Utilizing Simple Technology to Create an Instrument for Improved pH Measurements

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Background

pH is a metric used to describe the concentration of hydrogen ions present in a solution.[1] This value determines the acidity (or basicity) of a scientific sample and plays a key role in chemical, biological, environmental, and industrial applications.[1] Therefore, it is important that accurate and precise methods to measure pH are both scientifically and practically available; however, the two most common methods for pH measurements in undergraduate laboratories leave room for improvement. The aim of this project is to create a simple chemical instrument that produces reliable and standardized pH measurements via spectrophotometry and the direct application of pH indicator dyes. The complete assembly will be affordable, durable, easy to use, and include an accessible output. This project also serves as an example of multidisciplinary research and a proof-of-concept that effective and impactful instrumentation can be developed on small scales.

- **pH paper** is made from small strips of paper that have been saturated with dyes that change color in response to the proton concentration in a solution.[2]

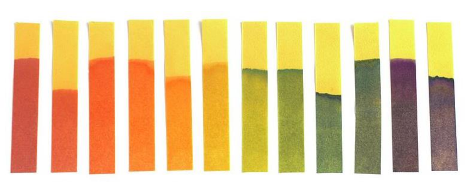


Figure 1: pH papers' response to solutions of varying pH

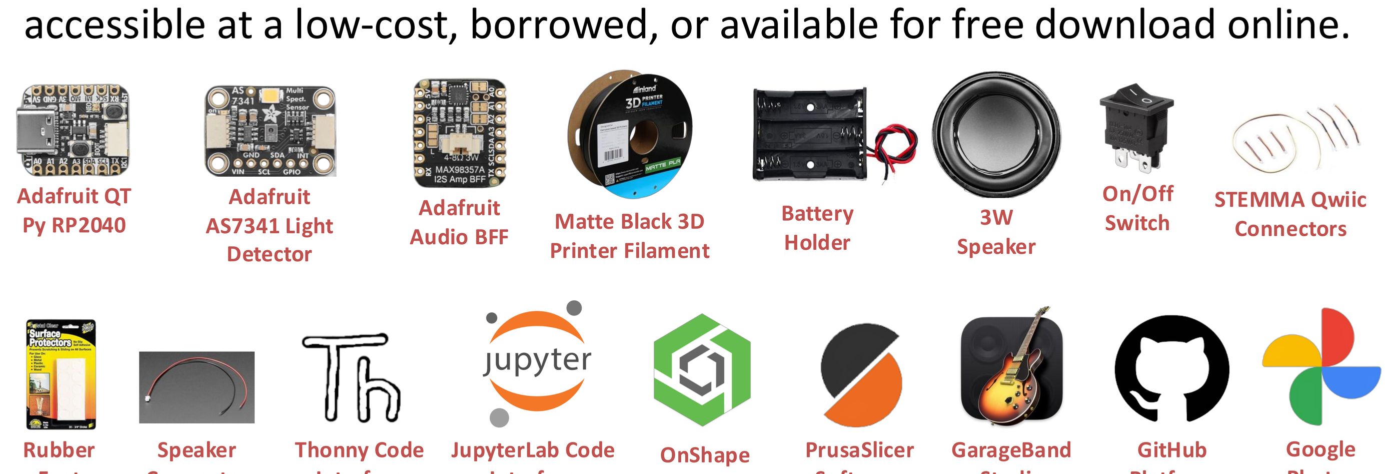
  - Easy to use, quick, durable, and affordable (~$10 per roll) [3]
  - Accuracy is reduced by human interpretation error, chemicals present in papers, and degradation
  - Inaccessible to blind and colorblind users
- **pH probes** translate the voltage difference between a reference and test electrode to a pH value and report it digitally. [4]

Figure 2: A typical pH probe

  - More accurate and accessible than pH paper
  - Delicate, bulky, difficult to use, time intensive, and expensive (~$70 and upwards per probe) [5]
  - Both pH paper and pH probes are not designed for use in aqueous mediums
- The design, construction, and implementation of simple instrumentation is a booming subject in the field of chemistry. It improves accessibility in lab settings, offers opportunities to explore sustainable research, and reduces costs.[6-10]

Materials and Methods

All materials and equipment used to complete this project were easily accessible at a low-cost, borrowed, or available for free download online.



