

Manual of using the REACTOR app

Real-time Experiment Analysis Control and Tracking for Optimization and Records

Make sure you have the test bench connected correctly before you load the app.

Make sure your computer is able to run the app.

A. Loading Arduino

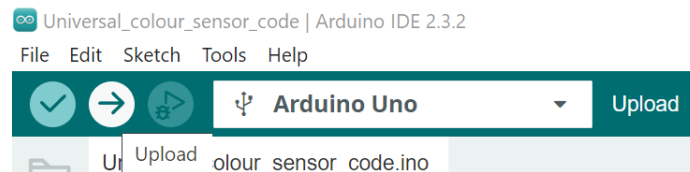
1. Clone the UTCV Reactions Github repo using the link:

<https://github.com/UTCV-github/Reactions.git>

2. Go to the folder where you saved the GitHub repo and open the GitHub folder.

3. Go to 'Reactions/Test_Bench_GUI/Universal_colour_sensor_code' folder and open the 'Universal_colour_sensor_code.ino' file with Arduino IDE

4. Select the Arduino board you are connecting. Click the 'Upload' button on the top left corner to upload the file to the Arduino board.

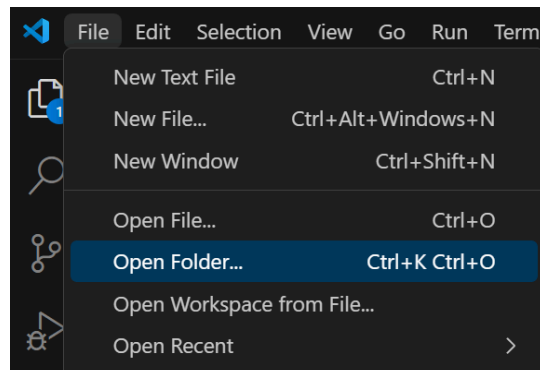


5. Once the upload is completed, close the file and exit Arduino IDE.

B. Loading Python Code

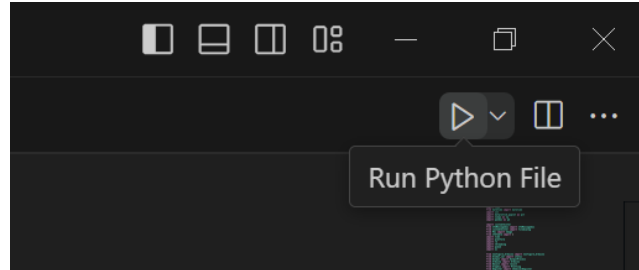
1. Under the "Test_Bench_GUI" folder, create a new folder and rename it as "Config". Place the "Config.json" file attached to the Hackathon package in the newly created folder.

2. Use VS Code to open the 'Test_Bench_GUI' folder by going to 'File' in the menu bar.



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3. Open the 'GUI_new.py' file by double-clicking the file located on the left side of the window. This is the main code file.
4. Make sure you have the configuration file ('Config.json') sent by the lab supervisor and place the file in the 'Config' folder under the 'Test_Bench_GUI' folder. The file is vital for running the app.
5. Click the 'Run' Button on the top right corner of the window



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C. Interacting with the app

a. The main window of the app is shown below. Red buttons are non-clickable unless certain conditions are met. The other colours are only used for differentiating different functions.

