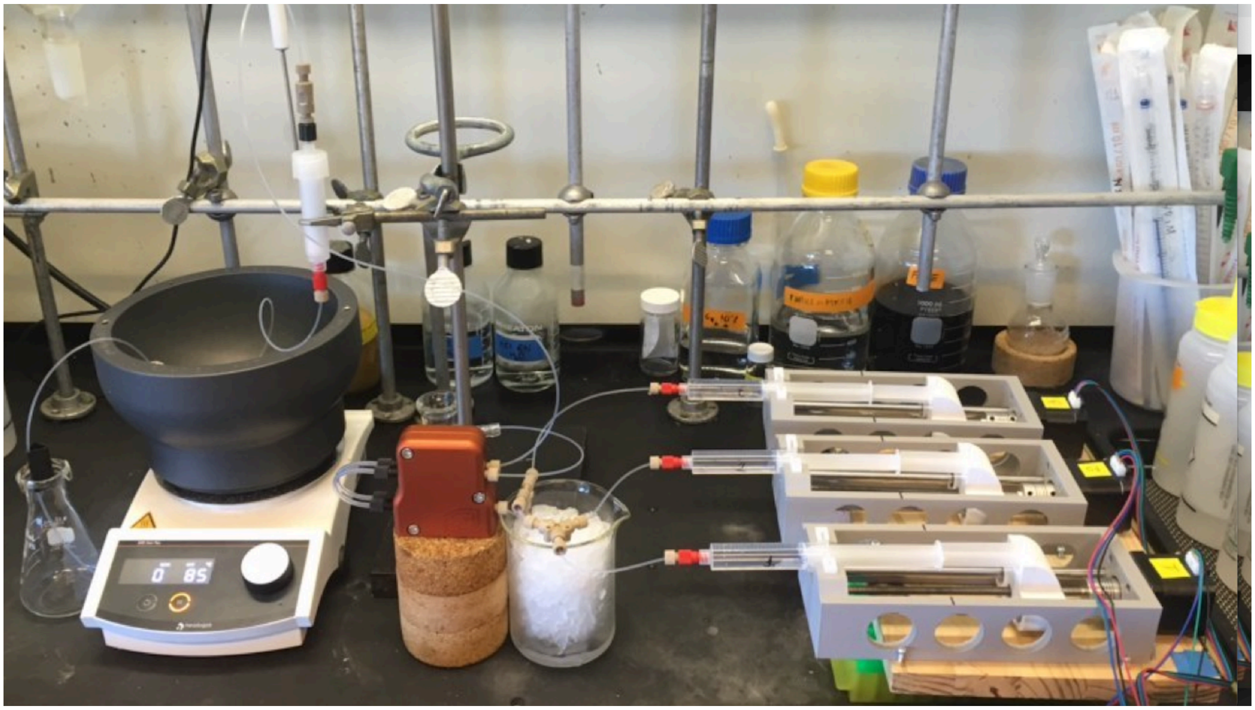
Designing a Flow System for Sustainable Chemistry



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Executive Summary

The practice of synthesizing chemicals has relied on low technology equipment such as glass flasks and pipettes for decades. Flow chemistry was invented in order to modernize and advance the practice of synthesizing chemicals in terms of both safety and efficiency. Flow chemistry consists of pumping reagents into converging tubing in which the reagents mix to form a product. Reactions conducted using flow chemistry techniques are safer due to the smaller volume of hazardous materials reacting at once, are more efficient due to the high surface area to volume ratio which increases the kinetics of the reactions, and exhibit better control because reactors can be kept at specific temperatures and pressures [1]. However, one large downside of flow chemistry is it's substantial price tag. Commercially available systems cost upwards of $20,000. This high price point makes it such that this technology is largely unavailable to academic laboratories and undergraduate students.

The sponsor of this project, Dr. Haim Weizman, a researcher and professor with the Department of Biochemistry and Chemistry, UCSD, hopes to make a chemistry flow system which is cost-effective and accessible to undergraduate laboratories. Various low-cost, DIY (Do It Yourself) flow chemistry systems have already been developed, however, these DIY systems have a number of shortcomings when it comes to ease of assembly and use. Dr. Weizman hopes to improve upon an existing DIY chemistry flow system by placing a greater emphasis on user-oriented design.

