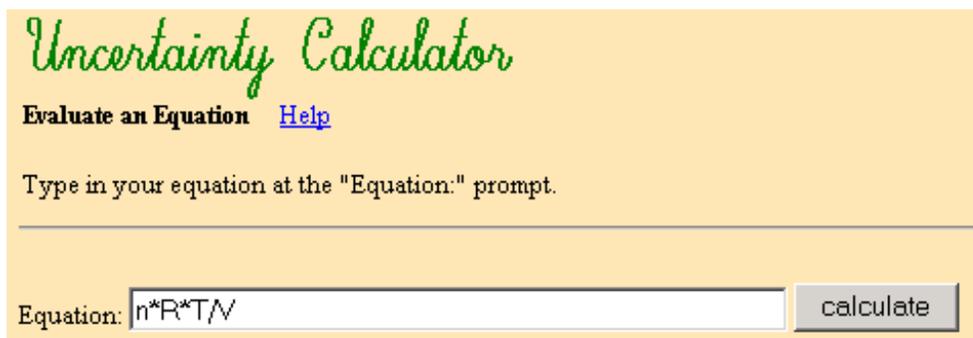# Uncertainty Calculator

Quick Start

The Error Calculator applet is a general purpose equation calculator. But, the real power of the Error Calculator program is that it does propagation of errors calculations. Lets start with a simple example. Assume that you wish to use the ideal gas law to calculate the pressure of a gas:

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

with   n=0.53 ± 0.02 mol
        T=298.2 ± 0.2 K
        V=10.12 ± 0.06 L

Start up the applet (http://www.colby.edu/chemistry/PChem/scripts/error.html) and then type the formula into the Equation box, without the equal sign as follows:

After pressing [calculate], the Variables window will be displayed:
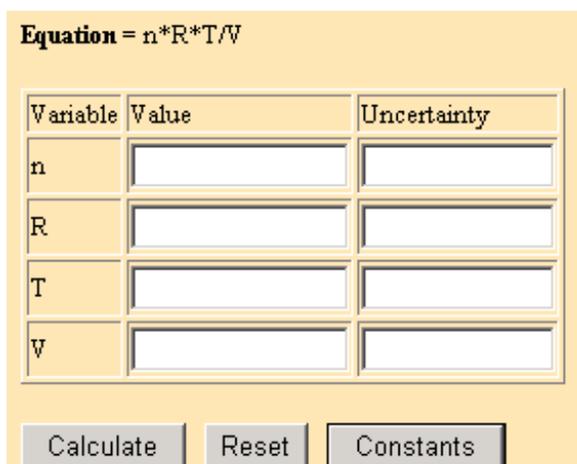
You then type in the values for the various parameters and their uncertainties. For example, you would type in 0.53 for n and 0.02 for the Uncertainty for n. The program also has available a table of constants and their uncertainties. Click the mouse in the R Value box, then click on the [Constants] button. The constants window will be displayed, as shown below.

☐ ao = 5.29177e-11 m	☐ π = 3.14159265359	
☐ c = 2.99792458e8 m s-1	☐ R = 8.31447 J mol-1 K-1	
☐ e = 1.60217733e-19 C	☐ R = 0.08205783 L atm mol-1 K-1	
☐ F = 9.6485309e4 C mol-1	☐ R_H = 2.1798741e-18 J	
☐ h = 6.6260755e-34 J sec	☐ To = -273.15 K	
☐ h/2π = 1.054573e-34 J sec	☐ 1 = 4.184 J/cal	
☐ hc/k = 1.43877 cm K	☐ 1 = 96.485309 kJ mol-1/eV	
☐ k = 1.38066e-23 J K-1	☐ 1 = 13.6057 eV/H	
☐ kT/hc = 207.226 cm-1	☐ 1 = 1e-10 m/Å	
☐ m_e = 9.1093897e-31 kg	☐ 1 = 2.54 cm/in	
☐ m_n = 1.6749286e-27 kg	☐ 1 = 1.609 km/mi	
☐ m_p = 1.6726231e-27 kg	☐ 1 = 0.4536 kg/lb	
☐ N_A = 6.0221367e23 mol-1	☐ 1 = 28.35 g/oz	
☐ P(atm) = 1.01325e5 Pa	☐ 1 = 0.9464 L/qt	

