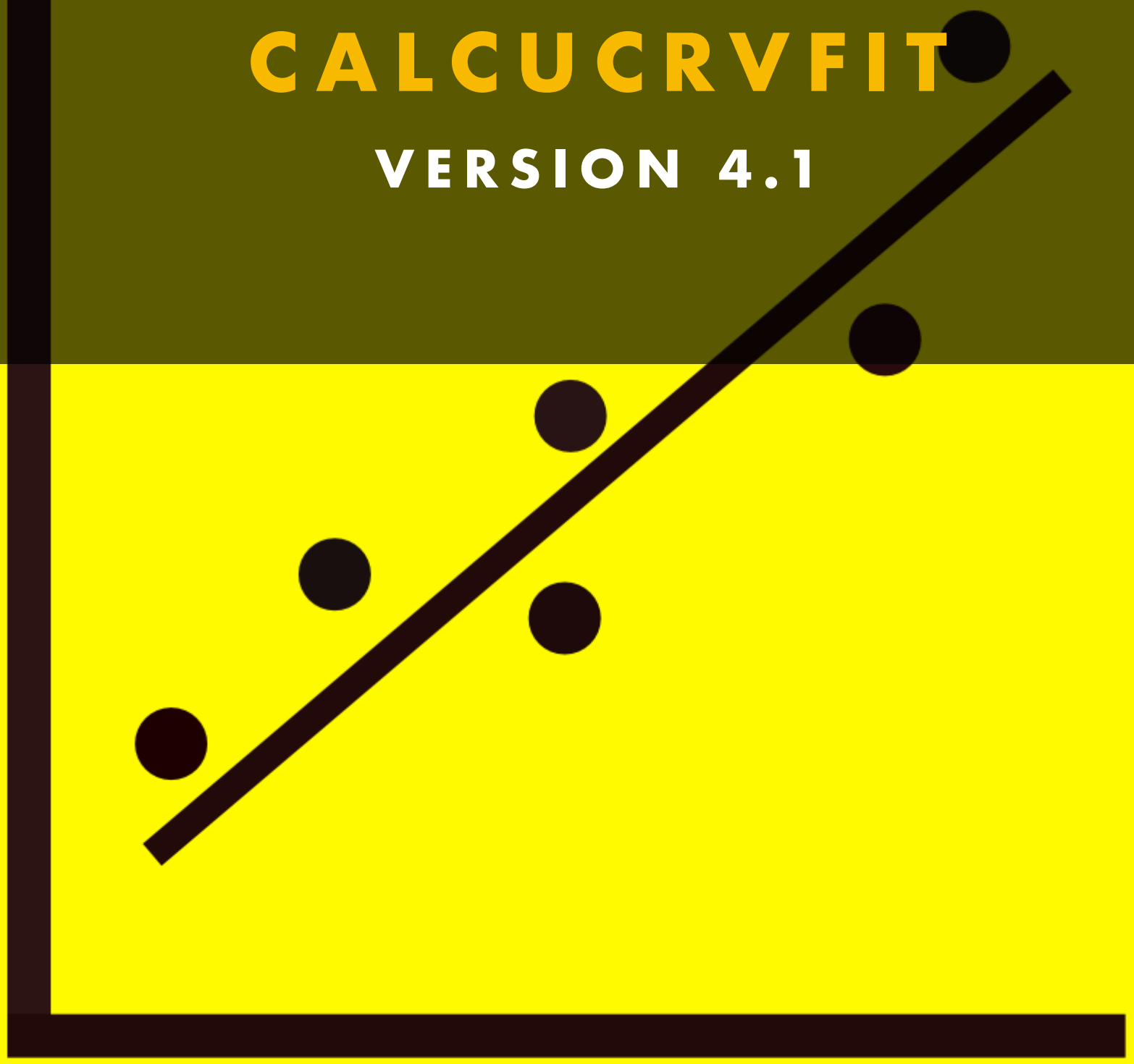
USER GUIDE

CALCUCRVFIT

VERSION 4.1



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USER GUIDE

OVERVIEW

WHAT'S NEW

Version 4.1 was updated to include the following capabilities:

- Dark mode support that is available in IOS 13.
- The PDF version of the graph can be converted into an image (JPEG, PNF, BMP, TIFF) for inclusion in reports.
- The calculator status is saved when you exit the application and restored the you reenter it so you can continue with the calculation where you left off. Things that are preserved are the numbers in the stack, the stored constant and unit conversion data.
- Import comma-quote delimited files.

Thank you for purchasing this app. Please send suggestions for improvements to JohnMDurand@icloud.com.

