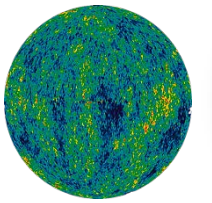

CBCAL 3

USER MANUAL

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1. DESCRIPTION

CBCAL is a Visual Basic.NET open-source code designed for the experimental collection of calorimetric data. In brief, it allows the simultaneous collection of the differential signal from, up to, four calorimetric cells, can perform electrical calibrations, and a trigger can be set to perform actions, e.g., using an Arduino setup. If you find this software useful for your research, please cite:

Carlos E.S. Bernardes; “CBCAL: Data Collection Program for Calorimetry Experiments”, *Zenodo*, **2022**, https://doi.org/10.5281/zenodo.6475251

The version currently available is working, however, it is not free from bugs. Any problems or questions do not hesitate to contact me.

CBCAL is free software, distributed in the hope that it will be useful, but WITHOUT ANY WARRANTY, without even the implied warranty of MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

In no event, the author will be liable to you for damages, including any general, special, incidental, or consequential damages (including but not limited to arising out of the use or inability to use the program, to loss of data or data being rendered inaccurate, or losses sustained by you or third parties, or a failure of the program to operate with any other programs), even if the author has been advised of the possibility of such damages.

2. Hardware Setup

A schematic representation of the hardware required to use the program is given in Figure 1. The program requires at least one multimeter, preferentially a Keysight 34420A meter to collect data. In this way, it is possible to connect each channel of the multimeter to one calorimetric cell. This enables the simultaneous collection of the data from two cells per multimeter. To read data from four cells, two Keysight 34420A meters are required.

The electric calibration system should be designed by connecting an electric resistance (inside the calorimetric cell) in a four-wire configuration (check scheme in Figure 1) to a power supply Agilent 6611C or Keysight E3642A and to a Keysight 34401A multimeter (other 6½ digit meters may be used). In this configuration, the power supply applies and reads the current flowing through the calibration circuit, while the multimeter measures the potential difference at the terminals of the resistance. The program will automatically compute the heat released by the resistance. In the current version of the program, only one cell can be calibrated at a time. Still, by using any commuter device to change between different calibration circuits, it is possible to calibrate several calorimetric cells under control by the program.

