Optimized Reactor Workbench

Muhammad Ziaur Rahman*, Md. Sakhawat Hossain*, Md. Mostafizur Rahman*,
Md. Mosaddik Mashrafi Mousum*, Sajid Ahamed* and Arafath Hossain*
Dept. of Computer Science and Engineering
United International University, Dhaka, Bangladesh
011202004*, 011221240*, 011221014*, 011221155*, 011221252* and 011173025*

***Abstract*—The Optimized Reactor workbench provides a framework for repetitive task minimization and safety assurance in modern-day chemical industries. It utilizes multiple techniques to create a prototype laboratory demonstrating how a chemical laboratory or factory should operate. Equipment for a specific experiment can be brought out using a real-time object detection mechanism. A researcher will also be obliged by the warning mechanism if he doesn't wear a safety apparatus while experimenting. After an experiment, the respective equipment will be systematically restored to their storage using object detection algorithms again. This will ensure the minimum need for human intervention in redundant tasks, and therefore, cost optimization on a large scale.**

***Index Terms*—Dispensing, Apparatus, YOLOV5 Tiny, OpenCV, TensorFlow Lite, Object Detection**

I. Introduction

Cost optimization and security maintenance are two major factors behind the success of modern-day chemical industries. In order to provide these industries with a sustainable solution, this paper will try to apply certain techniques in a prototype laboratory which is basically a miniature version of a large chemical facility. The aim of this project is to demonstrate how redundant tasks can be minimized to improve overall workflow of a laboratory. Apparatus selection, solvent dispensing, washing various equipment can be automated to take human intervention for these tasks out of the equation. On top of that, maintaining strict safety protocol such as wearing PPE, goggles, eyeglasses and deeply sanitizing an equipment after conducting an experiment will be demonstrated with the help of object detection algorithms implemented in Raspberry Pi single-board computer. Therefore, scientists and technicians will be able to focus entirely on their experiments rather than wasting their energy on mundane routines. The cumulative time and human resource saved in this process can ensure long-term optimization in scaled up industry.

Various research works have focused on automating chemical reactions and other necessary tasks. GMP (Good Manufacturing Practice) is a standard set by the World Health Organization. Velikyan et al. worked on automating the production of an imaging agent called [68Ga]Ga-DO3A-VS-Cys40-Exendin-4 which is used in PET (Positron Emission Tomography) to detect insulinomas, a tumor found on the human pancreas [1]. Such an approach will minimize the exposure to harmful radiation. Assuring safety is, after all, the primary goal to maintain GMP standards in any clinical manufacturing ecosystem. Harper et al. researched the optimized production of another PET imaging agent called technetium-94m [2]. Moreover, Bobrakov et al. (2013) discussed the optimized plasma treatment of low-level radioactive waste in shaft furnaces [3]. It can reduce the thermodynamic threats posed by harmful wastes in a nuclear powerplant. Mariam et al. (2015) also analyzed the fault-recovery system in the control system of plug-flow biomass reactors. It was automated by incorporating various strategies like Auger Jam Recovery Algorithm and Blower Algorithm. The authors reported that the pressure stability inside the reactor can be maintained efficiently to enhance overall safety [4]. These research works can be compared with each other to improve upon the lacking that have been found out in the context of this thesis.

Benchmark Analysis

Project/ Author	Safety Protocol	Object Detection	Cost Optimization	Use of Raspberry Pi	Sensor Integration
Velikyan et al. [1]	✓	✗	✓	✗	✗
Harper et al. [2]	✓	✗	✓	✗	✓
Bobrakov et al. [3]	✓	✗	✓	✗	✓
Mariam et al. [4]	✓	✗	✓	✗	✓
Optimized Reactor Workbench	✓	✓	✓	✓	✓

Fig. 1. Benchmark Analysis

Optimized workbench will incorporate the usage of Raspberry Pi in future which is uncommon in contemporary research works. The integration of object detection to ensure laboratory safety is also a key feature to take note of. Overall, the primary focus will be on fulfilling the gaps found in traditional approaches as well as presenting a miniaturized model in a unique way.

II. Proposed Method

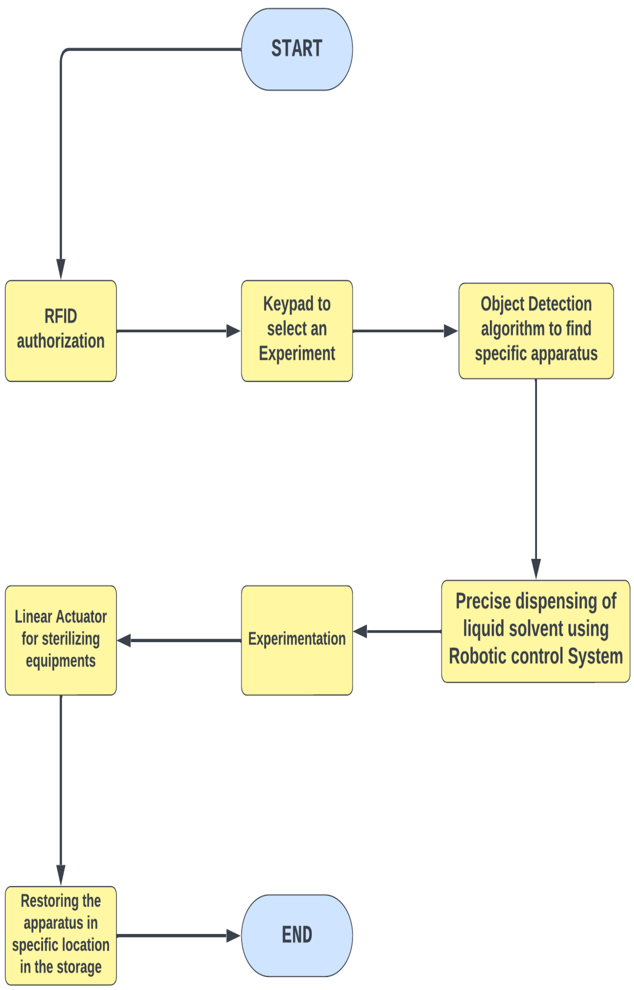


Fig. 2. Workflow Diagram

First of all, the researcher will pick a specific apparatus from the box manually. Three different equipment are available there: a beaker, a funnel, and a conical flask.

