

**USER GUIDE**  
**CALCUCRVFIT**  
**VERSION 4.0**



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# USER GUIDE

## OVERVIEW

### WHAT'S NEW

Version 4.0 now includes exponential and power curve fitting were included to offer more than the previous linear and polynomial regression curve fits. Also added is the ability to export the raw data, projected data and coefficients to a comma-quote delimited file. This file can be emailed.

Thank you for purchasing this app.

## CURVE FITTING MODULE

The curve fitting module is unique in that it has two modes, standard and calibration. In the standard mode you can:

### STANDARD MODE

Use this mode to:

- Predict any Y(ordinate) from an inputted X(abscissa).
- Determine the best fit for a dataset from a linear model up to a 9th degree polynomial model. This model is best when high degree polynomial fits are required.

### CALIBRATION MODE

Use this mode to:

- Predict any X(abscissa) from and inputted Y(ordinate). For example, if you have measured the absorbance of a given wave length of light with a spectrometer for a series of chemical concentrations in mg/L then the standard concentrations should be on the X axis and the absorbance (measurements with error) should be on the Y. You can then enter the absorbance of an unknown and calculate the concentration.
- Determine the best fit of a dataset from a linear to a third degree polynomial.

### BOTH MODES PROVIDE:

- Ability to store multiple datasets
- Virtually unlimited number of data points in a dataset

- goodness of fit calculations that include  $r^2$  (correlation coefficient) and the relative percent difference (RPD) between the given and predicted value.
- graphical representation of the fit
- PDF reports of the fit analysis and the graph of predicted versus given values that can either be printed or emailed.

## **LEAST SQUARES REGRESSION**

Space the x values equally for best results. This is to avoid high-leverage point errors. For instance, if you perform a linear least squares fit on a dataset, the fitted line will always pass through the average X, average Y point. If the points are spaced equally then they will contribute equally to the fit.

When performing calibration curves, do not use higher degree polynomials to compensate for detector saturation. In either mode, known values (for instance, standard concentration values) should be on the x-axis and the response variable (eg. instrument response measured with error) is on the y-axis. With this setup, the measurement errors are in the vertical direction and the least squares criterion works optimally.

# **DATASETS**

The following steps describe how to setup a curve, enter data, perform the best fit, graphs the predicted versus the given values and predict values based on user input.

Tap **Datasets** on the main menu to access the curve fitting module. This takes you to the **Curves Table** .

## **ADD A DATASET (CURVE)**

1. Tap the + menu item to create a new dataset (curve)
2. Enter the name of the dataset in the first text field, then press return.
3. Enter the X axis name in the second textfield, then press return.
4. Enter the Y axis name in the third text field and press return.
5. Tap the fit type: standard or calibration
6. Tap the **Save** menu item.

## **EDIT A DATASET (CURVE) SETUP**

1. Tap **Dataset** on the main menu to get to the **Curves** table.
2. Tap the **Title** of the dataset to enter the edit mode.
3. Tap the field or Fit Type to change the setting.
4. Tap **Save** menu item

When you change a curve then you will have to re-analyze it to be able to graph the results or predict values.

## **ADD DATA POINTS TO THE DATASET**

1. Tap the disclosure icon (ⓘ) of the dataset to which you want to add data. This will take you to the XY Data table.
2. You can add data in two ways: Using the + menu item or the calculator icon menu item
  - A. + Menu item method:
    - Tap the + menu item and this will take you to the **Data Entry** screen.
    - Type the X,Y values and either tap **OK** or press **Return** on the keyboard. Each time you enter a data point you will be returned to the XY Data screen. Repeat A & B for as many points as necessary. **Note: Don't add commas in large numbers because commas are used to identify the separation between the X and the Y value.**
  - B. Calculator icon in the menu method:
    - Tap the calculator icon in the menu bar.
    - Perform the following key strokes:
      - Type the Y value
      - press **ENTER**
      - Type the X value
      - Tap **DATA**
      - Alternatively, type X, type Y, press the **SWAP** (X<>Y) button, then press **DATA**.
      - Tap the XY Data back button to return to the dataset.