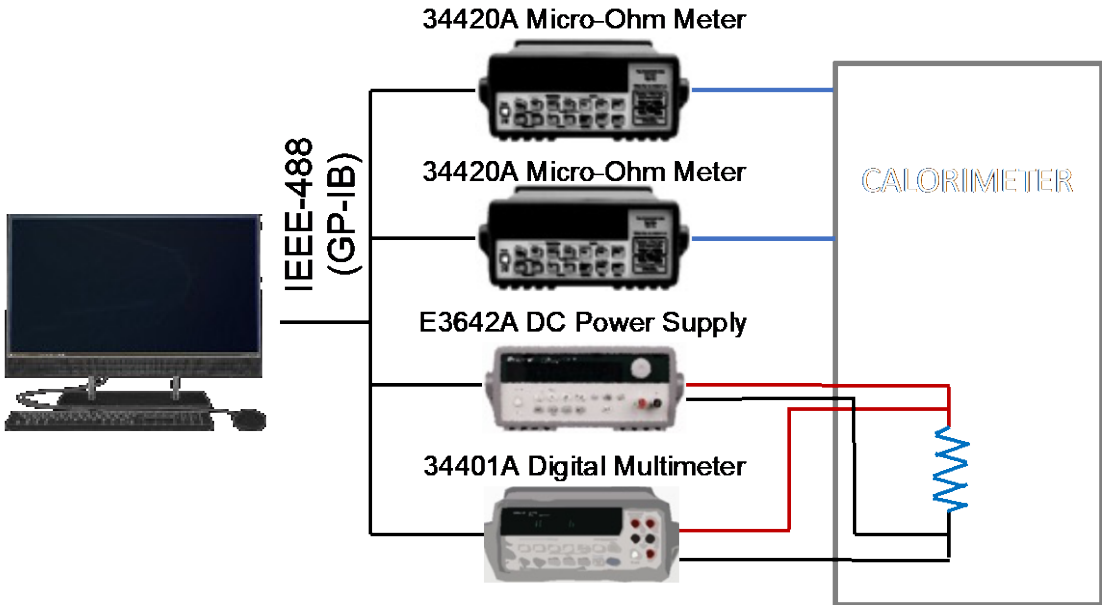


Figure 1. Hardware setup recommended for use with the CBCAL 3 software.

All multimeters should be connected to the computer by IEEE-488 GP-IB cables and the IO Libraries Suite must be installed on the Windows PC (the program was tested on Windows 7, 10, and 11).

Finally, the program contains a trigger that may be used to execute functions at regular intervals of time (see further details below).

3. Software

A snapshot of the program is given in Figure 2. As mentioned above, the program can collect the signal of, up to, four independent channels. The data acquisition process is controlled from different tabs in the main window. In each tab, 4 controls are used to collect data and control the experiments: (1) File selector; (2) Experiment start/stop; (3) Electric calibration control; and (4) Trigger control system, which, in this case, is designed for titration experiments. Additionally, during each experiment, an event log (5) can be used to record important information regarding the ongoing experiments. Records can be added by writing messages in the textbox and pressing the "Append" bottom (6).

All plots in the program are interactive. This means that, e.g., by using the mouse, the user can select an area of the plot to zoom in. Zoom out is activated by a double click over the plot. Additionally, the coordinates of the mouse when it is placed over the plot are given in the status bar of the program.

The calibration setup, Figure 3a, allows setting multiple sequential calibrations for a given channel. Note that, this