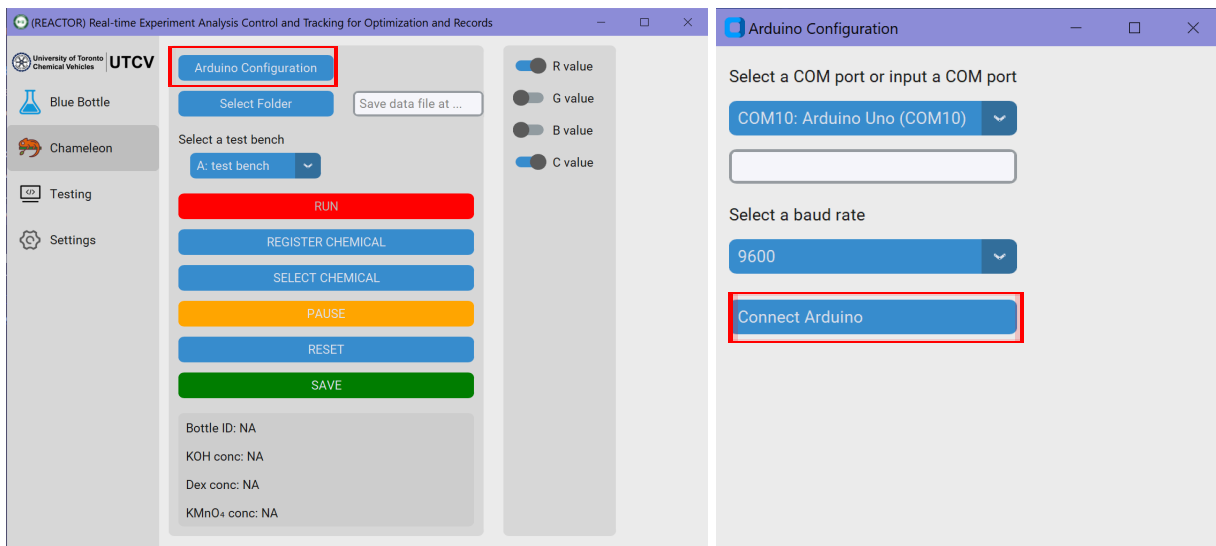
Closing the main window would result in the quitting of the app.



b. Configure Arduino.

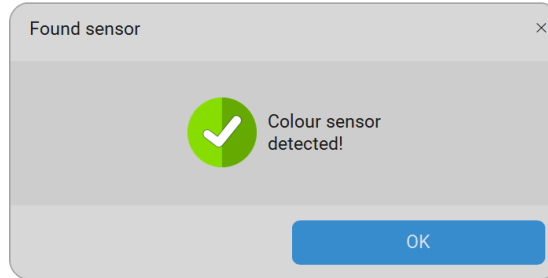
Note you have to have your test bench physically connected to your computer to complete the configuration.

To collect data from the test bench, you need to configure the connection between the computer and the Arduino. This step is mostly automatic but still requires manual confirmation. Click on the 'Arduino Configuration' button at the top of the window and a new window will open, as shown below:

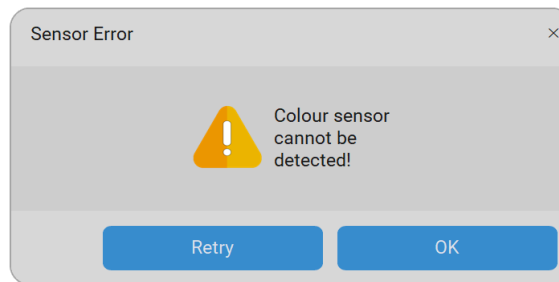


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Make sure the correct COM port and correct baud rate (usually 9600) are chosen and then click the 'Connect Arduino' button. The following window should pop up if the connection is successful. Click 'OK' and close the Arduino Configuration window.



If the connection failed, the following window would pop up. Click 'Retry' to try again. If the connection is still unsuccessful, notify the lab supervisor for help.



c. Chemical inventory management

The app provides you with an easy way to manage the chemicals/solutions you made in the lab. The inventory list is synchronized in real-time and saved on the UTCV network so you can easily share the list across the team and manage it on different devices. Note you don't need to connect to an Arduino device to use this feature.

c.1 Register chemical

Click the "REGISTER CHEMICAL" button in the main window to open the chemical register window

A form titled "Chemical registration" with standard window controls (minimize, maximize, close) in the top right. The form contains the following fields:

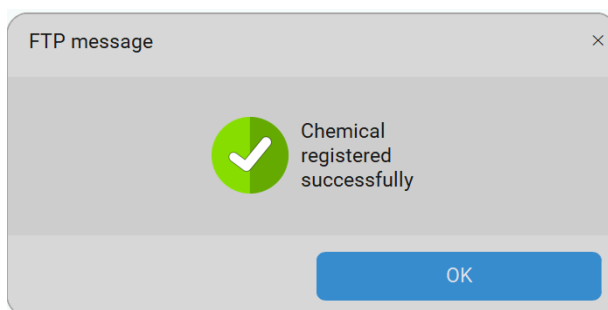
- "Input the KOH concentration": a dropdown menu set to "g/100mL" and a text input field labeled "KOH concentration".
- "Input the Dextrose concentration": a dropdown menu set to "g/100mL" and a text input field labeled "Dex concentration".
- "Input the KMnO₄ concentration": a dropdown menu set to "g/500mL" and a text input field labeled "KMnO₄ concentration".
- "The chemical is prepared by": a text input field with placeholder text "Your name (Optional)".
- "Note": a text input field with placeholder text "Note (Optional)".