The specific flow system being improved upon is the Croatt Research Group's DIY flow system [1]. This system is open access and can be manufactured using only a 3D printer and parts ordered from Amazon for a cost of around $150. The system consists of a carriage which pushes a syringe from within the chassis as can be seen in Figure 1. The motion of the carriage is actuated by a stepper motor which is controlled by an Arduino. The system is commanded by the user who inputs a string of commands to the Serial Monitor of the Arduino.

Issues with this system include non-intuitive user input commands to the Arduino, corrosion of the threaded rod, syringe holders specific to the syringe size as opposed to a single design which can accommodate multiple syringe sizes, and lack of a wire containment strategy.

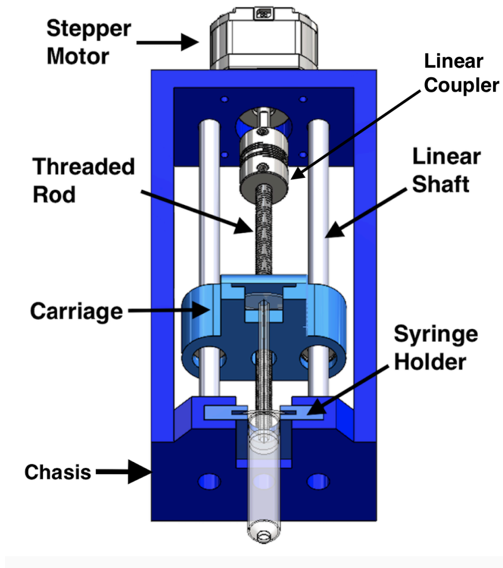


Figure 1. CAD model of Croatt Research Group's flow chemistry system

Specific improvements made to the system include a Graphical User Interface to enhance usability, exchanging the steel threaded rod for a stainless steel one which exhibits enhanced resistance to corrosion, designing a modular syringe holder which can hold syringes of various sizes, and implementing a wire containment strategy which includes an electronics box and cable sleeves. Additionally, servo motors were added to implement automated refill functionality.

The performance of the system [include performance].

Abstract

This project, sponsored by Dr. Haim Weizman of the Department of Chemistry and Biochemistry at UCSD, focuses on the improvement of the Croatt Research Group's DIY flow chemistry setup to enhance its usability. This project's motivation is to increase the prevalence of flow systems in undergraduate laboratories to grant students positive, hands-on experience with modern chemistry techniques. The Croatt Research Group's system includes a 3D printed chassis and carriage assembled with a threaded rod and linear shafts. A stepper motor is attached to the threaded rod which rotates to advance the carriage and depress the syringe plunger. The Croatt Research Group's system is controlled by Arduio and user input from the Serial Monitor. Major requirements for the improved system include a straightforward user interface, anti-corrosive materials, a modular syringe pump, and compact housing of the electronics. The system should be accompanied by a simple assembly and operations manual. To achieve these requirements, a GUI, modular syringe holder, and electronics containment box were integrated into the Croatt Research Group's flow system. Steel components were replaced with stainless steel to enhance resistance to corrosion. Major results of this project include an intuitive user interface that is capable of commanding multiple syringe pumps to dispense liquid at the desired rate.

Chapter 1: Project Description

Background:

The practice of synthesizing chemicals has relied on low technology equipment such as glass flasks and pipettes for decades. These practices are outdated in a world of modern technology and leave a great deal to be desired in terms of both safety and efficiency. Flow chemistry was invented in order to modernize and advance the practice of synthesizing chemicals. In flow chemistry, reactions are conducted continuously as reagents are pumped through tubing and mix to form a product. Figure 1 presents a schematic diagram demonstrating the process of flow chemistry.

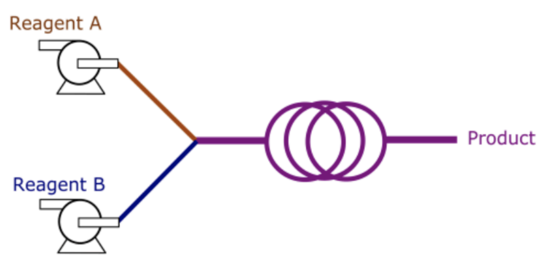


Figure 2. Flow chemistry schematic [2].