CURVE FITTING MODULE

The curve fitting module is unique in that it has two modes: standard and calibration. The difference in these two modes are described below:

STANDARD MODE

Use this mode to:

- Predict any Y(ordinate) from an inputed X(abscissa).
- Determine the best fit for a dataset using a linear, polynomial (up to 9th degree), exponential or power model. This mode 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 wavelength 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. Equation roots are used to predict X from the Y coordinate for polynomials.
- Determine the best fit of a dataset using a linear, polynomial (up to third degree), exponential or power model.

BOTH MODES PROVIDE:

- Ability to store multiple datasets
- Virtually unlimited number of data points in a dataset
- Goodness of fit calculations that include r2(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 graphic of predicted versus given values that can either be printed or e-mailed. PDF versions of graphs can be exported to an image.

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 though 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. Tab the **Save** menu item.

IMPORT A DATASET

1. Tap Dataset on the main menu to get to the **Curves** table.
2. Tap the disclosure icon (ⓘ) of the dataset.
3. Tap the Import button and select the file to import in the browser.

Import files must be comma quote delimited and the x and y data points must be the first two fields in each row. Import files must be in either .txt or .rtf format.

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 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 e-mail 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 inputed 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 e-mail the graph. Tap PIC to convert the PDF to an image (JPEG, PNF, BMP, TIFF).

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 e-mail the results.

EXPORT

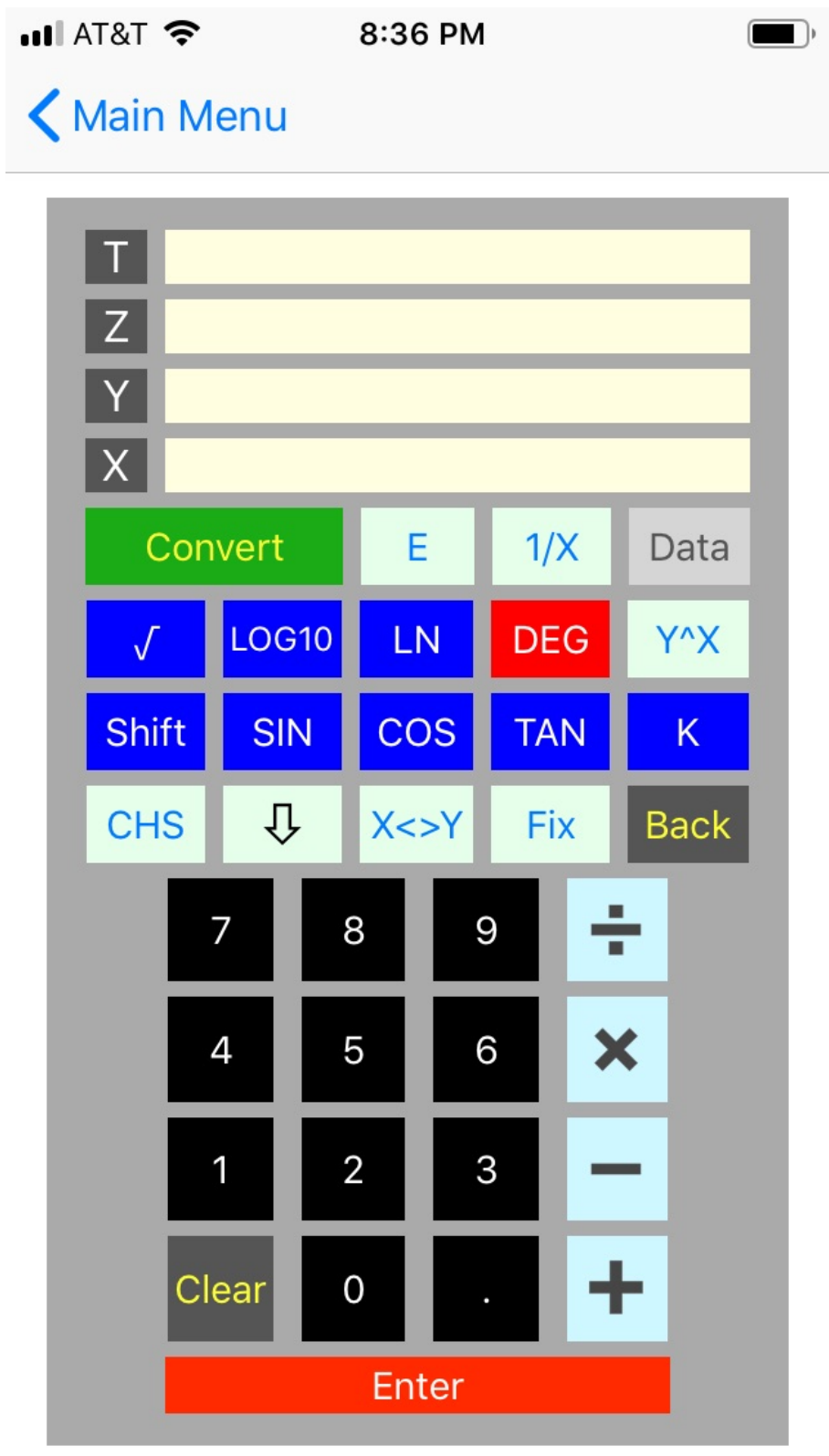
Access the Edit Curve screen by tapping the title of the dataset in the Curves screen. This will take you to the Export screen where you can create a comma-quote delimited file of the raw data (including projected values) or the equation coefficients. The Export button is disabled if there are no data 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.

