IDEAL GAS LAW - INTRO TO MATHCAD©

Created by
George Hardgrove
Chemistry Department
St. Olaf College
Northfield, MN 55057
hardgrov@lars.acc.stolaf.edu

Edited for Mathcad 8 by
Theresa Julia Zielinski
Monmouth University
400 Cedar Avenue
West Long Branch, NJ 07764
tzielins@monmouth.edu

Goal: To introduct students to Mathcad and some simple operations made possible by the software.

Objectives:

After completing this exercise you should be able to do the following with Mathcad:

1. Calculate the value of an independent variable from a simple equation where all the dependent variables are defined.
2. Calculate a series of values for an independent variable.
3. Prepare a simple 2D plot of dependent and independent variables.
4. Prepare a simple 3D plot of an independent variable and two dependent variables.
5. Explain the meaning of the axes in a 3D plot
6. Solve for a variable using symbolic mathematics
7. Differentiate a simple function with respect to one or another of the variables.
8. Do cut and paste operations in order to create equations as needed.

STUDENT INSTRUCTIONS: Welcome to MATHCAD! This program is a combination text editor and calculator. It could be used to write lab reports, lecture notes, etc. as any text editor can do, but it can also do calculations and even derive formulas which most text editors cannot do.

MATHCAD documents in this course come in sections (Some of the comments in this document are specific instructions for the St. Olaf students. Students at other campuses should follow the instructions of their own instructor.). The sections are::

1. A written set of instructions for a calculation (such as this one) with a filename ending in ...ins.mcd These instruction files are stored on the disk in case you need to print one out. It is a good idea to print this document so that you can use it while you are working with the executable worksheet for this assignment.

2. The actual calculations are done in a ...run file. The instructions in the gasins.mcd file are to help you perform the tasks in the file named gasrun.mcd.

3. If your calculations require tabulated data, these are often stored in .....PRN files.

So now let's get started. Find a computer with MATHCAD 8.0 available. On the program screen you should find an icon for Mathsoft app or Mathcad. With the mouse move the cursor to this icon and click on it. A new screen should appear and you then click on the MATHCAD PLUS 8.0 icon to start the program. A screen labeled Mathcad PLUS should appear with buttons at the top and an empty workspace.

At this point press the open file button (second from the left in the long row). Next select the disk drive (**c** for hard disk, **a** for floppy) where the MATHCAD programs documents are stored. Start the gasrun.mcd document. You can double-click, or click once on it and then click on the 'open' button to get the document to appear. At this point click on the 'View' menu and then on 'Regions'. You will note that each mathematical expression is in its own region, and that the sections of text are in their own regions. If you click on View, Regions again you return to the white page form of the document. You can edit in either form.

EXERCISE 1 (very easy)

You should note values of T, P, and V are given for a gas at what used to be called standard pressure and temperature. What units should be supplied to each of these quantities? Note the symbol := which appears in these expressions. This is the 'assign value' type of symbol - the values of the expressions on the right are assigned to the variables on the left. Press the F9 function key. This should cause the document to calculate values. Record the value for R. What are its units?

EXERCISE 2

Now we wish to calculate R in different units. Change the pressure to 101325 (in pascals) and the volume should correspond to m^3. 1 $m^3 = 10^3$ liters. To change a number place the cursor on the number. You may see a vertical line (called the insertion point) in among the numbers. You can eliminate characters to the left and right of the insertion point by pressing 'Backspace' or 'Delete.' Now type the new number. Press F9 to recalculate. What are the units of T, P, and V? What are the value and units for R? You should know how to associate units with a number. Place units on each of the state functions from Exercise 1. You can place units by just multiplying by the unit name. Check Mathcad's unit conventions in the Insert menu.

Subscripts

In the computational document we note the equation $V_i=RT/P_i$. For a given temperature T=300 K we wish to calculate values of V corresponding to a range of values for P. By typing i:=0..30 (Type a colon ':' to get the := symbol and type a semicolon ';' to get the ...) we choose to calculate values of P at 31 points. This is done on the next line where to get a subscript we typed '[' then the subscript immediately after the P, we then pressed the up arrow key to select the whole quantity rather than just the subscript. This means that we will have P values from 1 to 4 at intervals of 0.1. Next we calculate V_i for each value of P_i using the same technique for the subscript. Type P= and V= to see the arrays. Next we plot a graph of V vs. P. Do one or two calculations by hand with your calculator to check your work. Note well: do not confuse the variable index which is a step wise incremented variable with a subscript that is part of the name of a variable. They are created in two different ways and give two different results.

EXERCISE 3

Here you can test your understanding. Modify the computational document to calculate V for 21 temperatures from 200 to 400 K at a pressure of 1.00 atmosphere. Adjust the quantities on the graph to get the desired plot. You do the adjusting by clicking on the graph and then clicking on the axis label. Now you can change the label.

In the next part of the document you will see a 3-D plot where V is shown as a surface that is a function of P and T. Information about the 3D plot is included in the run document.

Next let's learn how to do simple symbolic operations with Mathcad. Go to page 3 of the **run** document.

Symbolic Operations

Solve for variable: Note the expression in the computational document 'PV=nRT'. (The type of equal sign in this expression, in bold, is the logical equal and to get it you type 'cntr =') To solve for V click on V, notice the blue outline below and to right of V. The means that V is now "selected." Then click on 'Symbolic', then 'variable' and then 'solve.' The answer will appear below the original equation.

To make this into an equation you need to select it and put it on the clipboard. You do this using the copy icon after surrounding the expression with the blue select lines. Click on the copy icon to put the expression on the clipboard. Then type 'Vcntr=' and then click on the paste button (9th from the left) and the expression will reappear.

Differentiate on Variable

Move the cursor down the page to an empty space and press either the 'paste' button or type 'cntr v'. The expression for V will then appear. Click on T to select it and drag the mouse to highlight the T in black. Then on the 'Symbolic' menu select 'Variable' and then 'Differentiate' and the derivative will appear below.

EXERCISE 4

Go back to the expression for V and find the derivative with respect to P.

You can add more lines to the page by pressing the 'Enter' button several time.

EXERCISE 5

Enter into the worksheet the equation PV=wRT/MP where w is the weight of the gas in grams and M is the molecular weight in grams/mole. Use the symbolic facility to solve for the molecular weight M. Find the derivative with respect to T. If the temperature of a gas sample should be 5 K too high calculate how far off the molecular weight will be.

Units

Note the illustration for units in the computational document. Units are considered quantities multiplied by the number. To enter 10 Kg you type '10' then * then press 'cntr u'. Usually you can find the units you are looking for in the right-hand column. Select the unit kg and then click on 'insert'.

EXERCISE 6

The root mean square velocity of a molecule is given by

$$vel := \sqrt{\frac{3 \cdot R \cdot T}{M}}$$

Set up the constants with their units and calculate the root mean square velocity for O_2. Hint: the square root sign is on the arithmetic pallet (the button that looks like a calculator). The values of constants with their units are: R=8.314 joule/(K*mole), T=300 K, and M=0.032 kg/mole.