difficult to determine V for a given n, T, and P.

Determining V requires solving a cubic equation:

$$P = \frac{nRTV^2 - n^2a(V - nb)}{(V - nb)V^2}$$

$$P(V - nb)V^2 = nRTV^2 - n^2a(V - nb)$$

$$PV^3 - nbPV^2 = nRTV^2 - n^2aV + n^3ab$$

$$PV^3 - (nbP + nRT)V^2 + n^2aV - n^3ab = 0$$

Let's look at CO_2 at 300 K for which a = 3.59 L^2-atm/mol^2 and b = 0.0427 L/mol. What is the volume of one mole of CO_2 at 100. atm?

If CO_2 were an ideal gas, determining the volume would be a very easy calculation. Rearranging the ideal gas equation gives

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

$$\frac{(1.00\text{ mol})(0.0821\text{ L - atm/K - mol})(300.\text{ K})}{100.\text{ atm}} = 0.246\text{ L}$$

Using the Solver to Determine the Volume of van der Waal's gas

1. Enter the van der Waal's equation into Y1.

- Press the [Y=] button.
- Use the [ALPHA] button and operation buttons to type NRT/(X–NB)–N^2A/X^2.
- Note that X is the volume variable. See Figure 1.

2. Enter the equation to be solved into Solver.

- Notice that there is no need to rewrite the equation in the form of a cubic equation.
- Press [MATH] [▲] to 0:Solver, and press [ENTER] (or you can simply press [0] after pressing [MATH]).
- If Figure 2 does not appear on the TI-84 Plus screen, scroll up until the words EQUATION SOLVER appear, and then press [CLEAR].

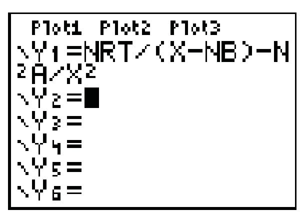

Figure 1

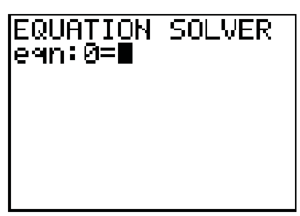

Figure 2

- Enter equation 0 = P – Y1 (to get Y1, press [VARS] [▸] [ENTER] [ENTER]). See Figure 3.

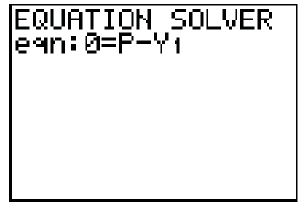

Figure 3

- Press [ENTER], and then type in the values of P, n, R, T, *a*, and *b*. See Figure 4.

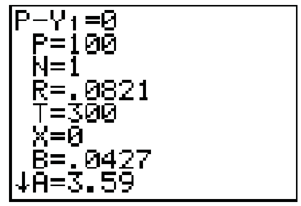

Figure 4

3. The volume for the ideal gas at 100 atm was 0.246 L. Enter this value as an initial guess for X (note X = volume). See Figure 5.

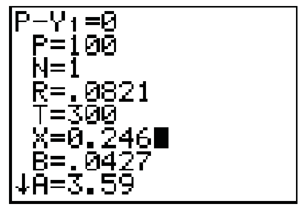

Figure 5

4. Press [ALPHA] [ENTER] (for [SOLVE]).

- Solver does a numerical search for the root of P – Y1 and finds the volume of a van der Waal's gas to be 0.0798 L. See Figure 6.
- Notice how much smaller V_{VdW} = 0.0798 L is compared to V_{ideal} = 0.246 L.

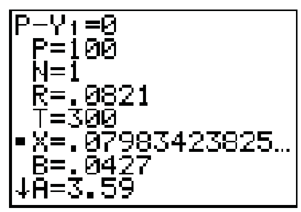

Figure 6

5. With Solver, you can solve for any of the parameters listed. For example, find the pressure for which the volume is equal to 0.100 L.

- Replace the X value 0.0798 with 0.100.
- Move up to P.
- Press [ALPHA] [ENTER] (for [SOLVE]). The result is P = 70.84 atm. See Figure 7.

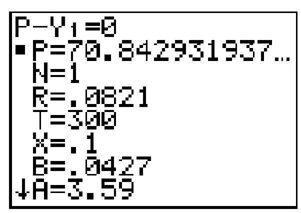

Figure 7