Clicking on the check box for the line that reads "R=0.08205783" will automatically enter the value and its uncertainty in the Variables window. After you type in the values for T and V the Variables window should appear as shown below:

Equation = n*R*T/V

Variable	Value	Uncertainty
n	0.53	0.02
R	0.08205783	1.0e-8
T	298.2	0.2
V	10.12	0.06

[Calculate]   [Reset]   [Constants]

Now if you click on the [Calculate] button the final result and its uncertainty will be displayed:

Equation = n*R*T/V

Variable	Value	Uncertainty
n	0.53	0.02
R	0.08205783	1.0e-8
T	298.2	0.2
V	10.12	0.06

Calculate   Reset   Constants

```
        Variable         Resultant
       Uncertainty       Uncertainty
n          0.02          +-0.04836
R          0.0           +-0.0
T          0.2           +-0.00086
V          0.06          +-0.00759

_____

Result = 1.282 +- 0.049 uncorrelated
                     +- 0.057 correlated
```

Your final pressure would be 1.282 atm with an uncertainty of ±0.049. See the Details section for a discussion of the propagated error for correlated variables.

Details

What are the allowable variable names?
Input your expression using a one or two character name for each variable that is uncertain. For example, the Clausius Clapyeron equation for the vapor pure of a pure liquid is:

$$\ln\left(\frac{P_2}{P_1}\right) = -\frac{\Delta_{vap}H}{8.314}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

To solve for $\Delta_{vap}H$, knowing P_1, P_2, T_1, and T_2, you would first rearrange to solve for $\Delta_{vap}H$:

$$\Delta_{vap}H = -\frac{\ln\left(\frac{P_2}{P_1}\right)8.314}{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

You would then type this into the program as:

LNe(P2/P1)*8.314 / (1/T2-1/T1)

Examples of valid variable names are A, df, and G6. The name must start with a letter. For two character names the second character can be a letter or a number. Variable names are not case

sensitive, that is "r" and "R" are the same variable. Remember that LOG is base 10 and LNe is base e. So use LNe(X) for ln(X).

How should I enter my equations?

The equation input syntax follows "BASIC" programming language rules. For example:

- ï Exponentiation is indicated by ^ or **, for example $V^2 = V\char94 2$.
- ï LOG() is base 10, LNe() is base e (or LNE)
- ï Allowed functions are ATN, COS, EXP, LNe, LOG, SIN, SQR, TAN. (ATN is arctan.)
- ï No implicit multiplication is allowed. For example ((X+Y)Z) is not allowed. Instead this expression should be written as ((X+Y)*Z). Another example is P = nRT/V, which would be typed in as n*R*T/V.
- ï Scientific notation: 1.23×10^{-3} is written as 1.23E-3.
- ï You can also clarify your equations by using parentheses. For example: ((X+Y)*Z) is different than X+Y*Z, because the multiplication is done first unless parentheses are present.
- ï Enter your equation without an '=' sign.

An example of a complex equation is the temperature dependence of the equilibrium constant. Lets assume we wish to evaluate K_2, knowing K_1, $\Delta_r H$, R, T_2, and T_1 in the equation:

$$\ln\left(\frac{K_2}{K_1}\right) = - \frac{\Delta_r H}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

You would first solve for K2:

$$K_2 = K_1 * e^{(-\Delta_r H \, / \, R*(1/T_2 - 1/T_1))}$$

You would enter Equation:

K1*EXP(-H/R*(1/T2-1/T1))

where H is used for $\Delta_r H$.

What kind of errors or uncertainties should I input?