Project Timeline

Concept → Learning → Construction → Calibration → Prototype 1

The Grace pH Box

Enclosure

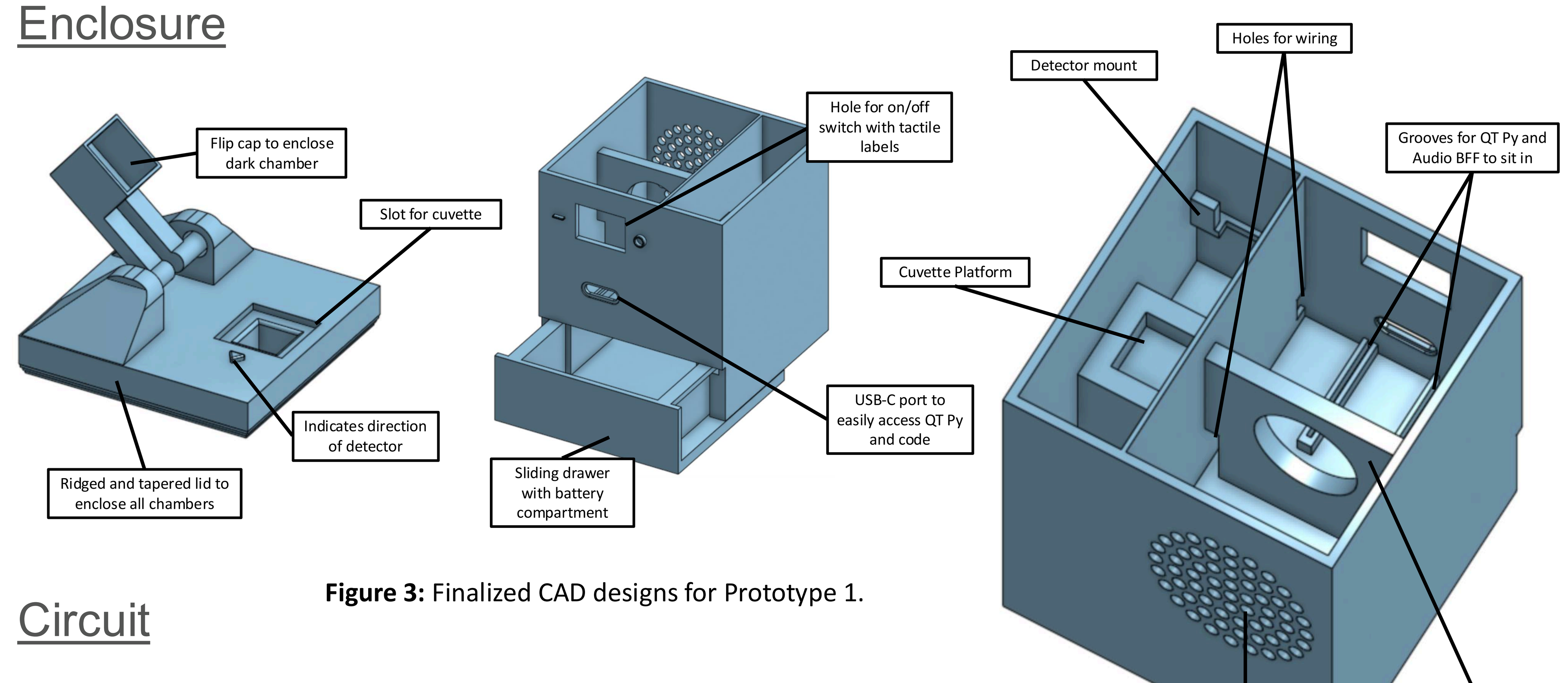


Figure 3: Finalized CAD designs for Prototype 1.