Unlike the + method, you will not be returned to the dataset after each point. This is easier for large numbers of data points. However, the data are not saved until you return to the XY Data screen.

## **EDIT A DATA POINT**

Tap the data point on the **XY Data** table that you want to edit. Edit the values then press **Return** on the keyboard or tap **OK**.

## **ANALYZE A DATASET**

At the bottom of the data point list is a tool bar with menu items. If the dataset is large you will have to scroll down to the bottom.

1. Tap **Analyze** on the bottom tool bar. This takes you to the **Analyze Screen**.
2. Choose the fit type by tapping either Linear, Polynomial, Exponential, or Power. Since the exponential and power fits utilize logarithms these options are not always available. These will be gray if not available and indicate that negative or zero numbers appear in

critical areas.

Once the calculation is done the program displays:

- The equation and coefficients
  - the correlation coefficient
  - X and Y data that were inputted
  - Projected values. If Standard Mode is selected then Y is projected. If Calibration mode was selected then X is projected.
  - The relative Percent Difference (RPD) between the real and projected value for each data point.
3. Polynomial degrees of fit are increased or decreased with the +/- button
  4. Tap PDF if you want to print or email the results of the analysis. You will be prompted to select the paper size, then the report will appear in PDF format. Tap the **Print** or **Email** icons as needed.
  5. Tap the **<Analyze** back button at the top menu to return to the **XY Data** screen where the **Graph** and **Calculate** buttons in the bottom tool bar are now enabled.

## **GRAPH THE POINTS AND FIT LINE**

1. Tap the **Graph** button in the bottom tool bar. The inputted points will show as a solid dot. The projected points will show as a circle. The program computes many other projected points to create a smooth line showing the fit to the data. The line is red for **Standard Mode** and it is green for **Calibration Mode**.
2. Tap PDF to print or email the graph.

## **CALCULATE POINTS FROM USER INPUT**

1. Tap the **Calculate** button on the bottom tool bar. If the curve is in **Standard Mode** then the button will be titled **Calculate Y**. If the curve is in **Calibration Mode** then the button will be titled **Calculate X**. This will bring you to the **Calculate Screen**.
2. Choose the **Significant Figures** for the result in the segmented buttons at the bottom of the screen.
3. Tap the field that says either Enter X (Standard Mode) or Enter Y (Calibration Mode)
4. Enter the value of X or Y depending on the prompt then, either tap **Return** on the keyboard or tap the **Calculate** button. The results will be displayed in the yellow field below.
5. The PDF button allows you to print or email the results.

## **EXPORT**

Access the Edit Curve screen by tapping the title of the dataset in the Curves screen. This will take you to the Export screen where you can create a comma-quote delimited file of the