At the bottom of the form is a blue button labeled "REGISTER".

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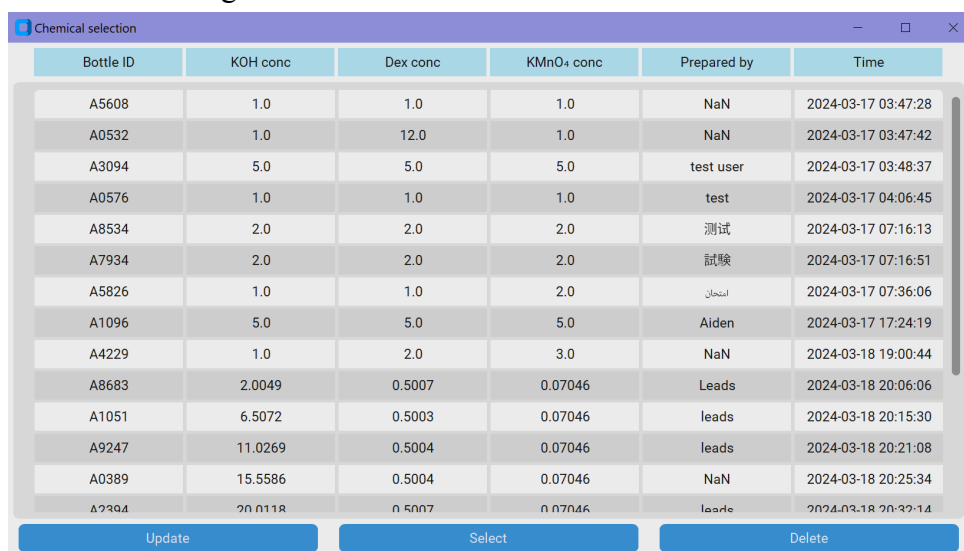
Input the concentration of the chemicals. Note that the concentration refers to the concentration of the solution you made before being added to the reaction vessel.

Please choose the correct concentration unit and only enter numeric values for concentrations. Once all information is input, click the “REGISTER” button to save the information. The pop-up window shown below will appear if the chemical information is successfully saved.



c.2 Select registered chemicals

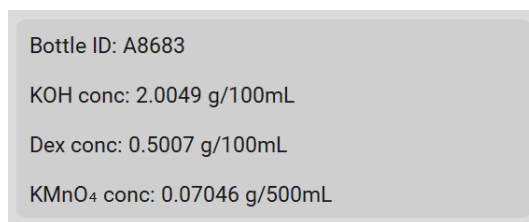
Click on the “SELECT CHEMICAL” button in the main window to open the data sheet of the chemicals that have been registered.



Bottle ID	KOH conc	Dex conc	KMnO ₄ conc	Prepared by	Time
A5608	1.0	1.0	1.0	NaN	2024-03-17 03:47:28
A0532	1.0	12.0	1.0	NaN	2024-03-17 03:47:42
A3094	5.0	5.0	5.0	test user	2024-03-17 03:48:37
A0576	1.0	1.0	1.0	test	2024-03-17 04:06:45
A8534	2.0	2.0	2.0	测试	2024-03-17 07:16:13
A7934	2.0	2.0	2.0	試験	2024-03-17 07:16:51
A5826	1.0	1.0	2.0	المجان	2024-03-17 07:36:06
A1096	5.0	5.0	5.0	Aiden	2024-03-17 17:24:19
A4229	1.0	2.0	3.0	NaN	2024-03-18 19:00:44
A8683	2.0049	0.5007	0.07046	Leads	2024-03-18 20:06:06
A1051	6.5072	0.5003	0.07046	leads	2024-03-18 20:15:30
A9247	11.0269	0.5004	0.07046	leads	2024-03-18 20:21:08
A0389	15.5586	0.5004	0.07046	NaN	2024-03-18 20:25:34
A2394	20.0118	0.5007	0.07046	leade	2024-03-18 20:32:14