Fig. 3. Dispenser Front View

Three different types of chemical elements are available in their liquid form: Hydrogen, Oxygen, and Sulphur. A mobile application to control the Bluetooth module can be run by the researcher to dispense a specific amount of chemical compound or element. As for the prototype, three different samples of compounds can be produced automatically: Sulphuric Acid (H2SO4), Hydrogen Sulphide (H2S), and Sulphur Dioxide (SO2). If a user wants to create a 5 ml solution of Sulphuric Acid (H2SO4), he will simply have to press the "H2SO4" button from the mobile application. The automated mechanism will trigger the motors to dispense from the containers containing the three basic elements in such way timed way that the necessary amount of liquid from all the relevant containers will be dripped into the beaker or conical flask. Moreover, a user can also dispense a particular element (not exceeding 9 ml in this case), not just a compound. Finally, the user will take the solution to a mixer manually and the mixer will mix the entire solution with the help of stepper motors for around 10 seconds. The mixing can be initiated by the mobile application, and all these dispensing and mixing procedures will be demonstrated synchronously on an LCD monitor.

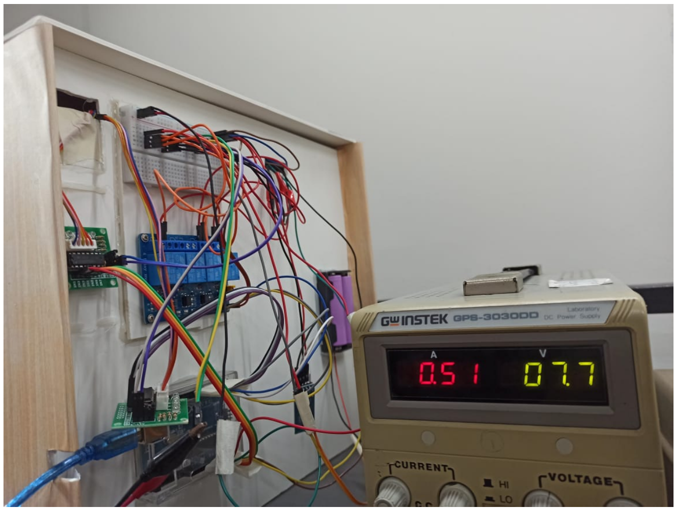


Fig. 4. Dispenser Rear View

The washing procedure of the apparatus will take place right after an experiment is finished. User will have to place an apparatus on the ultrasonic sensor panel at the rightmost side of the washing station. The ultrasonic sensor can easily detect the presence of an object right above it to eventually initiate the washing process. A robotic hand will grab the equipment and place it right under the washer at the leftmost side of the washing station. After washing the equipment, the robotic hand will bring it back on the ultrasonic sensor pad to activate the drier fan. Finally, a servo motor-powered handler will put the equipment right back to its place it was taken from. That is how a full cycle of the entire experiment will take place.

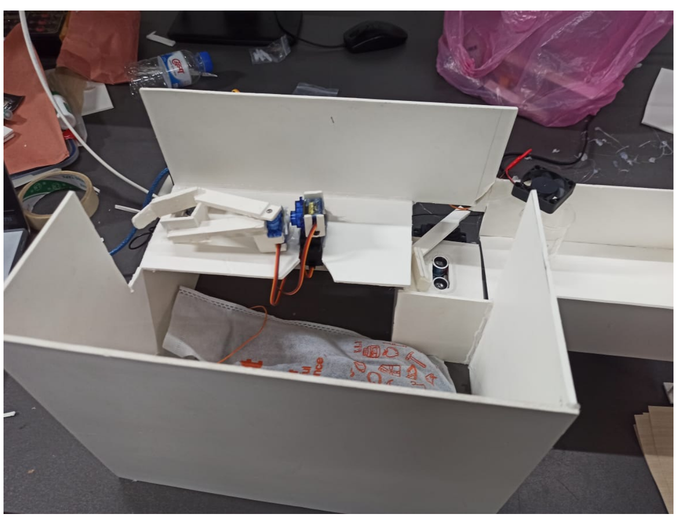


Fig. 5. Washing Station

III. Component List

A comprehensive overview of the key components is provided here. They play a critical role in order to achieve overall functionality and efficacy. Only the major components are described further.