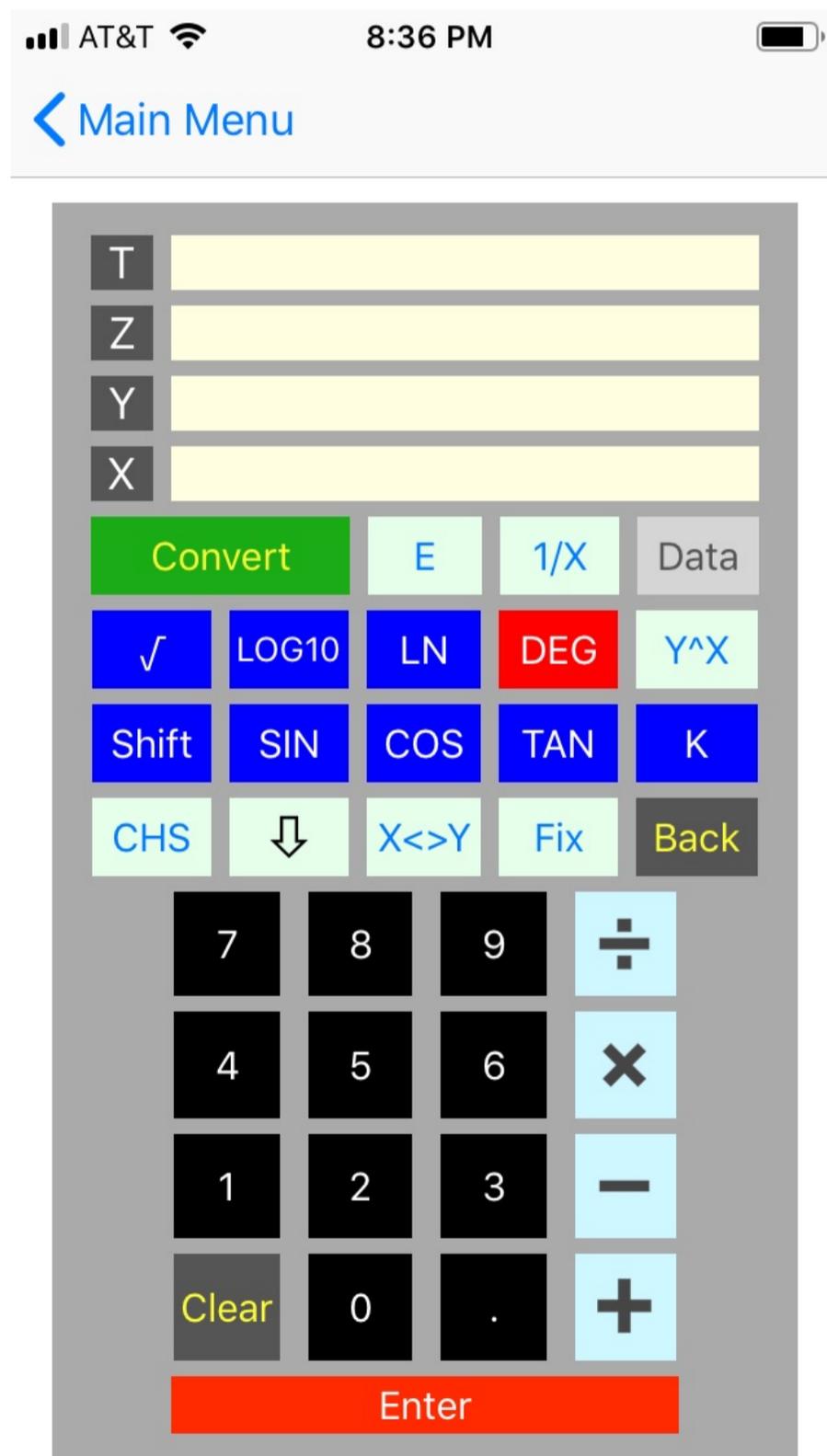
raw data (including projected values) or the equation coefficients. The Export button is disabled if there are no data in the dataset.

# CALCULATOR

## REVERSE POLISH NOTATION

The calculator uses reverse polish notation (RPN) where parentheses are not used. Rather, a number stack is used to store and separate intermediate calculations. Four stack registers are shown on the screen (X,Y,Z,T) but the stack is only limited by the device memory.

Calculator Screen



When you begin keying in a number it is placed in the X Register. You press the Enter button to push that number into the Y Register and if there is a number in the Y Register it is pushed to the Z register and so on.

## **CALCULATIONS**

If you want to perform a simple calculation such as  $2+3$  you would execute the following key strokes:

2  
Enter  
3  
+

The result 5 appears in the X Register.

A slightly more complex example is  $(2 + 3) * (4 - 2)$  is performed as follows:

2  
Enter  
3  
+  
4  
Enter  
2  
-  
X

The result 10 appears in the X Register.

Let's look at starting a calculation with one of the function keys:  $\text{Log}_{10}(100) * 5$ . Perform these keystrokes:

1  
0  
0  
Log10  
5  
X

The result 10 appears in the X Register.