Circuit

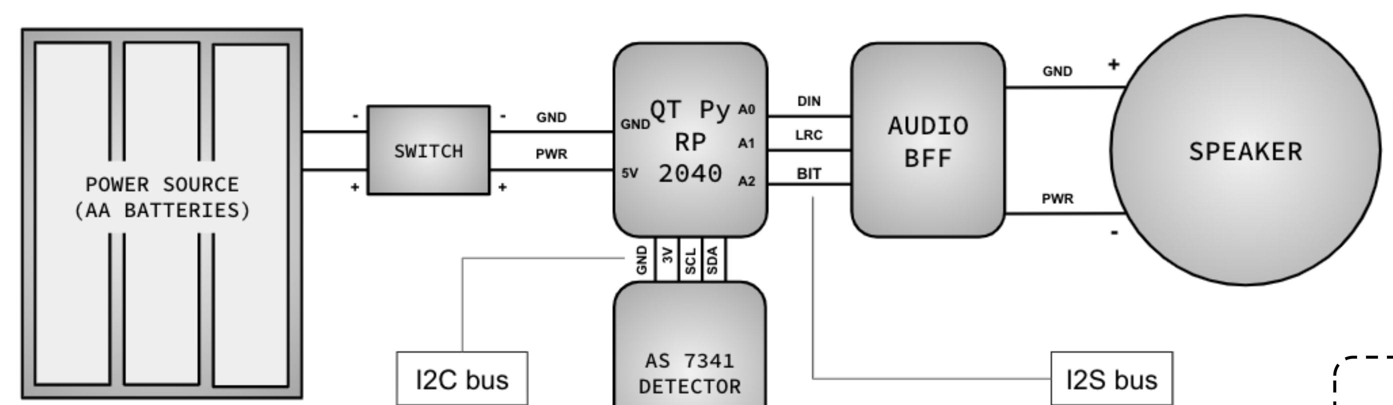


Figure 4 (left, above): Finalized circuit for Prototype 1.

Code

```python
#----------MAIN LOOP

while True:
    sleep(5) #wait 5 seconds then repeat
    if is_closed(): #check to see if sensor is in the dark
        reading = get_reading() #gather a reading from the sensor
        ph = compute_ph(reading) #convert the sensor reading to a pH value
        speak_ph(ph) #play pH value out loud
```

Figure 5 (left, below): The main loop of the Prototype 1's code. The yellow comments explain each of the main functions carried out to make the box operate.

Equation 1: Calibration operation generated by the machine learning model. A dot product between the values gathered from each channel and their corresponding calibration coefficients produce a scalar that is then added to an additional calibration constant.

Calibration

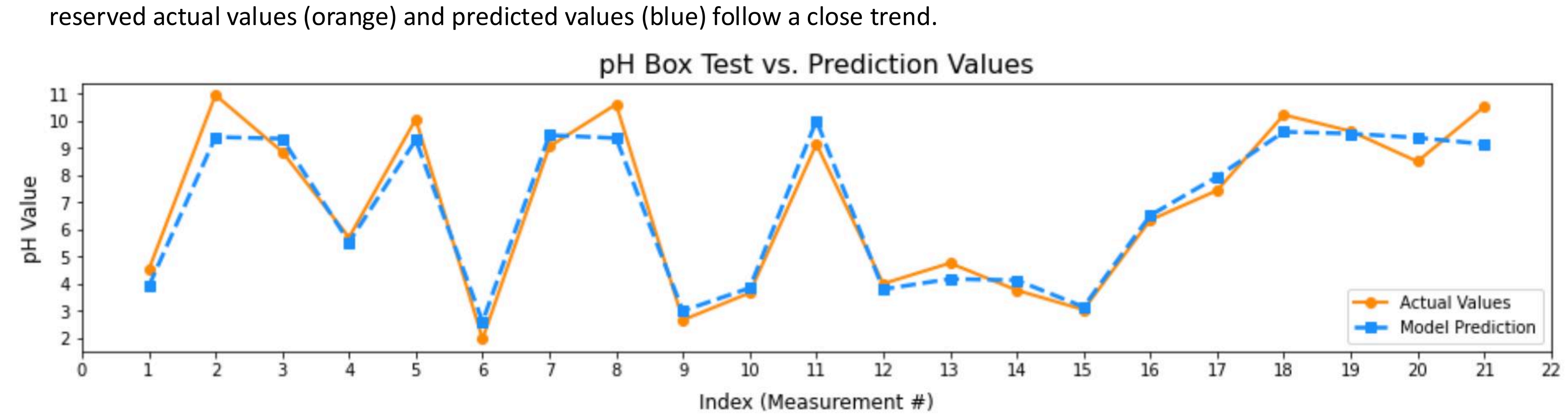
A linear machine learning model (Equation 1) was developed using the scikit-learn Python library and 81 aqueous pH measurements gathered with a pH probe and universal indicator. The model was generally able to predict a pH value within 1 pH value of an actual measurement.