A. Primary Components

1) Arduino UNO
2) Arduino NANO
3) Servo Motors
4) Stepper Motors
5) Robotic Arm/Linear Actuators
6) I2C LCD Display
7) Keypad
8) Breadboard
9) Jumper Wire
10) Water pump
11) PVC Board

B. Chemical Dispenser and Mixer

12) Mixing Motors (DC/Stepper Motors)
13) Chemical-Resistant Tanks
14) Flow/Pressure Sensors

C. Advanced Cleaning Solution

15) Chemical Rinsing system
16) Drying System
17) Robotic Arm
18) Drier Fan

D. Software used for testing purpose

19) Machine learning for Object detection.
20) Yolov5 Tiny model
21) TensorFlow lite and OpenCV is used (library)
22) 110 already pre-trained machine learning model
23) Algorithm type: Single shot multi-box detector
24) Confidence level: Up to 60
25) Image preprocess : 30 shorts for per pre train

IV. Primary Components

A. Arduino Microcontroller

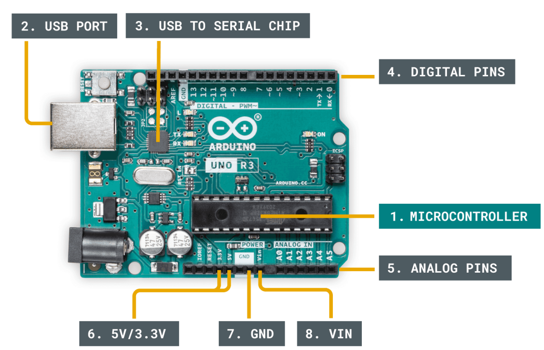


Fig. 6. Arduino UNO R3

The Arduino Uno R3 is the central processing board that uses ATmega328P microcontroller operating at an effective clock speed of 1 MHz. It has 14 digital input/output pins numbered from 0 to 13. The pins numbered 3, 5, 6, 9, 10, and 11 can generate PWM(Pulse with Modulation) output.

Moreover, the analog input pins (A0-A5) can convert analog signals into digital ones. It comes in handy while measuring voltage from different types of sensors. 0 (RX) and 1 (TX) are the serial communication channel pins. The LED of RX turns on when the Arduino board receives a signal from an external source. The TX, on the other hand, turns on during any activity that sends data to an external device. The 5V and 3.3V pins for respective voltages provide sufficient voltage to power up a connected device through these pins. Multiple GND pins provide ground connections for the negative terminals of those devices. The UNO board itself, however, needs power through an external power supply port or the USB port. The board also has a reset button for program reinitialization.

B. Servo Motor MG-996R

Fig. 7. Servo Motor MG-996R

This motor can rotate from 0 to 180 degrees according to requirements. It is mainly used in this project to implement the robotic arm for grabbing any equipment in the washing station. Here is a code snippet to explain the mechanism:

```
#include <Servo.h>
#define SERVO_PIN 13
Servo servo;
void setup() {
  servo.attach(SERVO_PIN);
}
void loop() {
  servo.write(90);
  delay(1000);
  servo.write(0);
}
```

The servo motor's signal pin is connected to pin 13 of the Arduino board. Initially, It will rotate to 90 degrees from its initial position within 1 second. Then, it will rotate back to its initial position.

C. Ultrasonic Sensor HC-SR04

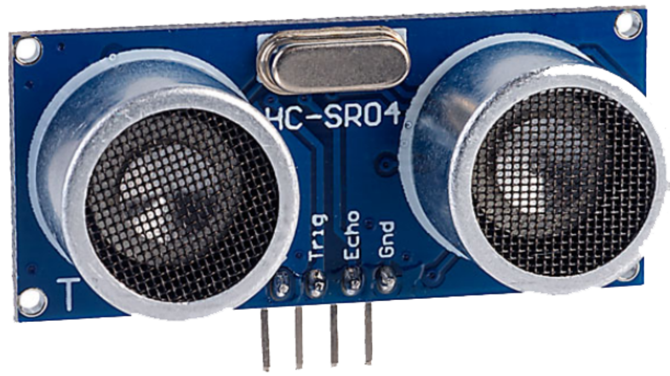


Fig. 8. Ultrasonic Sensor HC-SR04

The ultrasonic sensor is primarily used to measure certain distances. A short burst of high-frequency sound waves is generated from the Trigger pin, which is reflected back from a solid obstacle to be listened to by the Echo pin. The amount of time for the waves to travel back and forth is used to calculate the distance between the sensor and the obstacle. In the following code, we are categorizing objects according to their heights by an ultrasonic sensor:

```
#define TRIG_PIN_1 12
#define ECHO_PIN_1 13

#define TRIG_PIN_2 10
#define ECHO_PIN_2 11

#define TRIG_PIN_3 8
#define ECHO_PIN_3 9

#define distance_to_slate 30
bool ultra_1 = false;
bool ultra_2 = false;
bool ultra_3 = false;

void setup() {
  Serial.begin(9600);
  pinMode(TRIG_PIN_1, OUTPUT);
  pinMode(ECHO_PIN_1, INPUT);

  pinMode(TRIG_PIN_2, OUTPUT);
```

```
  pinMode(ECHO_PIN_2, INPUT);


  pinMode(TRIG_PIN_3, OUTPUT);
  pinMode(ECHO_PIN_3, INPUT);
}

void loop() {

  ultra_1 = object_detected
  (TRIG_PIN_1,ECHO_PIN_1);
  delay(25);
  ultra_2 = object_detected
  (TRIG_PIN_2,ECHO_PIN_2);
  delay(25);
  ultra_3 = object_detected
  (TRIG_PIN_3,ECHO_PIN_3);
  delay(25);
  if
  (ultra_1 && !ultra_2 &&  !ultra_3)
  Serial.println("Small Object");
  else if
      (ultra_1 &&ultra_2&&!ultra_3)
  Serial.println("Medium Object");
  else if(ultra_1&&ultra_2&&ultra_3)
  Serial.println("Tall Object");

  delay(1000);
}


bool object_detected
(int TRIG_PIN, int ECHO_PIN)
{
  long duration, distance_cm;

  // Send a short pulse
  //to the TRIG pin
  digitalWrite(TRIG_PIN, LOW);
  delayMicroseconds(2);
  digitalWrite(TRIG_PIN, HIGH);
  delayMicroseconds(10);
  digitalWrite(TRIG_PIN, LOW);

  // Measure the time it takes
  //for the echo to return
  duration = pulseIn(ECHO_PIN, HIGH);

  // Calculate distance in cm
  distance_cm = (duration / 2) * 0.0343;

  // Print the distance
 // Serial.print("Distance: ");
  //Serial.print(distance_cm);
  //Serial.println(" cm");
  int upper_limit =
  (distance_to_slate/2) + 5;
  if(distance_cm <= upper_limit)
   return true;
  return false;
  //delay(1000); // Wait 1 second
  //before taking the next measurement
}
```