Flow chemistry exhibits numerous benefits over traditional laboratory techniques. Reactions are safer due to the smaller volume of hazardous materials reacting at once, are more efficient due to the high surface area to volume ratio which increases the kinetics of the reactions, and exhibit better control because reactors can be kept at specific temperatures and pressures [2]. Additionally, flow chemistry is more environmentally friendly and has generated new ways to manufacture sustainable materials. However, one large downside of flow chemistry is it's substantial price tag. Commercially available systems cost upwards of $20,000. Figure 2 displays a $20,000 chemistry flow system located in the Burkart Laboratory, UCSD. This high price point makes it such that this technology is largely unavailable to academic laboratories and undergraduate students.

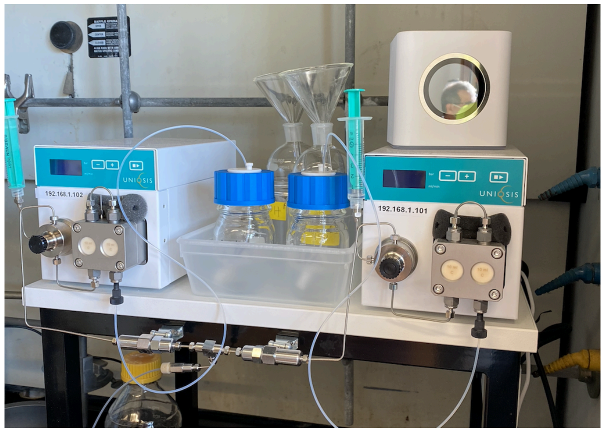


Figure 3. $20,000 flow chemistry system.

The sponsor of this project, Dr. Haim Weizman, a researcher and professor with the Department of Biochemistry and Chemistry, UCSD, has primary research interests of improving organic chemistry instruction at a college level and developing comprehensive laboratories to better train chemistry majors. Dr. Weizman hopes to use this flow system to advance these interests. By developing a chemistry flow system which is cost-effective, it will be more accessible to undergraduate laboratories. Although many universities are capable of securing high-end equipment for their laboratories, this equipment is often restricted for use by graduate students and professors. Therefore, undergraduates miss out on valuable learning opportunities due to the limited availability of high-end equipment, and due to the restrictions placed on its usage out of caution so that untrained students do not damage the costly equipment. However, with the introduction of low-cost flow systems, it will be easier for labs to acquire multiple systems for undergraduate students to use. Additionally, if an untrained student were to break the system, each component is low-cost, so that no major financial burden would be induced on the university or the student.

Dr. Weizman has also emphasized the importance of creating a flow system which is user-friendly to improve chemistry instruction. With chemistry being an already difficult major, Dr. Weizman wants to introduce no further obstacles in the path of student's completion of their education. The Croatt Research Group's system, as well as many other DIY flow systems, require users to input commands to the Arduino Serial Monitor. This may be out of the comfort range of many undergraduate chemistry students and add a level of complexity which may deter them from future chemistry labs. By creating a simple, aesthetic, and straightforward user interface, Dr. Weizman aims to remove any difficulties or mental blocks associated with the Arduino Serial Monitor chemistry flow system. With a pleasing and intuitive GUI design, student's will hopefully be inspired to pursue chemistry as their major and future career path.

Review of Existing Design Solutions:

Other researchers and professionals have likewise recognised the need for a cost-effective alternative to the costly commercially available flow systems. Therefore, various low-cost, DIY (Do It Yourself) flow chemistry systems have been developed. Namely, the Croatt Research Group at UNC, Greensboro has developed a DIY flow system which is open access and can be manufactured using only a 3D printer and parts found on Amazon. This system costs around $150 total - roughly a 100th of the cost of commercial systems which can cost up to $20,000 for a high end system. The system consists of a syringe pump actuated by a stepper motor which is controlled with an Arduino by sending commands through the serial monitor. Figure 3 displays a model of the Croatt Research Group's system [1].

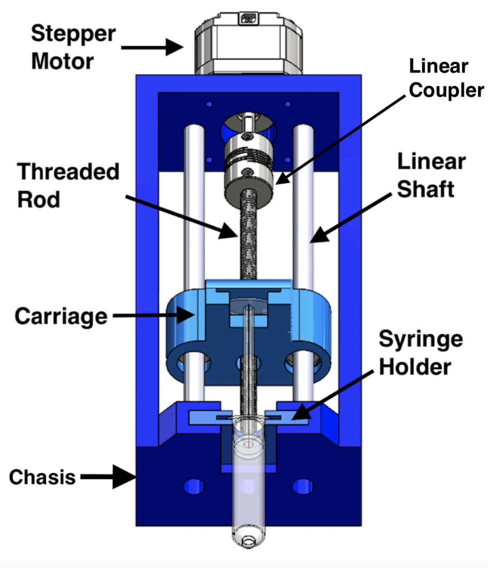


Figure 3. CAD model of Croatt Research Group's flow chemistry system.

