# Recursion Method

In solving chemical systems, often equilibrium systems, it is sometimes necessary to solve expressions that are cubic or above or worse. Such equations can be solved by numerical solvers found in various programs. However, often these equations can be solved recursively. This method involves solving the desired equation for one of the variables and expressing it as an equation that still has the variables within the expression. One then makes a "guess" of the x within the expression and solves for the isolated x. One then takes the answer, replaces it back within the expression in place of the x as the new guess values to produce still another value for x. This is repeated until the answer produced matches the guess value entered to whatever degree of accuracy is desired.

For example, consider the expression: $1.6x10^{-4} = 4x^2(x + 0.0200)$

Here, I will select a convenient x on the right hand side for which to solve. The x I choose may be the x that is squared. Solving for that x, I get:

$$x = \sqrt{\frac{1.6x10^{-4}}{4(x+0.0200)}}$$

Now, see that there is still an x in the right hand side expression. This makes it impossible to find an answer because I have to know the answer to get the answer! To circumvent this, I will guess a value for x. If I guess "0" to start. I can then get a value for the expression. (Guessing "0" may not be the case in every instance. You intuition as to the what the answer should be close to will be helpful. This can be deduced from the problem that is being solved.) The equation then becomes:

$$x = \sqrt{\frac{1.6x10^{-4}}{4(0+0.0200)}} = 4.47 \text{ x } 10^{-2}$$

Now, the answer is not "0" as we guess. Therefore, I'll take my new value for x and use it as a new guess value. This produces the expression:

$$x = \sqrt{\frac{1.6x10^{-4}}{4(4.47 \text{ x } 10^{-2}+0.0200)}} = 2.49 \text{ x } 10^{-2}$$

Once again, the calculated number does not agree with the guess value. Thus, we repeat this process. This is continued until the number calculated matches the guess value. The nature of the equation and the quality of the guess wll combine to determine how many cycles you must perform in addition to your desired accuracy. For this equation, the successive answers are asa follows:

$4.47x10^{-2}$ $2.49x10^{-2}$ $2.99x10^{-2}$ $2.83x10^{-2}$ $2.88x10^{-2}$ $2.86x10^{-2}$ $2.87x10^{-2}$ $2.87x10^{-2}$.. Converged!

This process is easily accomplished in Excel or an alphanumeric scientific calculator. The instructions are given below.

## TI Calculator (and some others) Recursion Method

1.) In the calculator, enter the solution of the equation to be solved, as manipulated for the desired variable. Enter "0" for the initial guess explicitly.

Example: $1.6x10^{-4} = 4x^2(x + 0.0200)$

Solving for one of the x's in the numerator…

$$x = \sqrt{\frac{1.6x10^{-4}}{4(x+0.0200)}}$$

In your calculator, enter the right hand side of the expression above and put "0" in the place of the "x" in the radical.

2.) Hit "enter" to produce an answer.

3.) Hit "2nd" and "enter" to get your original expression back on the screen. Edit this expression, replacing the value of "0" with the keystrokes "2nd" and "Ans". This will bring your answer into the expression. You will see "Ans" within the equation on the screen.

4.) Hit "enter" repeatedly until the numbers you get back converge to a single answer.

For this example, you should get 4.47 x $10^{-2}$ as an initial answer. After executing steps 3.) and 4.) the answers, in order are found to be as listed above.

## Modifications for Casio Calculator (and some others)

For some calculator, recalling the equation is not necessary. Alter Step 3 as follows:

3.) Using the back arrow key, move the cursor to the "0" you entered in the place of "x" in Step 1.) Hit 2nd "Ans" key, replacing the "0" with "Ans". Hit enter and continue as above.

# Operation in Excel Spreadsheet

In Excel, follow the steps on a fresh sheet.