Here, 3 ultrasonic sensors are attached equidistantly to a perpendicular holder. the bottom-most sensor is connected to Arduino pins 12 and 13 and the topmost one is to pins 8 and 9. A slate is placed at a distance of around 30 centimetres from the perpendicular holder. An object is placed in between the holder and the slate. If the height of the object is small, only the bottom-most sensor will detect a distance within 15 to 20 centimetres. For medium objects, it will happen for both bottom-most and middle sensors, except for the topmost sensor. Any tall object will provide a distance of 15 to 20 centimetres for all 3 sensors.

D. I2C LCD

We used a 16x2 LCD monitor for the user interface. The resolution 16x2 means that there is a total space for 32 characters. As we are using an already soldered LCD monitor, an I2C adapter will be used to establish communication between the LCD and the Arduino board. The SDA pin is the data transfer

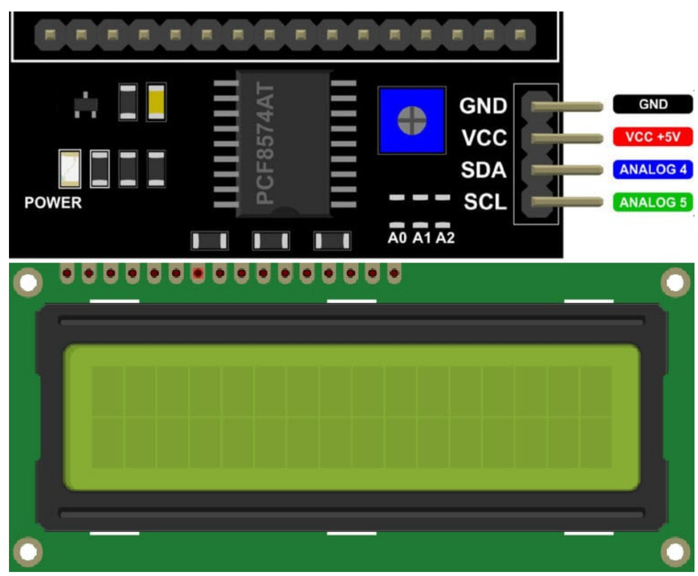


Fig. 9. I2C Adapter

line that receives signals to generate characters on the LCD screen. The SCL pin provides clock pulses to synchronize the data transfer. A potentiometer is situated(blue color) on the back of the panel to adjust the screen's brightness. The LCD screen has 16 columns and 2 rows. In order to set the starting point of the screen, we used the setCursor(col, row) method. Here, "col" and "row" denote the indices of the column and row from where the output string will start to show up. For example, setCursor(10,1) will indicate that the first character

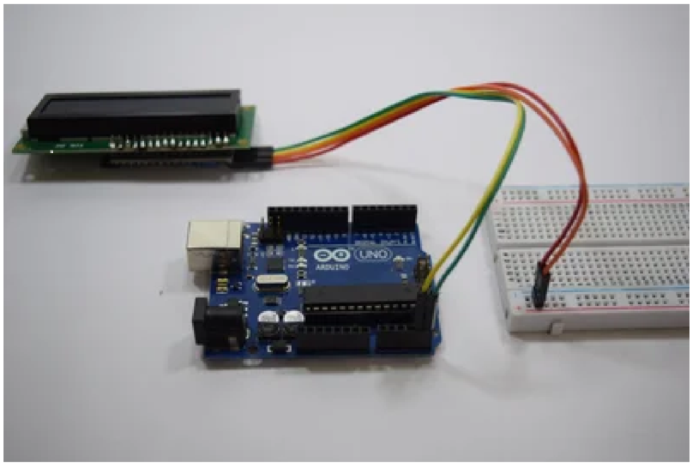


Fig. 10. LCD Screen Connection

of the output string(s) will start to show up from the eleventh column of the second row.

E. 4x4 Matrix Keypad

Researchers will communicate with the system through this keypad interface. It will help them to input the serial number of the experiment they want to conduct. It is very user-friendly to demonstrate various pre-programmed lab activities. The

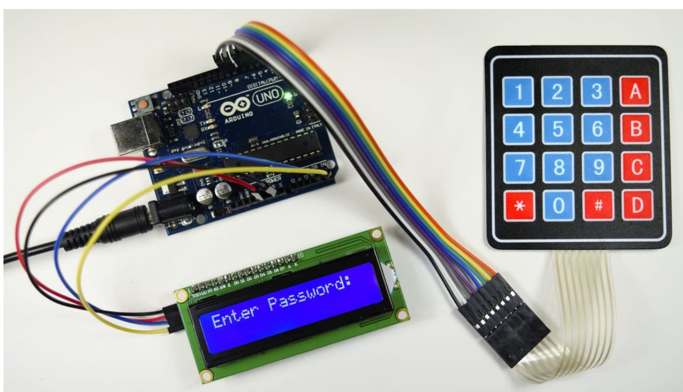


Fig. 11. 4x4 Matrix Keypad

following code snippet demonstrates the basic setup of a 4x4 keypad:

```
#include <Keypad.h>

const byte ROW_NUM    = 4;
const byte COLUMN_NUM = 4;

char keys[ROW_NUM][COLUMN_NUM] = {
  {'1', '2', '3', 'A'},
  {'4', '5', '6', 'B'},
  {'7', '8', '9', 'C'},
  {'*', '0', '#', 'D'}
};
```