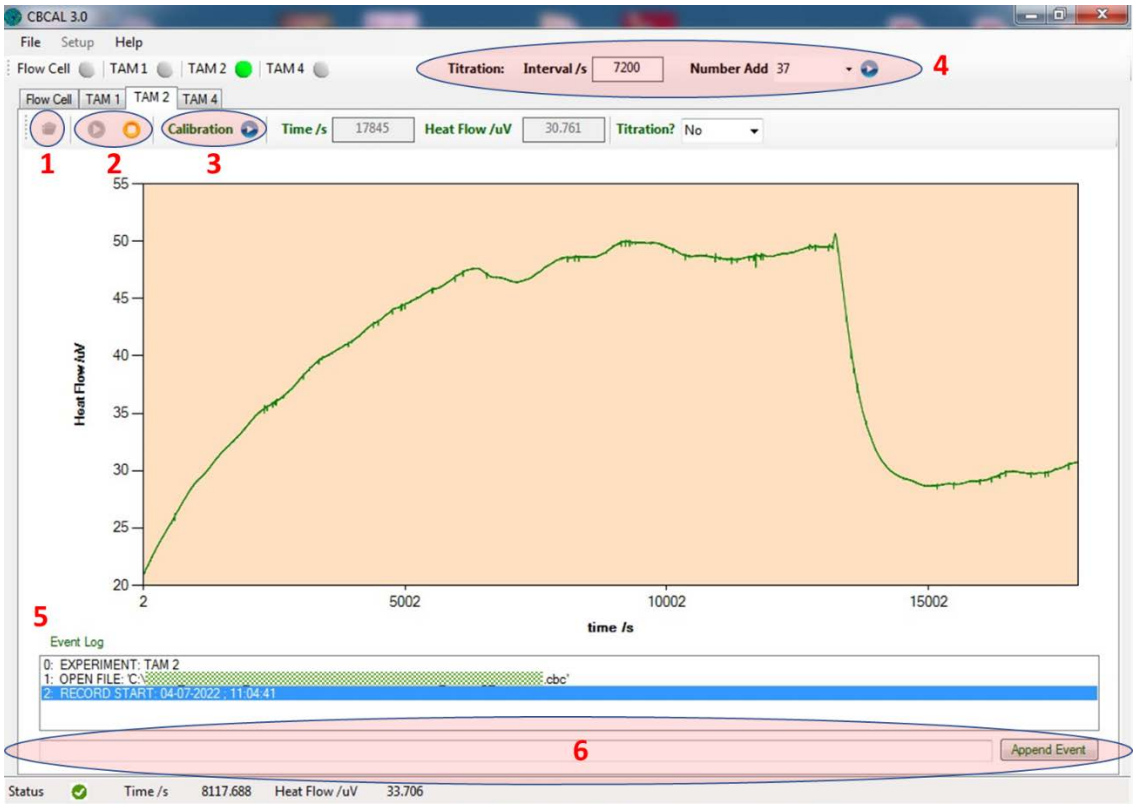
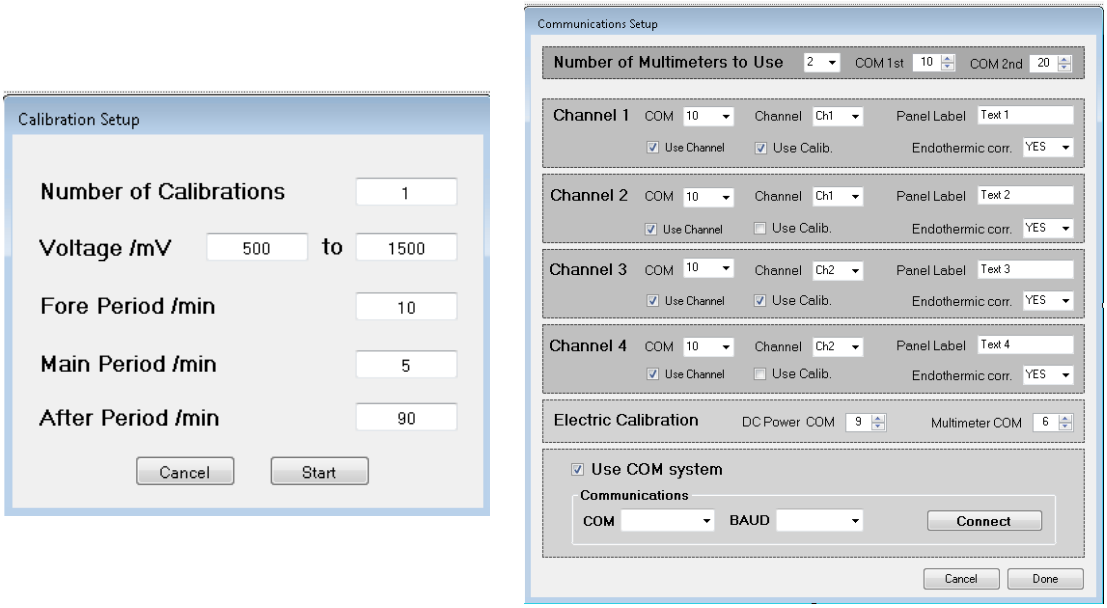


Figure 2. Snapshot of the CBCAL 3 software main window.



(a) (b)

Figure 3. Snapshot of (a) the calibration and (b) setup windows.

option becomes disabled for the remaining channels once calibration is started for one of them. In this menu, the user sets the number of calibrations to be run, the range of potential values to be scanned (a value is randomly selected by the program within this range of values), and the time to be used in the fore, main, and after periods of the calibration run.

