Simplify Uncertainty Analysis Using Excel Macros

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Introduction

Estimating and reporting reliability in experiments and calculations is an important part of engineering design and analysis. Reporting results from calculations and experiments without some estimation of reliability may invalidate our results. To illustrate, if we report a volume from designing a chemical reactor without taking into account the uncertainty in the design parameters, we risk under sizing a cooling system, which can have catastrophic consequences for exothermic runaway reactions. One measure of reliability comes from uncertainty analysis. Chemical engineering students learn simple concepts of experimental error and uncertainty analysis in physics and chemistry labs. Their first impressions and experiences with uncertainty are not positive. In some cases, this is their first taste of statistics. Students find the process tedious, labor intensive, and sometimes irrelevant in the context of their limited science and engineering experience. When we bring up the topic of uncertainty analysis in our engineering labs, students groan in anticipation of the laborious, monotonous calculations.

To reinforce the principles of uncertainty analysis and provide students with tools for uncertainty calculations that help to alleviate their anxiety, we have incorporated uncertainty analysis earlier in our program in a one-semester required course on computational methods for engineering problem solving. Our students typically take this course in the second half of the sophomore year, about mid way through their chemistry and engineering lab sequences. Prior to our computational methods course, students receive a basic introduction to descriptive statistics and uncertainty in their chemistry and physics courses. Most students in the course have also completed another course on statistical design of engineering experiments.

In our computational methods course, we introduce students to concepts of random and systematic uncertainty in measurements, degrees of freedom, propagation of uncertainty, and expanded uncertainty (confidence intervals). We outline a recipe for uncertainty analysis and develop spreadsheet tools to simplify the implementation. We use a simple, hands-on classroom demonstration to generate experimental data and help students experience the differences between uncertainties in analog and digital measuring instruments. The example involves calculating the density of an object from replicated measurements of dimensions and weight. The students first perform the steps of uncertainty analysis in an Excel worksheet to experience the calculations "by hand."

In a follow-up class-exercise, students create an Excel macro that calculates the expanded propagation of uncertainty according to the conventional Guidelines for Analysis of Uncertainty in Measurements (GUM).[1] The macro incorporates basic programming methods of loops, logical statements, input and output, user functions and subroutines. Students finish the course with a deeper understanding and appreciation of their responsibility for reporting reliability of results in terms of uncertainty. They also move on equipped with tools for simplifying the

implementation of uncertainty analysis for most situations they will encounter in their undergraduate experience.

Recipe for Basic Uncertainty Analysis

In an interactive lecture, we derive the well-known principles of uncertainty analysis from Taylor series analysis.[2] We also present case studies to promote the value of uncertainty analysis, including an example of a nuclear reactor.[3] For brevity in this paper, we skip theories of uncertainty analysis that are readily available in the literature and outline a simple recipe for students to follow when calculating the propagation of uncertainty through their engineering calculations. The reader is encouraged to review the literature for background information on uncertainty analysis.[4] The recipe presented here is limited by the assumptions of normally distributed random errors in replicated measurements with no bias or correlation between independent variables. We also assume that systematic errors are uniformly distributed between the limits of precision the measurement. Students learn to reduce bias and correlation between independent variables by careful calibration of instruments and randomization of experiments. Equation (1) summarizes the functional relationship between inputs, x (e.g., experimental measurements), and the output, y:

$$y = f\left(x_1, x_2, \ldots\right) \tag{1}$$

The function, f, represents any series of calculations that incorporates the input values from experimental measurements needed for obtaining y. The following calculation steps are illustrated in an example.

1. Model the uncertainty in the inputs form the combined effects of random and systematic errors:

$$x = \bar{x} \pm u_x \tag{2}$$

   where $\bar{x}$ is the expected value for x calculated from the mean value of n replicated measurements

$$\bar{x} = \frac{1}{n}\sum x \tag{3}$$

   and u_x is the combined uncertainty due to random (u_R) and systematic (u_Z) errors in the measured values:

$$u_x = \sqrt{u_R^2 + u_Z^2} \tag{4}$$

2. Assume random errors are normally distributed and use the standard error in Equation (5) for the random uncertainty in terms of the standard deviation s, and the sample size, n:

$$u_R = \pm \frac{s}{\sqrt{n}} \tag{5}$$

   Students discover that they may reduce the random uncertainty in Equation (5) by taking more measurements. However, this revelation is tempered by Equation (4) when they

realize that systematic uncertainties are always present for any measurement due to the limitations of precision in our instrumentation.