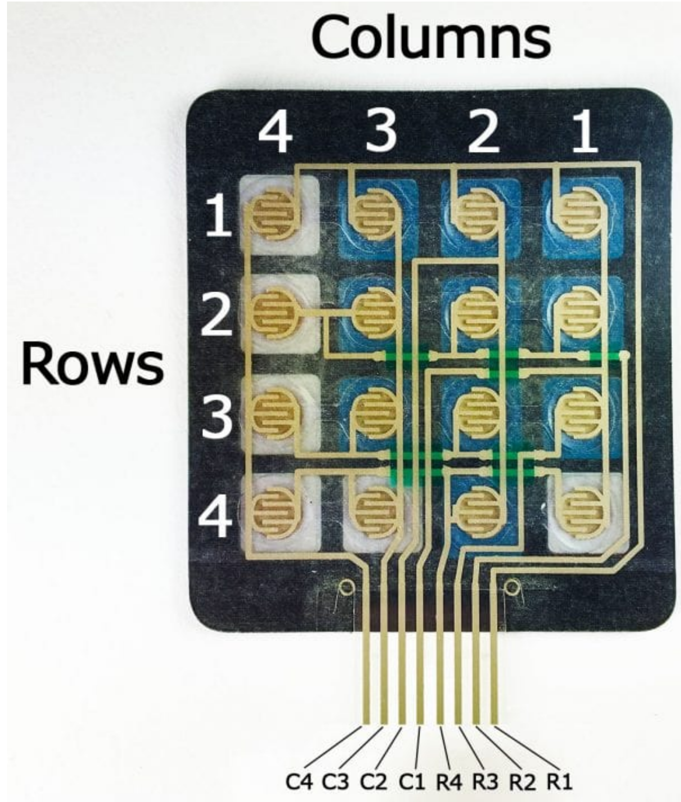


Fig. 12. Wiring (Rear View)

```
byte pin_rows[ROW_NUM]={6, 7, 8, 9 };
byte pin_column[COLUMN_NUM]={10,11,12,13};

Keypad keypad = Keypad(makeKeymap(keys),
pin_rows, pin_column, ROW_NUM, COLUMN_NUM);



void setup() {

  Serial.begin(9600);

}

void loop() {
  char key = keypad.getKey();
  if(key)
  Serial.println(key);

}
```

Viewing from the front of the keypad, the leftmost wire is connected to Arduino pin 6. The rightmost wire is connected to pin 13. Pins for the keypad rows: 6,7,8,9. Pins for the keypad columns: 10,11,12,13. A Two-dimensional character array named ”keys” and the library function makeKeymap(keys) are used to establish proper connection mapping to the Arduino pins.

F. Water Pump

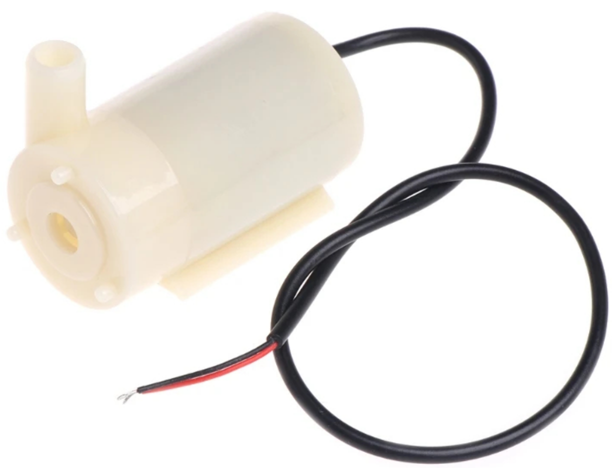


Fig. 13. 5V DC Water Pump

Multiple 5V DC water pumps are used in this project to dispense a calculated amount of liquid reactants into various containers. Four 100 ohm resistors are used in parallel combination to create an equivalent resistance of 25 ohm. It will help the pump achieve a voltage drop of around 2 volts for more precise dispensing. The amount of delay in the code segments is calculated through several trials and errors. The pump will run for these amounts of time to flow out a certain amount of liquid.

G. RFID Scanner RC522

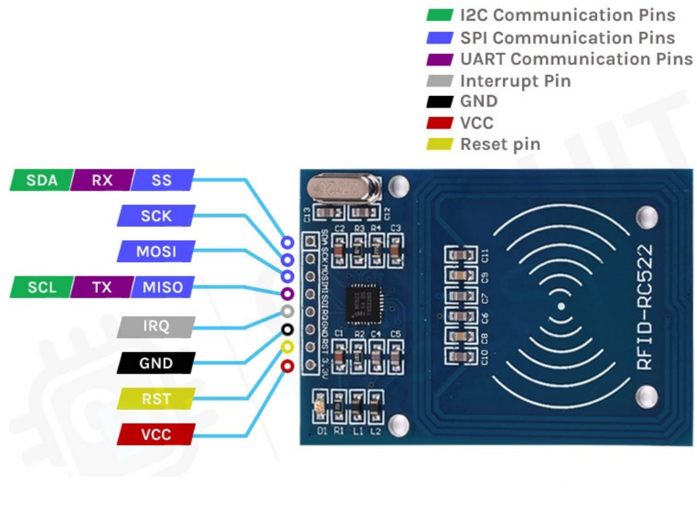


Fig. 14. RC522 Pinout

The RFID scanner(MODEL RC522) is utilized to detect the identity card(model SPI S50) of authorized personnel. Only registered users can use the chemistry lab in this project.