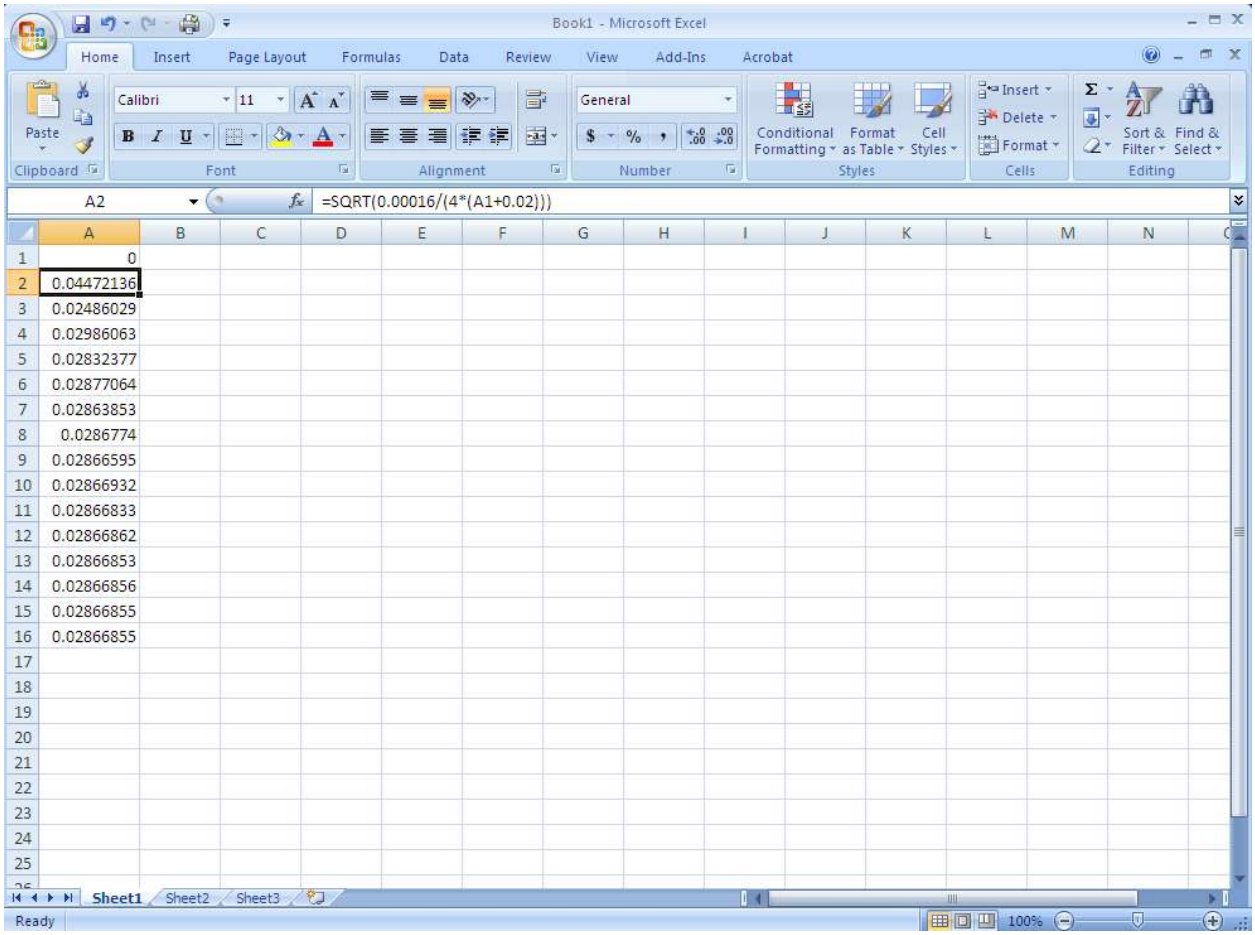
1.) Enter your initial guess in cell A1.
2.) In the next cell, enter your equation. Don't forget to begin with the "=" command to start. When you get to the "x" in the expression, replace that with the cell location number. In this instance, enter A1. For the example above, the cell should look as follows:

In cell A2, enter "=sqrt(1.6E-4/(4*(A1 + 0.0200)))

When you hit the "Enter" key, the number, $4.47 \times 10^{-2}$, will show up.

3.) Select and copy cell A2.
4.) Select cells A3 down as far as you like and hit "Paste"

You will see, in each successive cell, the recursed values. These values should converge to your answer. The screen will look as follows:




| | A |
|---|---|
| 1 | 0 |
| 2 | 0.04472136 |
| 3 | 0.02486029 |
| 4 | 0.02986063 |
| 5 | 0.02832377 |
| 6 | 0.02877064 |
| 7 | 0.02863853 |
| 8 | 0.0286774 |
| 9 | 0.02866595 |
| 10 | 0.02866932 |
| 11 | 0.02866833 |
| 12 | 0.02866862 |
| 13 | 0.02866853 |
| 14 | 0.02866856 |
| 15 | 0.02866855 |
| 16 | 0.02866855 |