   The uncertainties you input can be standard deviations, confidence limits, or just rough guesses. The final calculated uncertainty will be on the same basis as the input uncertainties. For example, if you input standard deviations for the Uncertainties, the final propagated uncertainty will be a standard deviation. If you input rough guesses, the final uncertainty will be just as rough a guess.

Why does the program list two different uncertainties?

   If the variables are uncorrelated, the uncertainty of the result is the "uncorrelated" uncertainty. Uncorrelated means that the error in one variable is not related to the error in another variable. For example, in P=nRT/V if the errors in T and V both tend to be positive or negative together then the errors would be correlated. If the variables are correlated, the ëuncorrelated" uncertainty is not valid, only an upper limit on the uncertainty can be specified. This upper limit is listed as the "correlated" uncertainty. The uncorrelated uncertainty is calculated with the variance:

$$\partial^2 f = (\frac{\partial f}{\partial x})^2 \partial^2 x + (\frac{\partial f}{\partial y})^2 \partial^2 y + ... \qquad (1)$$

The maximum uncertainty, which is listed as the "correlated" uncertainty, is

$$\partial f = \left|\frac{\partial f}{\partial x}\right| \partial x + \left|\frac{\partial f}{\partial y}\right| \partial y + ... \qquad (2)$$

What is the Resultant Uncertainty *column in the output?*
After clicking on [Calculate] the third column in the output is labeled "Resultant Uncertainty."
This column is the contribution to the error in the final result caused by the particular variable.
For example, in the P=nRT/V problem, above, the largest contribution to the error in P is from the
uncertainty in n, at ±0.048. Scanning this column then tells you what the predominate source of
error is for your experiment.

How accurate are the error calculations?
   The derivatives in Eqs. 1 and 2 are calculated in a very approximate manner in this program.
However, we usually only have rough guesses for the errors in our experimental values, so any
error in the calculations in Eq. 1 or 2 are unimportant by comparison. Therefore, the calculations
will be close enough for an error analysis.

A Complete Example

An example of a common calculation is the temperature dependence of the equilibrium constant.
Lets assume we wish to evaluate $\Delta_r H$, knowing K_2, K_1, R, T_2, and T_1 in the equation:

$$\ln\left(\frac{K_2}{K_1}\right) = - \frac{\Delta_r H}{R} \left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

where $K_1 = 0.0322 \pm 0.0007$ at 298.2 and $K_2 = 0.473 \pm 0.006$ at 353.2 K with $\delta T = \pm 0.2$ K. (This is
the same algebraic form as the Clausius Clapeyron example above.)
Solving for $\Delta_r H$:

$$\Delta_r H = - \frac{R \ln\left(\frac{K_2}{K_1}\right)}{\left(\frac{1}{T_2} - \frac{1}{T_1}\right)}$$

R can be entered by clicking on the constants button. The units are J/mol. Here is the result:

Equation = -R*lne(K2/K1)/(1/T2-1/T1)

Variable	Value	Uncertainty
R	8.31447	1.0e-5
K2	0.473	0.006
K1	0.0322	0.0007
T2	353.2	0.2
T1	298.2	0.2

[Calculate]   [Reset]   [Constants]

```
        Variable            Resultant
        Uncertainty         Uncertainty
R           0.00001         +-0.05146
K2          0.006           +-201.84362
K1          0.0007          +-345.75682
T2          0.2             +-131.30615
T1          0.2             +-184.34316

Result = 42780 +- 460 uncorrelated
                 +- 860 correlated
```

You would give the final result as 42.8 ± 0.5 kJ/mol.

Installation

You can save the applet on the hard drive of your computer for use at any time, even if you are not on the network. From the ì http://www.colby.edu/chemistry/PChem/scripts/î directory, copy the error.html and constants.html files to a directory on your computer. Then double clicking on the error.html file icon will start the applet. Or, from your browser pull down the File menu and choose OpenÖ