Fig. 15. SPI S50 Identity Card and Keychain

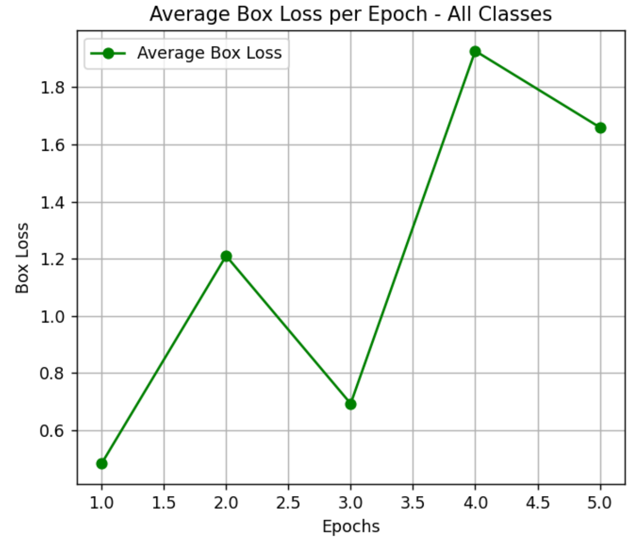
H. Stepper Motor with Driver

Fig. 16. Stepper Motor and Driver

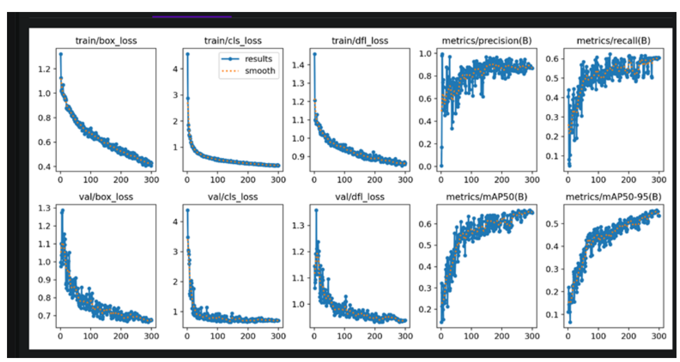
A stepper motor operates by converting electrical energy to mechanical movement. It consists of multiple coils arranged in phases around a central rotor. When the motor receives an electrical pulse, the coils are energized in a specific sequence, generating magnetic fields that attract the rotor's teeth to align with the energized coil. As the pulses continue, the rotor advances in discrete steps, resulting in controlled rotation. A stepper driver is a related component that controls the movement of the stepper motor. This component is particularly necessary as it provides extra external power for rotation. The driver interprets digital signals originating from a microcontroller and converts them into the specific electrical current patterns necessary to drive the coils within the stepper motor. By issuing a series of pulses to the stepper driver, the motor is directed to move in precise steps.

V. Analysis

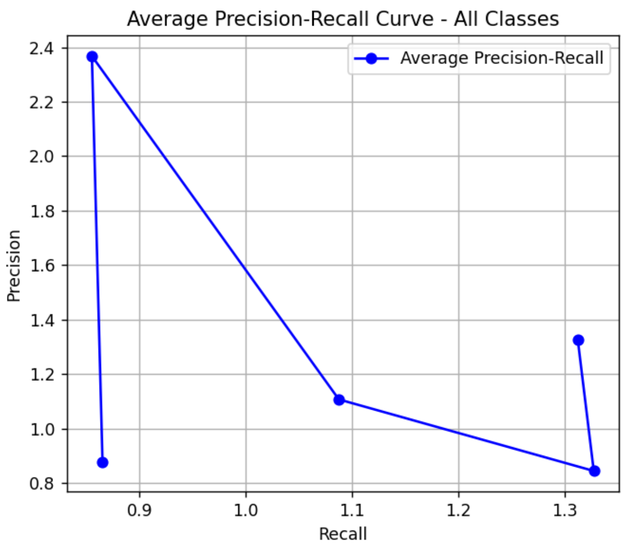
The apparatus was selected from the appropriate location and tested to perform in an automated environment. Digital Image Processing techniques and the deep learning model YOLOv5 tiny were utilized for this purpose. Here are the results of the overall analysis in a graphical format:



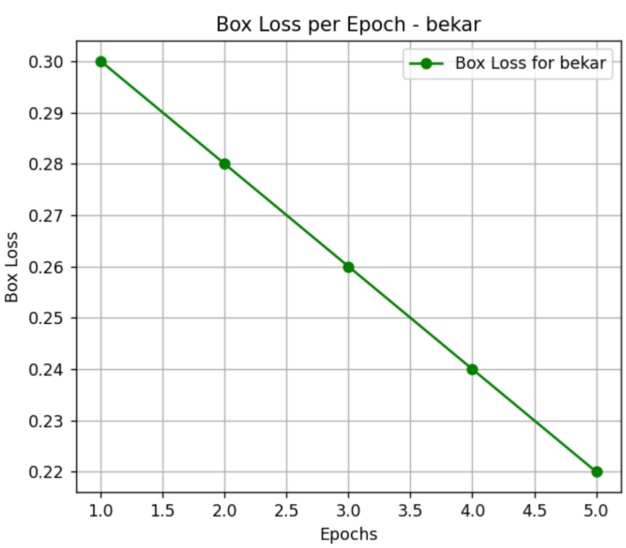
The graph shows all the class's epochs. The machine is trained with 50 epochs, and the x-axis shows the box losses as we used the box model here. Average box losses are 1.2. The maximum box losses are 2.3. A value of 2.3 indicates that the model is still learning and might need further tuning to optimize performance. The more we feed data to the model the more it will train in a more optimized way and it will decrease the losses of boxes in all classes.