3. Assume that systematic errors are uniformly distributed between the limits of readability of the instrument of measurement, δ:

$$u_Z = \pm \frac{\delta}{\sqrt{3}} \qquad (6)$$

4. The conventional method for calculating the propagation of measurement uncertainty employs the law of uncertainty propagation (ignoring parameter correlation):

$$u_y = \sqrt{\sum_i (c u_x)_i^2} \qquad (7)$$

where c is the sensitivity coefficient, defined as the partial derivative of the function with respect to x evaluated at the mean value:

$$c = \left. \frac{\partial f}{\partial x} \right|_{\bar{x}} \qquad (8)$$

5. Finally, calculate the expanded uncertainty to give a level of confidence for the interval of uncertainty by multiplying the standard uncertainty by the 95% coverage factor, or Student t-statistic:

$$U_y = \pm t_{95\%, v_y} u_y \qquad (9)$$

where the degrees of freedom, v_y, are calculated from the Welch-Satterthwaite formula[1]:

$$v_y = \frac{u_y^4}{\sum \left[\frac{(c \cdot u_x)^4}{v_x} \right]} \qquad (10)$$

The degrees of freedom for each variable in Equation (10) are also calculated from the reduced form of the Welch-Satterthwaite formula assuming infinite degrees of freedom for systematic errors, and n-1 degrees of freedom for the mean value:

$$v_x \cong \frac{(n-1) u_R^4}{u_x^4} \qquad (11)$$

After working through the recipe, you may experience the same anxiety that our students report about uncertainty analysis, and have your own questions about the need for it. Although the "ingredients" of the calculations appear complicated and tedious to implement, the ubiquitous spreadsheet software Excel is primed to carry out these steps with relative ease using built-in statistical functions and macros. We illustrate the implementation of the recipe with a simple exercise that students complete in a 50-minute class period using easily obtained materials and measuring instruments. A second class period is used to provide students with Visual Basic for Applications (VBA) macros designed to simplify and automate the analysis in an Excel worksheet.

Classroom Exercise: Calculation of Wood Density

A simple classroom experiment was devised to allow students to generate random and systematic data for calculating the density of a wood sample from the dimensions of rectangular wooden blocks with a cylindrical hole drilled through their centers, as shown the schematic of Figure 1. Prior to the class, the instructor makes 12 rough copies of the small wood blocks from the same piece of wood, with slight deviations from the mean values of each dimension to introduce noise into the experimental data.
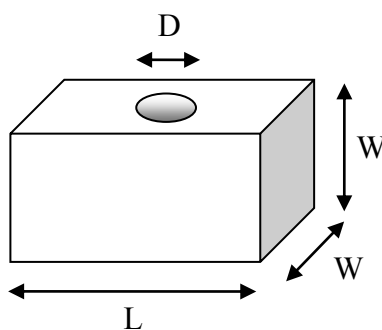

Figure 1 Schematic of wooden block with length L, width W, and hole diameter D.

This example extends the simpler exercise proposed by Yates, who distributed sheets of paper with hand-drawn rectangles to chemistry students for measuring the circumference and area.[5] The chemistry students used a ruler to measure the lengths of the sides of the rectangle. In our labs, however, students use combinations of analog and digital meters for collecting data. By extending the exercise to a density calculation, we allow for two different types of instruments of measurement. We also limit the number of measurements to four, which forces students to assume that the widths of the cross section are equal, a uniform hole diameter, and that the length of the hole is equal to the width of the block.

Students first derive an expression for the density of the block from the ratio of the mass to volume in terms of mass (m), length (L), width (W), and diameter (D).

$$\rho = \frac{m}{V} \tag{12}$$

The volume is calculated from the dimensions of the block:

$$V = W\left(LW - \frac{\pi D^2}{4}\right) \tag{13}$$

Students form teams with a minimum size of three. Each team is provided with a similar block of wood, an inexpensive plastic ruler for measuring length dimensions, and a portable digital scale for measuring the mass, as shown in Figure 2.
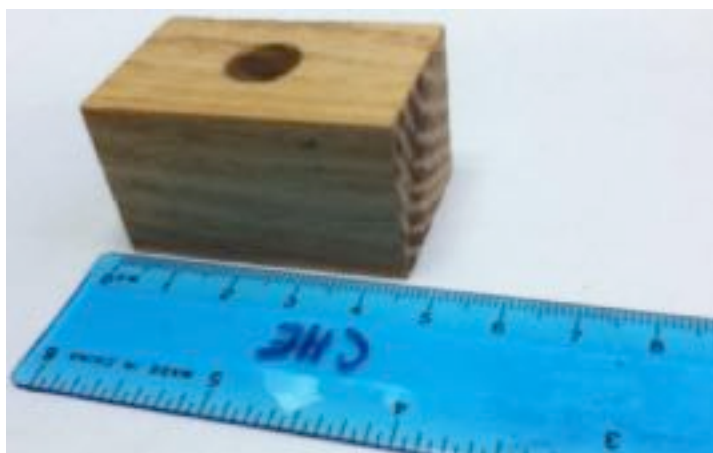
| | (a) | | (b) |

Figure 2 (a) Analog ruler for measuring length dimensions. The precision is 0.1 cm. The readability is ±0.05 cm. (b) Digital scale for measuring mass in grams. The precision is 0.1 gm, with a readability of ±0.05 gm.

The ruler serves as a simple example of an analog instrument. Students must visually interpolate between the graduation marks on the scale for a measurement reading. Examples of analog instruments in our labs include liquid thermometers, titration pipettes, Bourdon tube pressure meters, rotameters for fluid flow rates, manometers, and barometers. The electronic balance is an example of a digital meter that interpolates the signals for the student. Examples of digital meters in our labs include conductivity meters, refractometers, thermocouple digital thermometers, pressure guages, flow meters, and humidity meters, to name a few.

	A	B	C	D	E
1	Team	L(cm)	W (cm)	D (cm)	m (gm)
2	1	4.6	2.65	1.12	18.4
3	2	4.6	2.75	1.15	19.4
4	3	4.5	2.6	1	18.7
5	4	4.6	2.85	1.1	18.8
6	5	4.5	2.7	0.9	18.6
7	6	4.5	2.7	0.9	19.2
8	7	4.45	2.71	0.96	18.4
9	8	4.6	2.6	1.1	19.8
10	9	4.6	2.7	0.95	18.6
11	10	4.6	2.75	1	18.9
12	11	4.65	2.7	1.1	18.9
13	12	4.6	2.75	0.95	18.7

Figure 3 Student derived experimental data for wooden block dimensions.

The student teams pool their measurement results and record the values in an Excel worksheet, like Figure 3. Although this is a student-team exercise, each individual student saves a copy of the Excel worksheet for personal reference and use later in the program and future lab courses.

The precision of the graduation marks on the ruler is 0.1 cm, but students report the readability of the ruler as ranging from ±0.05 cm down to ±0.025 cm (depending on a student's confidence in his or her ability to interpolate the scale). The precision and readability of the digital balance scale is 0.1 gm, for a uniform systematic uncertainty of ±0.05/√3 gm. With this information, students are able to calculate the combined uncertainty in each variable using worksheet functions. To illustrate, we refer to the data for the measurement of length (L) of the block listed in column B on the Excel worksheet, shown in Figure 3. Table 1 contains a summary of the measurement uncertainty calculations including the Excel formulas and worksheet functions for L.

Table 1   Excel formulas for calculating measurement uncertainty.

Variable	Symbol	Excel Worksheet Function	Result
Average Length	L	= AVERAGE(B2:B13)	4.57 cm
Number of measurements	n	= COUNT(B2:B13)	12
Average DoF (n-1)	DoF	=B15-1	11
Standard Deviation	s	=STDEV(B2:B13)	0.06155 cm
Random Uncertainty	u_R	=B17/SQRT(B15)	0.0178 cm
Systematic Uncertainty	u_Z	=0.025/SQRT(3)	0.0144 cm
Combined Uncertainty	u_x	=SQRT(B18 + B20)	0.0229 cm
Combined DoF	v	=(B15-1)*(B21/B18)^4	30

The volume and density of the wood are calculated from the average values for the dimensions and mass in Equations (12) and (13). Figure 4 shows the results in the Excel worksheet. The uncertainty analysis uses these values for evaluating the derivatives in the sensitivity coefficients.

	A	B		B
33	V/cm³	31.21	33	=C14*(C14*B14-PI()*D14^2/4)
34	ρ/(gm/cm³)	0.605	34	=E14/B33

Figure 4   Wood block volume and density values and formulas in column B evaluated at the average values for the experimental measurements of L, W, D, and m.