$$pH = \begin{bmatrix} 415nm & 445nm & 480nm & 515nm & 555nm & 590nm & 630nm & 680nm \end{bmatrix} \begin{bmatrix} -0.29185504 \\ -0.00273654 \\ 0.04974995 \\ 0.00562701 \\ -0.01471374 \\ -0.00918647 \\ 0.01269146 \\ 0.01608802 \end{bmatrix} + 3.868977986033828$$

$$\sigma = 0.7$$

$$R^2 = 0.9434$$

Figure 6: To test the calibration, 25% of the dataset (21 readings) was set aside to be compared with values predicted by the model. When plotted against one another, the reserved actual values (orange) and predicted values (blue) follow a close trend.



Conclusions and Next Steps

Prototype 1:
- ✓ Accessible
- ✓ Yields a standardized pH reading (could still be improved)
- ✓ Affordable:

Protype 1:	Compare to:
Price Per Unit: $44.77 Materials Cost: $82.17 Total Project Cost: < ~$400	Vernier GoDirect Spectrophotometer: $460 [11] PerkinElmer ScanLambda 650: ~ $20000 [12]

Future Prototypes:
- Alternative displays or detectors
- Compact and rounded enclosure
- Manufactured circuit board
- Alternate internal layout or materials

Future Calibrations:
- Larger dataset
- Varying indicator concentrations

Future Applications:
- Organic solvents
- Additional indicators
- Field work

Figure 7a (left): Back of Prototype 1 including on/off switch, USB-C access, and open cap

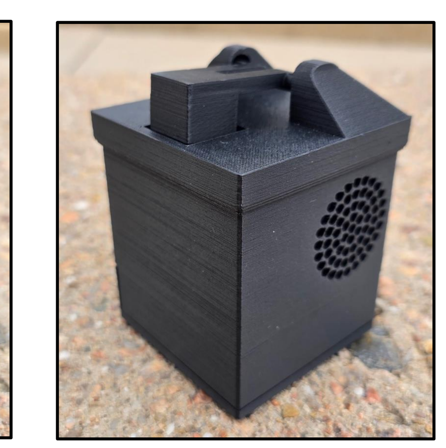


Figure 7b (middle): Front of Prototype 1 including speaker output and closed cap

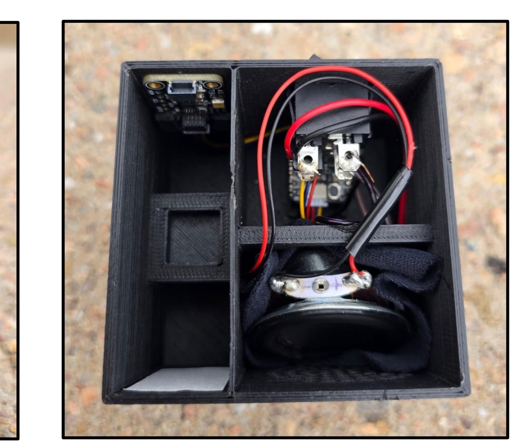


Figure 7c (right): Interior components of Prototype 1 including circuitry and dark chamber

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