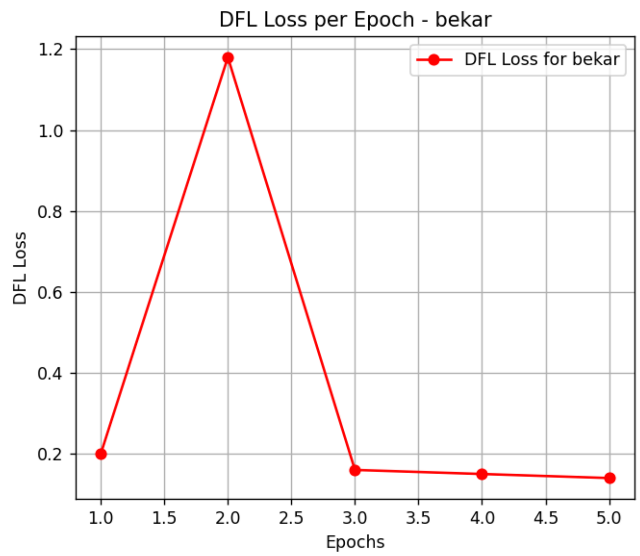
Here, an overall graph analysis is given of this model how it trained how it tested with the test result, how it validated with the result, and the overall performances are shown with the clustering of pixels and color gradients.



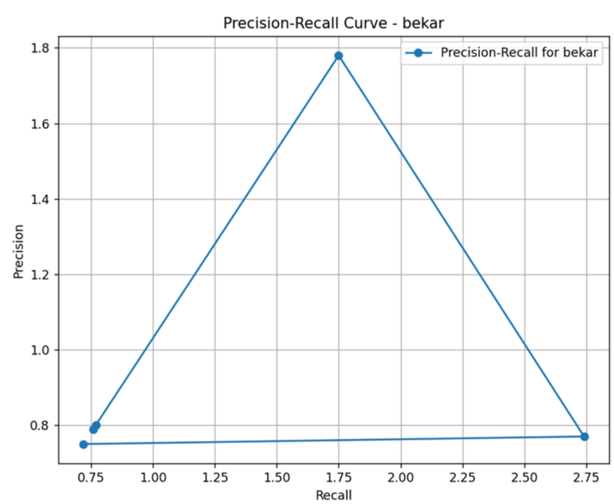
Average Precision (AP) denotes precision across all recall thresholds. It is the area under the precision-recall curve. Recall represents the ratio of true positives detected by the model out of all actual positives.



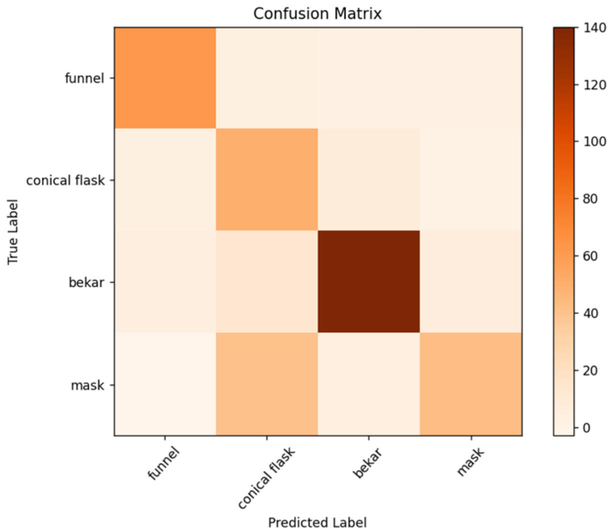
In our machine learning model, we worked with 4 major classes and the beaker is one of them. Here, we micro-analyzed the model of each class where the gradient is in a linear decreasing order. Also, 5 is the maximum range, but a model cannot make that kind of loss so it is not showing that a model is losing the performance. It shows the range of performance which depends on feeding the data to a model.



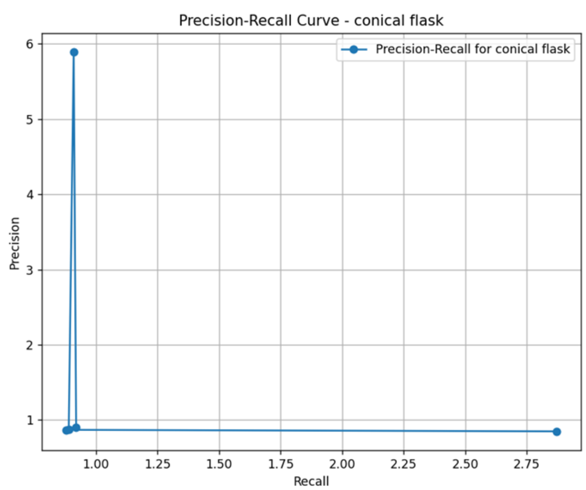
DFL (Distribution Focal Loss) is a loss function used in advanced object detection models, such as those based on the YOLOv5 or YOLOv8 architectures, to improve the accuracy of bounding box predictions. It's designed to address the issue of accurately predicting bounding box coordinates, leading to better localization of objects.



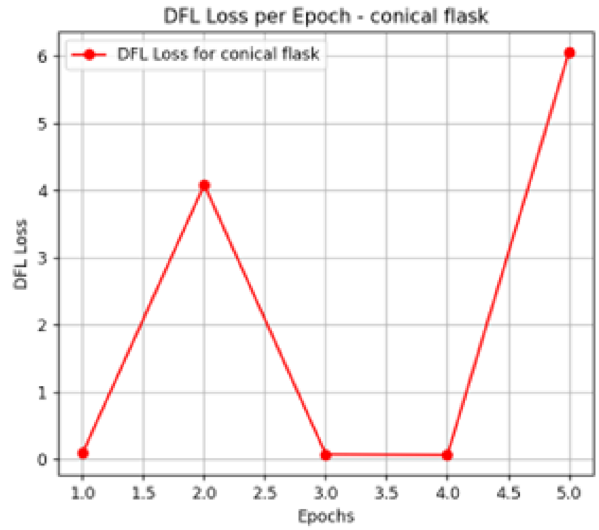
High precision and low recall from this graph indicate we should lower the threshold further to classify a beaker.