The analytical formulas for the sensitivity coefficients are listed in Equations (14) to (17):

$$c_L = \frac{\partial \rho}{\partial L} = -m\left(\frac{W}{V}\right)^2 \tag{14}$$

$$c_W = \frac{\partial \rho}{\partial W} = -m\left[\frac{1}{WV} + \frac{LW}{V^2}\right] \tag{15}$$

$$c_D = \frac{\partial \rho}{\partial D} = \frac{\pi DWm}{2V^2} \tag{16}$$

$$c_m = \frac{\partial \rho}{\partial m} = \frac{1}{V} \tag{17}$$

The results for c using the average values of the variables are shown in row 23 of the Excel worksheet in Figure 5.

	A	B	C	D	E
14	x_{ave}	4.57	2.71	1.02	18.87
15	n	12	12	12	12
16	DOF	11	11	11	11
17	s	0.0615	0.0690	0.0900	0.4163
18	u_R	0.0178	0.0199	0.0260	0.1202
19	δ	0.025	0.025	0.025	0.050
20	u_z	0.0144	0.0144	0.0144	0.0289
21	u_x	0.0229	0.0246	0.0297	0.1236
22	v	30.31	25.61	18.84	12.31
23	c analyial	-0.1417	-0.4628	0.0839	0.0320
24	c finite difference	-0.1417	-0.4628	0.0839	0.0320
25	c macro	-0.1417	-0.4628	0.0839	0.0320

Figure 5 Measurement uncertainty and sensitivity coefficients for the wood density exercise, evaluated in an Excel worksheet.

Unlike the simple linear derivative results of the perimeter and area of a rectangle in the uncertainty exercise of Yates [5], the derivative formulas for density in terms of mass and block dimensions are nonlinear, and prone to formulation errors in a worksheet calculation. At this juncture, it is important to remind the students that uncertainty analysis is "uncertain." High precision calculations for the sensitivity coefficients are unnecessary. We can take our first step toward simplification of the process of uncertainty analysis by introducing first-order, finite difference approximations for the derivatives of the sensitivity coefficients.

$$c_i = \frac{\partial \rho}{\partial x_i} \cong \frac{\rho(x_i + \varepsilon) - \rho(x_i)}{\varepsilon} \tag{18}$$

where ε is a small value used to perturb the average value of a variable in the formula for density. The perturbation value must be small relative to the magnitude of the variable. In our exercise, a value of $\varepsilon = 10^{-4}$ is sufficiently small to yield good values for the sensitivity coefficients of each variable. We use a VBA user function of the density to simplify the calculations in a worksheet.

```
Public Function DENS(L, W, D, m)
      DENS = m / (L * W ^ 2 - W * WorksheetFunction.Pi() * (D / 2) ^ 2)
End Function
```

We use the following worksheet formula to illustrate the calculation of the sensitivity coefficient relative to the wood block length measurement using finite difference derivative approximation:

$$B24 = (DENS(\$B\$14 + 0.0001, \$C\$14, \$D\$14, \$E\$14) - DENS(\$B\$14, \$C\$14, \$D\$14, \$E\$14))/0.0001 \quad (19)$$

By using absolute worksheet cell references for the average values of the variables, we can fill the formula in Equation (19) across the row of cells in the worksheet for each variable. Then, we simply change the addition of the perturbation value for each variable in turn to get the complete set of sensitivity coefficients. The values in rows 23 and 24 compare the results from the analytical formulas to the finite difference approximations where we observe good agreement. Finite difference derivative approximations become important for obtaining good sensitivity coefficients for complicated calculations that involve multiple mathematical operations between the inputs to the output. For working with more complicated problems, we help the students write a VBA macro like the listing in Figure 6 to automate the evaluation of the sensitivity coefficients.