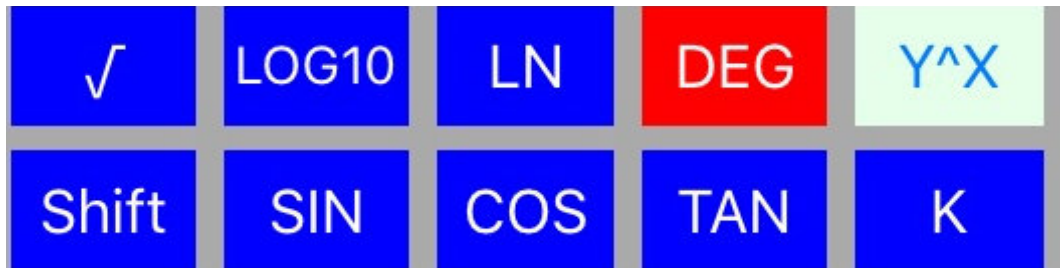
A slightly more complex example is (2 + 3) * (4 - 2) is performed as follows:

2
Enter
3
+
4
Enter
2
-
X
The result 10 appears in the X Register.

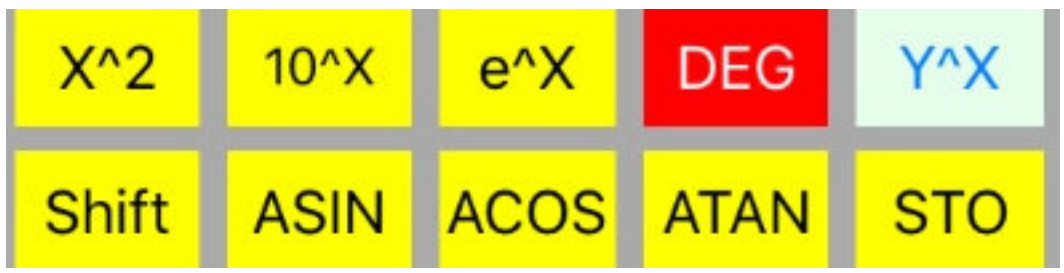
Let’s look at starting a calculation with one of the function keys: Log10(100) * 5. Perform these keystrokes:
1
0
0
Log10
5
X
The result 10 appears in the X Register.

FUNCTION KEYS

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



After shift it tapped:



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.
⇩ - 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 i 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.

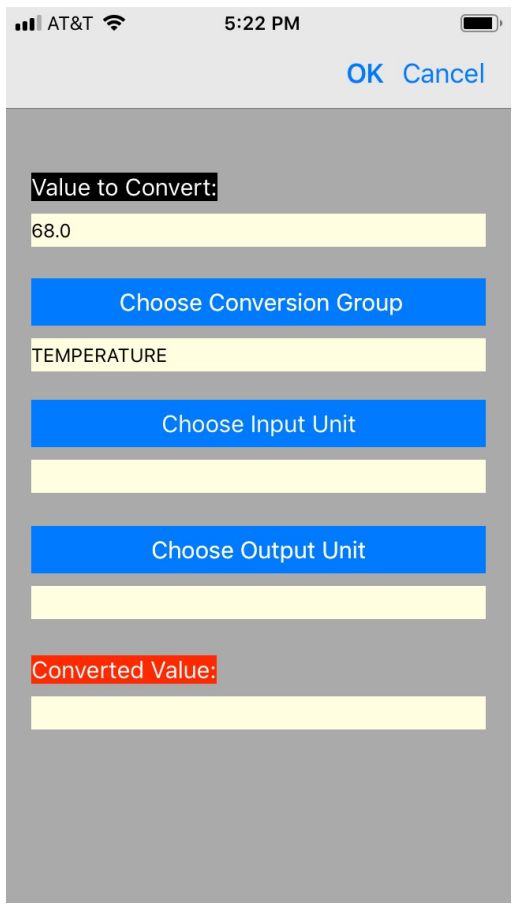
DEG RAD

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.