The program is configured from the Setup menu, Figure 3b. From top to bottom:

- The first context menu requests the details about the micro-ohm meters, namely, if one or two apparatus will be used and the corresponding communication GP-IB ports.
- Next, the context menus contain the definition of each channel: a check to set if the channel will be used, another to set if it will be used in electric calibration experiments, COM port and channel of multimeter to be used, a label for ID in the program, and a check to set if an endothermic correction is required (i.e., the signal of the output is or is not multiplied by -1).
- It follows the settings of the GP-IB ports for the calibration DC power supply and the multimeter, used in the electric calibration.
- Finally, at the bottom of the window, it is possible to set RS-232 communications related to the trigger system (see details below).

It should be mentioned that the **CBCAL program does not perform data analysis**. This needs to be executed using other programs. For example, the freeware EASYGRAPH program is designed to natively open the CBCAL files (https://doi.org/10.5281/zenodo.4450358).

4. Trigger System

The current version of the program uses a trigger system based on RS-232 communications with an Arduino board. An example of the Arduino code is as follows:

```
const int ADD = 13;    // ADD solvent channel
int incomingByte = 0;
String myString;

void setup() {
    pinMode (ADD, OUTPUT);
    pinMode (FILL, OUTPUT);
    Serial.begin(9600);
    Serial.println("ON");
}

void loop() {

  if (Serial.available() > 0) {
    // read buffer:
    incomingByte = Serial.read();
    myString = char(incomingByte);
  }

   // ADD SOLVENT
   if (myString == "A") {
      Serial.println("OK");
      digitalWrite(ADD, HIGH);
      delay(500);
      digitalWrite(ADD, LOW);
   }
   delay(500);
}
```

In brief, CBCAL sends a trigger signal “A” to the board (see Figure 4). Once this signal is received, the board makes a 5V pulse during 500ms in terminal 13. As can be observed in Figure 4, this channel is connected to a MOS MODULE-MH. At this point, this event closes the circuit and/or passes a DC current that can be used as an analog trigger, for example, for a titration system.

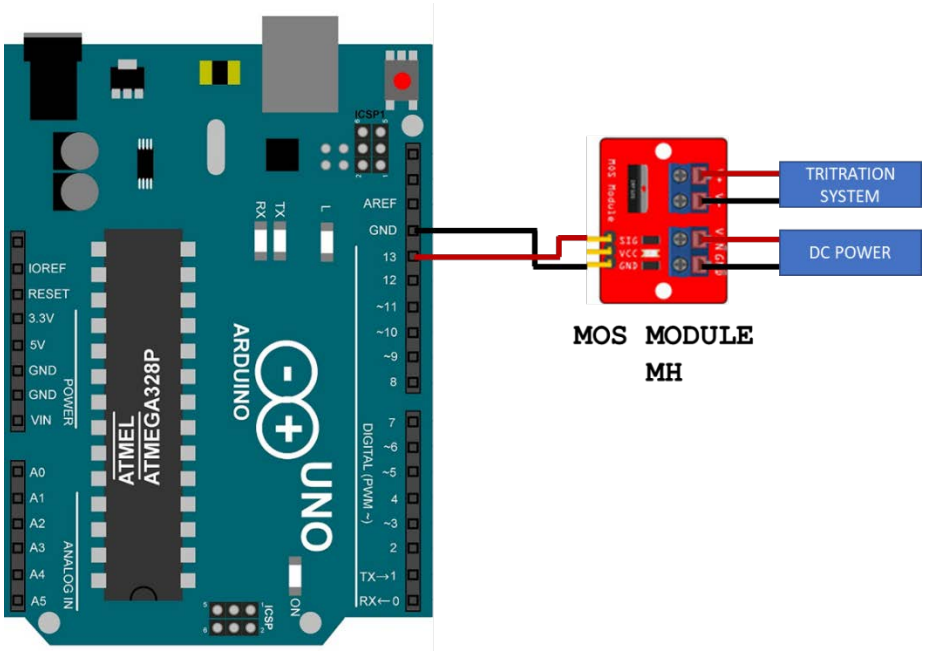


Figure 4. Schematic representation of the Arduino circuit used for the control of a titration system.