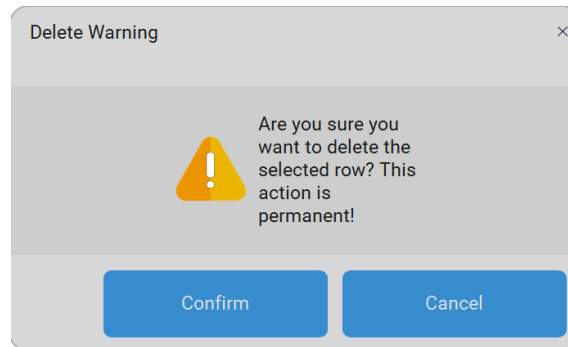
Note that the “Bottle ID” is generated when you register the chemical. It is used to identify different data files for further data processing.

To select a chemical combination, click on the row you want to select and then click the “Select” button, the chemical you selected will appear in the button part of the new window under the “SAVE button”



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To delete a row, click on the row you want to delete and click on the “Delete” button, a pop-up will ask you to confirm your choice. Click “Confirm” if you do want to delete the data. Click “Cancel” to cancel.

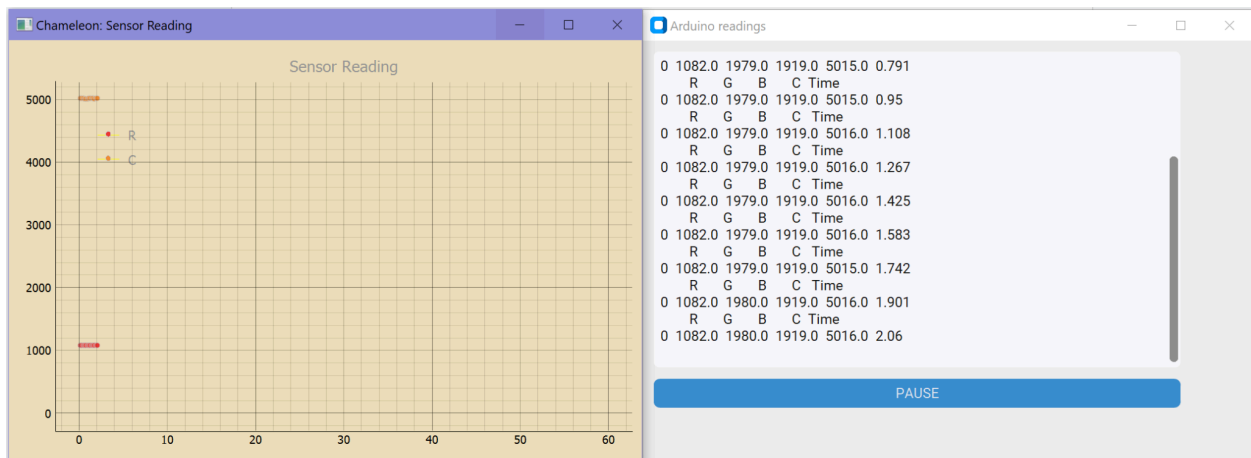


D. Collecting, visualizing and saving data

a. Before start collecting data, make sure Arduino has been configured successfully and the “RUN” button is green. Click “RUN” to start data collecting.

A real-time plotting window and an output printing window will be open.

Once the “RUN” button is clicked, it will be disabled until being reset manually or automatically to avoid mis-clicking.



b. To stop the data collection, press the “PAUSE” button in the output printing window or the “PAUSE” button in the main window.

Note that once the data collection is paused, it cannot be resumed.

c. During the data collection, a pop-up window might appear to indicate the endpoint of the reaction. The window has to be closed (by clicking “OK”) before further action can be taken.

d. Close both plotting and output windows and click the “Reset” button before you start a new round of data collection.

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- e. To save the data, click the “SAVE” button after the data collection has stopped. Make sure to click the save button before you start a new round of data collection, as clicking the “RUN” button will clear all the caches.
- f. You can choose what variable to show in the real-time plot by toggling on/off the variable switches on the right side of the main window.