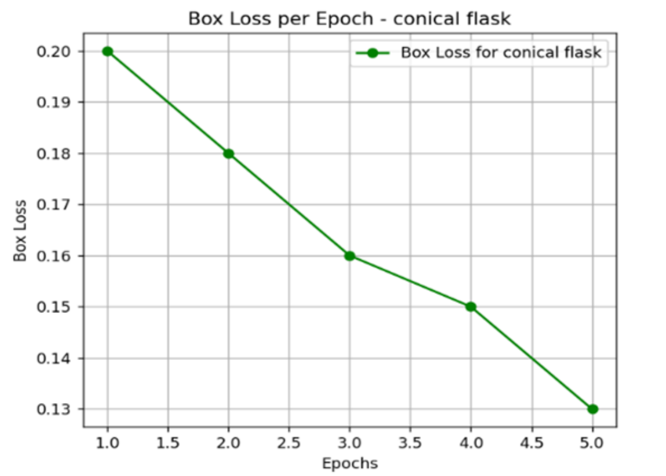


The confusion matrix concludes that the model performs best for beakers and worst for masks.



The Precision-Recall curve of a conical flask shows a value below 1. It's not a negative value that results in a fair prediction.





Here, the box Loss per epoch of a conical flask is in decreasing order. The DFL loss per Epoch of a conical flask increases in the first 20 epochs. Then it decreases the gradient in the 30 to 40 range of epochs. As it gets less feeding on that time, other classes get much data on that time and it decreases the gradient. However, in the last 10 epochs, it increases the DFL loss epoch.

VI. Future Scopes

The test results from the YOLOv5 Tiny proved satisfactory. This is an assurance that there will be further integrations based on Raspberry Pi or any other portable microprocessor systems to implement object detection and many other critical functionalities. The entire procedure will enhance the safety and precise object placement to increase the range of benefits this project can add to our scientific ecosystem.

VII. Discussion

To maintain the standards while solving a complex engineering problem, the following matters raised concerns:

A. P1 - Depth of Knowledge

Sufficient knowledge about the available components has been acquired. However, the knowledge of the Robotic Control System is beyond the reach of the ongoing laboratory course the authors are enrolled in.

B. P2 - Conflicting Requirements

Although the project is for demonstration purposes of a future-large scale industry application, the current prototype has much slower performance than expected due to hardware limitations. The current progress has come with a trade-off between cost and performance.

C. P3 - Depth of Analysis

The analysis of the project and ML model has been done precisely to reach meaningful conclusions.

D. P4 - Familiarity of Issues

The security and productivity issues have already raised a concern among the authors. Therefore, they were familiar with all the latest trends in this field of research.

E. P5 - Extent of Applicable Codes

The current project will try to maintain GMP (Good Manufacturing Practices) standards set by the World Health Organization. It is a set of rules that must be followed in every chemical industry to maximize the safety of technical personnel.

F. P6 - Stakeholder Involvement

Opinions from familiar researchers and lab technicians were taken to set a clear goal for the project. The necessary optimizations were suggested by people in both academia and industry so that the project could demonstrate real-life solutions.

G. P7 - Module Dependency

Hardware and software modules are dependent on each other. For example: the accuracy of the apparatus restoration at the end of an experiment depends on the performance of the linear actuator. If the actuator accidentally malfunctions during the sanitization process, the object detection mechanism to store a piece of particular equipment will fail even though the algorithm behind it is fully functional.

P1	P2	P3	P4	P5	P6	P7
	✓	✓	✓	✓	✓	✓

References

[1] Velikyan I, Rosenstrom U, Eriksson O. Fully automated GMP production of [68Ga]Ga-DO3A-VS-Cys40-Exendin-4 for clinical use. Am J Nucl Med Mol Imaging. 2017 Jul 15;7(3):111-125. PMID: 28721305; PMCID: PMC5511121.

[2] Ross Harper, Derek R. Morim, Dhyey Mehta, Veronika Rosecker, Stephen J. Archibald, Richard Southworth, Philip J. Blower, Karin A. Stephenson, Karin M. Nielsen, Optimised production of technetium-94m for PET imaging by proton-irradiation of phosphomolybdic acid in cyclotron liquid target, Applied Radiation and Isotopes, Volume 210, 2024, 111381, ISSN 0969-8043, https://doi.org/10.1016/j.apradiso.2024.111381. (https://www.sciencedirect.com/science/article/pii/S0969804324002094)

[3] Bobrakov, Anton Kudrinskii, A. Pereslavtsev, A. Polkanov, M. Shiryaevskii, V. Artemov, A.. (2015). Thermodynamic analysis of the processes of plasma treatment of low-level radioactive waste in shaft furnaces. Rossijskij Khimicheskij Zhurnal (Zhurnal Rossijskogo Khimicheskogo Obshchestva Im. D.I. Mendeleeva). 85. 1575-1581. 10.1134/S1070363215060377.

[4] Jacob, Mariam (2024). DEVELOPMENT OF AUTOMATED FAULT RECOVERY CONTROLS FOR PLUG-FLOW BIOMASS REACTORS. Purdue University Graduate School. Thesis. https://doi.org/10.25394/PGS.25606401.v1