The Croatt Research Group's system functions as a basic flow system, however, the overall user-friendliness of the system leaves something to be desired. A computer must be connected to the Arduino in order to control the system. Space is highly limited in many laboratories, so having a laptop connected to the system poses an inconvenience. And while the electronics will be outside of the fume hood and away from chemicals, it would be better to avoid having an expensive laptop in close proximity to the chemical workspace. Therefore, a stand-alone syringe pump system is more desirable in a lab environment and or when there is no access to a laptop. Additionally, the user input commands to the serial monitor on the laptop are not intuitive, especially considering that many chemistry students have limited experience with coding. Furthermore, the Croatt Research Group's system offers little in terms of wire management. As can be seen in Figure 4, many wires are needed to connect the components of the system, resulting in a large nest of wires. Having exposed and mismanaged wires is inconvenient and unsafe to have in a chemistry laboratory. Another issue with the system is that the steel threaded rod experiences corrosion after being left in the fume hood while reactions take place. The system fits syringes of size 1,3,5, and 10 mL. The syringe holder is specific to the size of syringe being used, so multiple differently sized syringe holders are required, along with steps to exchange them when a different syringe is used.

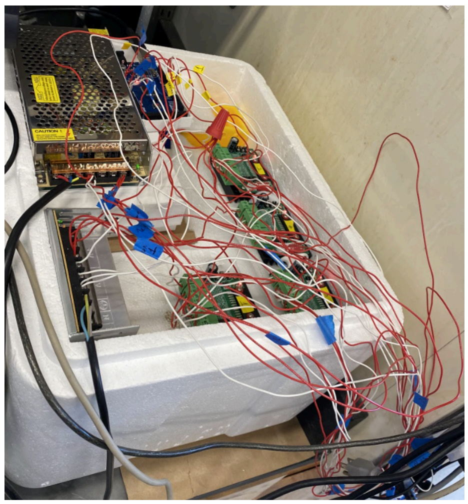


Figure 4. Arduinos and power supplies used to run four flow systems simultaneously. Picture taken from the Burkart Laboratory, UCSD. .

A second cost-effective solution to flow chemistry was created by engineer David Florian and published on his website Dr. D-Flo. This system is similarly open access, and can be created with a 3D printer and parts ordered from McMaster-Carr and Amazon for a total cost of $200. Also operated with a stepper motor and Arduino, the main external difference between this system and the Croatt Research Group's is the use of an aluminum rail as opposed to a fully 3D printed chassis. Figure 5 displays David Florian's syringe pump design as manufactured by the Burkart Laboratory, UCSD.

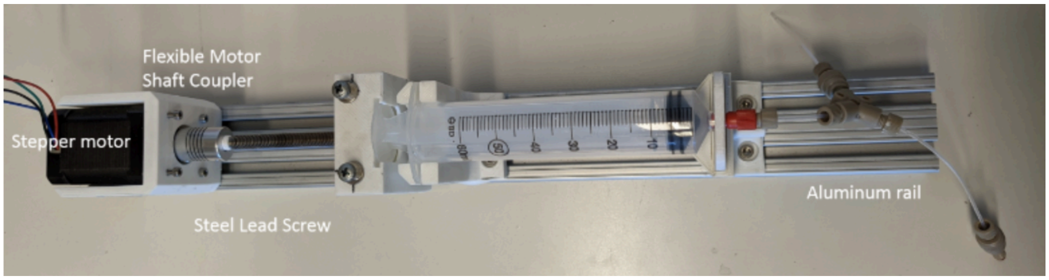


Figure 5. David Florian's syringe pump design.

This design presents the same issues as the Croatt Research Group's in terms of non-intuitive user-input commands, limited wire management solutions, and corrosion of the steel lead screw. Syringes of sizes ranging from 15 to 50 mL can be used with this system. However, changing the size of the syringe requires modifying the 3D printed syringe holders.