Students create their macros in the same workbook that contains their worksheet for uncertainty analysis of the wood density calculations. The macro employs input boxes for selecting the ranges of data and writing the results on the worksheet. The algorithm cycles through the variables perturbing the average values one at a time to calculate the derivative approximation. The average value of the variable is reset to its original cell contents before perturbing the next variable for partial derivative evaluations. By default, Excel worksheets automatically recalculate the value of the density function for each small change in the variables. Be sure to turn on automatic calculations if it is not previously set in the Excel worksheet.

```
Public Sub dfdx()
' Calculate sensitivity coefficients from
' finite difference derivative approximations

' Get input from the worksheet
Set x = Application.InputBox(Type:=8, Prompt:="Range of average variables:")
Set f = Application.InputBox(Type:=8, Prompt:= "Cell with function result:")
Set sc = Application.InputBox(Type:=8, _
         Prompt:="Range of sensitivity coefficients:")

' Specify number of variables, perturbation factor & save function value
n = x.Count: eps = 0.0001: fi = f

' Loop through variables to calculate sensitivity coefficients
For j = 1 To n
    temp = x(j).Formula      ' save worksheet formula for average variable j
    x(j) = x(j) + eps        ' perturb value of variable j in worksheet
    sc(j) = (f - fi) / eps   ' calculate sensitivity coefficient for j
    x(j) = temp              ' replace value/formula of j in worksheet
Next j
End Sub
```

Figure 6   VBA macro for calculating sensitivity coefficients in an Excel worksheet.

With the sensitivity coefficients, we now have all of the information needed to calculate the propagation of the uncertainty in the measurements for the variables (L, W, D, and m) through the calculation of density. First, we calculate the standard uncertainty from the law of propagation of uncertainty. Figure 7 shows the values for the product of the sensitivity coefficient and combined uncertainty required by Equation (7).

	A	B	C	D	E
26	$c \cdot u_x$	-0.003245	-0.011378	0.002493	0.003961
27	$(c \cdot u_x)^2$	1.05E-05	1.29E-04	6.22E-06	1.57E-05
28	u_y	0.013			

Figure 7   Excel worksheet calculation of standard uncertainty

The results for the square of the product $(c \cdot u)^2$ guide the student in identifying which variable(s) contribute most to the uncertainty in y. We find that the contribution from the width measurement in column C is larger than the other variables by at least an order of magnitude. We can take steps to reduce the uncertainty in the width by taking more measurements, or using a higher precision ruler. We report the density with standard uncertainty as

$$\rho = 0.605 \pm 0.013 \; gm/cm^3 \; \left(\text{standard uncertainty}\right) \tag{20}$$

Some practitioners recommend the retention of just one significant figure in the uncertainty, rounded up for $\rho = 0.61 \pm 0.02 \; gm/cm^3$.

Finally, students calculate the expanded uncertainty for a 95% confidence interval. We need the degrees of freedom from the Welch-Satterthwaite formulas in Equations (10) and (11). Table 2 summarizes the worksheet formulas and functions for calculating the propagation of uncertainty and coverage factor. Note how we rounded the result for the combined degrees of freedom down to the nearest integer value for a conservative value of the coverage factor:

Table 2 Excel worksheet formulas for calculating the propagation of uncertainty in the wood density exercise.

Variable	Symbol	Excel Worksheet Function	Result
Standard Uncertainty	u_y	=SQRT(SUMSQ(B26:E26))	0.013 gm/cm^3
Degrees of Freedom	v_y	=ROUNDDOWN((B28^4)/(SUM(B29:E29)),0)	38
Coverage Factor	t	=TINV(0.05,B30)	2.02
Expanded Uncertainty	U_y	=B28*B31	0.026 gm/cm^3

We now have the expanded uncertainty for wood density:

$$\rho = 0.61 \pm 0.03 \; gm/cm^3 \; (95\% \, confidence) \tag{21}$$

or

$$\rho = 0.61 \; gm/cm^3 \pm 5\% \; (95\% \, confidence) \tag{22}$$

	A	B	C	D	E
29	$(c \cdot u_x)^4 / v$	3.66E-12	6.54E-10	2.05E-12	2.00E-11
30	v_y	38			
31	t	2.024394			
32	U_y	0.026			

Figure 8 Excel worksheet with results for expanded uncertainty in density.

Jitter Macro

A VBA macro JITTER that automates the complete recipe for uncertainty propagation is provided to the students. [6] The macro incorporates the VBA code from the student-generated macros from the class exercises. To use the macro, students must set up a worksheet with a cell containing the final value of the function ultimately calculated from the average values of experimental inputs. In addition, the worksheet must include ranges of values for the average variables, random uncertainties, readability, and degrees of freedom. In most cases, the degrees of freedom for averaged values are the number of replicated experiments, less one (n-1). An example of a different number of degrees of freedom is the use of least-squares regression parameters, such as the slope or intercept of a line, where the degrees of freedom is the number of regression data points less two. The macro uses input boxes to prompt the user for the

required information. The input boxes displayed in Figure 9 show the cell and range addresses used for the wood density exercise.