## FUNCTION KEYS

The Shift Button changes the function the dark blue keys to their inverse function:

$\sqrt{\quad}$	LOG10	LN	DEG	$Y^X$
Shift	SIN	COS	TAN	K

After shift it tapped:

$X^2$	$10^X$	$e^X$	DEG	$Y^X$
Shift	ASIN	ACOS	ATAN	STO

For the function keys simply key the number if it is not already displayed and tap the function.

To store a constant tap Shift so the **STO** button is visible, key the number to store then tap **STO**. To recall the number tap Shift so the **K** (constant) button is visible and tap **K**. The constant is pushed into the stack.

Here is a description of some of the other functions:

**CHS** - changes the sign of a number.

$\Downarrow$  - Rolls the stack down and discards the number in the X Register.

**X<>Y** - Swaps the X and Y registers.

**FIX** - sets the number of decimals to show. Calculations are performed on the unrounded number.

To set the decimals at three places press 3 then Fix. To show the unrolled number press 1 CHS FIX. Entering -1 turns off the FIX function.

**$Y^X$**  - This calculates value in the Y register to the X power and the result is displayed in the X Register.

**E** - Allows you to add an exponent (10 to the E power) to your number. For instance, the following key strokes equals 1000: 1, E, 3.

## TRIGONOMETRIC FUNCTIONS

You have to tell the calculator if you are working in degrees or radians when using trigonometric functions. The calculator defaults to degrees. To change to radians, tap the red **DEG** button and a Green **RAD** button appears. This shows the calculator is in radians mode. Tap it to switch back.

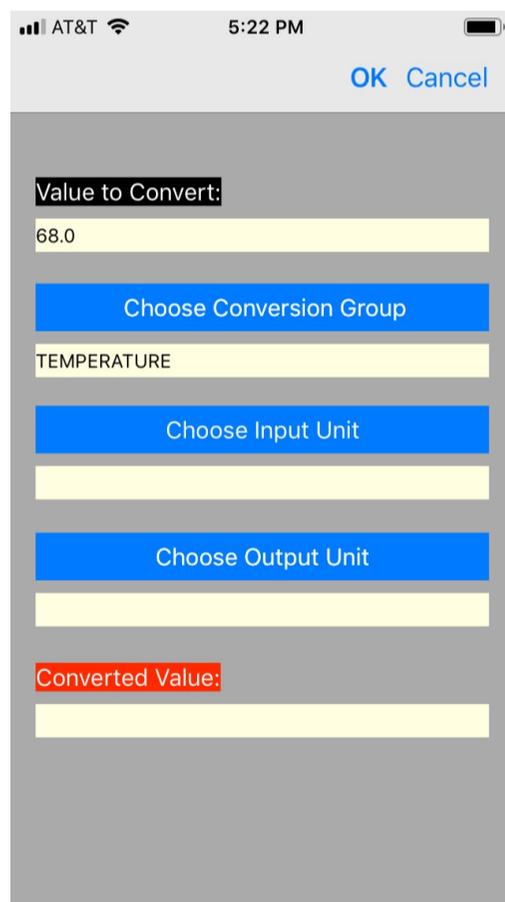


If you want to convert degrees to radians and vice versa you use the Convert button which will be discussed later.

## UNIT CONVERSION

The **Convert** button on the calculator give you access to a powerful conversion tool with hundreds of potential conversions. First, key the number you want to convert into the X Register then tap the **Convert** button. You are then taken to a screen where you select the conversion type (e.g. temperature), input unit and output unit.

Let's convert 68 degrees Fahrenheit to its equivalent Celsius value as an example. First key 68 into the X Register then tap **Convert**. You are taken to the following screen:



Tap the Choose Conversion Group and select Temperature.

Tap the Input Unit and select Fahrenheit

Tap the Output Unit and select Celsius.

Tap OK to accept the conversion

You will see 20 degrees presented in the X Register.

Subsequent conversion of the same type are simpler in that all you have to do is key the new value, tap Convert and tap OK in the menu and the conversion is computed.