Figure 9   JITTER macro input boxes with worksheet ranges for wood density exercise.

The JITTER macro output for our class exercise in Figure 10 shows the absolute and relative expanded, standard, and maximum uncertainties. In addition, the output includes the sensitivity coefficients and contributions from each variable to the propagation of uncertainty. We see that variable 2, corresponding to width, contributes approximately 80% of the uncertainty and should be a target for refining the experiments to reduce uncertainty in our density calculation.

$U_{95\%} = \pm$	2.6E-02	$= \pm$	4.261%
$U_{max} = \pm$	2.1E-02	$= \pm$	3.486%
$u = \pm$	1.3E-02	$= \pm$	2.105%
$t_{95\%} =$	2.02	DOF =	38
$c_1 =$	-1.42E-01	$(c \cdot u_1)^2 =$	6.50%
$c_2 =$	-4.63E-01	$(c \cdot u_2)^2 =$	79.97%
$c_3 =$	8.39E-02	$(c \cdot u_3)^2 =$	3.84%
$c_4 =$	3.20E-02	$(c \cdot u_4)^2 =$	9.69%

Figure 10 Results from macro JITTER for the propagation of uncertainty in the wood density exercise.

Results

Students develop tools in these exercises that are applicable to a wide variety of problems involving uncertainty analysis in their remaining course work, but particularly in our program's lab courses. Armed with an understanding of the basic assumptions and data requirements, students may use other software tools for uncertainty analysis available freely on the internet or commercially.

We evaluate our students' ability to transfer the recipe and tools for analysis of a new exam question where they are allowed to use their Excel worksheets and macros from the class exercises. We find that over 90% of the students are able to transfer their skills from class in the exam.

We are also beginning to see improvements in uncertainty analysis by students in our lab courses. Evidence includes an increased discussion and application of analysis of uncertainty in lab reports. Students are also careful to include estimates of uncertainty in all final reported values. Although we warn the students that they will need these tools in courses later in the program, some students are in the habit of compartmentalizing their learning. Once they are finished with the computational methods course, they do not automatically make the connection of applying the recipe later in the program. However, when we provide them with a copy of the Excel worksheet and macros from the wood density exercises, they are able to quickly relearn and apply these skills.

In one particularly complicated lab analysis, students use the macro to estimate the uncertainty in the calculation of chemical equilibrium constants. Experimental measurements of volume and mass to calculate reagent concentration and extent of reaction are fed into a worksheet set up to perform a complex series of stoichiometric mass conservation calculations to arrive at a value of the equilibrium constant. These calculations may be spread across multiple worksheets. Propagating the uncertainty through this involved series of calculations by hand is tedious and prone to mistakes. The JITTER macro efficiently performs the analysis requiring little effort setting up the worksheets for the macro inputs. The students also appreciate the additional VBA programming skills developed as part of this exercise and report using this additional skill in academic and industrial settings.

Conclusions

A simple hands-on active-learning exercise provides students with experience collecting and analyzing experimental data with random and systematic uncertainties. Students create an Excel worksheet that serves as a template of a recipe for calculating the propagation of measurement uncertainty in engineering analysis. This worksheet template, coupled with VBA macros, gives the students powerful tools for including measures of reliability in their calculated results. By making the process simple, relatively easy, and painless, students who formerly avoided uncertainty analysis are now more willing and able to conduct proper uncertainty analysis.

Similar tools may be developed in other computational tools, such as Mathcad or Matlab. However, we focus on Excel knowing that most of our graduates will have access to this software and make extensive use of it for engineering calculations wherever they are employed.

Nomenclature

c	=	sensitivity coefficient
D	=	diameter, cm
f	=	relationship between input variables and output variable
L	=	length, cm
m	=	mass, gm
n	=	number of replicated measurements

s	=	sample standard deviation
t	=	coverage factor, or Student's t-statistic
u_R	=	random uncertainty or standard error
u_x	=	combined uncertainty in measurements
u_Z	=	systematic uncertainty
V	=	volume, cm^3
v_x	=	degrees of freedom
W	=	width, cm
x	=	input variable from experimental measurements
y	=	output value calculated from input values
δ	=	readability
ε	=	perturbation in x
ρ	=	density, gm/cm^3

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Biography

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