A much more expensive syringe pump system that was found during the research process is the Standard Infusion Only PHD Ultra Syringe Pumps. They usually cost in the range of 2,500 to 5,000 USD which is 5 times the maximum set cost to make the current system. This system uses a mechanical driving mechanism that resembles the Croatt Group's mechanism as it features a lead screw that when rotated by a stepper motor pushes a carriage that pushes the plunger of a syringe. This system also includes two low-friction guiding linear shafts for the carriage and a modular syringe holder design. The main changes we made to the Croatt Research Group's design include a design change in the syringe holder to facilitate the use of different size syringes.

Figure XX. Standard Infusion Only PHD ULTRA™ Syringe Pump

Statement of Requirements and Deliverables:

High Priority Objectives:

1. Implement an intuitive user-interface to control the system
2. Design a modular syringe pump that can fit various sizes of syringes (1,3,5,10 mL).
3. Enhance resistance to corrosion of threaded rod.

Second Priority Objectives:

4. Provide an alternative design for refilling the syringe that doesn't rely on expensive check valves.

WOW Design Solution:

5. A system that can detect leaks and shut down the system when they occur.

Deliverables:

1. Flow Chemistry System
    a. Two complete syringe pumps, including syringe holder and refill mechanism
    b. Graphical User Interface
    c. Display Holder
    d. Electronics Containment Box
2. Documentation
    a. User Manual
    b. Manufacturing procedures
    c. Code files
    d. CAD (Computer Aided Design) and STL files
    e. BOM

Chapter 2: Description of Final Solution

Functional Requirements

The chemistry flow system must have the following functional requirements:

- Conduct reactions in a continuous flow stream
- Refill syringes
- Be controlled by an intuitive user interface
- Accurately dispense chemicals for flow rates from (add range here)
- Accommodate syringe sizes of 1, 3, 5, and 10 mL
- Control four syringe pumps simultaneously

Design Solution

The final design solution consists of a total of four major components: the syringe pump, the refill mechanism, the electronics and associated coding, and the electronics containment box. Modifications were made to the Croatt Research Group's design to meet the functional requirements of the system.

Syringe Pump

This design was taken directly from the Croatt Research Group's system due to its proven efficacy and simplicity of design. It is easy to understand how the system works and it is very inexpensive to manufacture. There are not that many different kinds of chemical containers, and syringes would work well if the rate the plunger is pushed is carefully controlled. Stepper motors are very reliable at regulating their steps, so they can be used in the system for this purpose of carefully regulating the linear motion of the syringe plunger. Based on the Croatt Research Group's design, there is a mechanism that translates this rotational motion of the motor into a linear one, so their existing design was taken as the base and modifications were made to enhance the performance of the system. These changes included modifying the syringe holder so that syringes of size 1, 3, 5, and 10 mL can fit in a single holder. Minor changes were made to the carriage as well in order to accommodate the changes made to the syringe holder. The threaded rod, previously made from steel, was replaced with a stainless steel threaded rod in order to enhance resistance to corrosion.

The first component is the syringe pump system itself. The system consists of a 3D printed chassis, carriage, and syringe holder, as well as two linear rods, a threaded rod, a linear coupler, and a Nema 17 Stepper motor, as can be seen in Figure xx. The threaded rod in conjunction with a nut embedded in the carriage translates the rotational motion of the stepper motor into linear motion of the carriage which is guided by linear rods. As the stepper motor rotates, so does the threaded rod and the carriage is either advanced forwards or backwards depending on the direction of rotation. The plunger of the syringe is mated in a slot on the carriage and so as the carriage moves so does the plunger of the syringe in order to draw in or extrude chemicals from the syringe. The motion of the system can be seen in Figure xx.

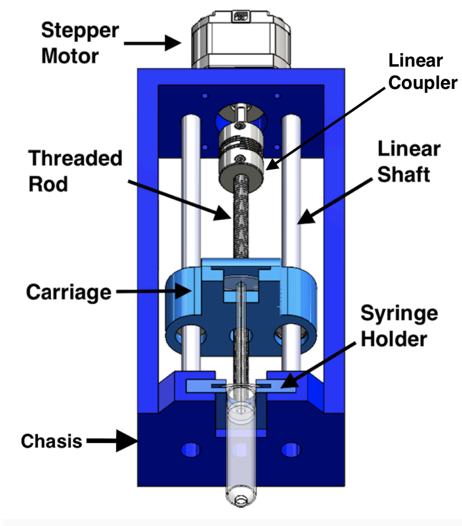


Figure xx. Main Syringe Pump Components.

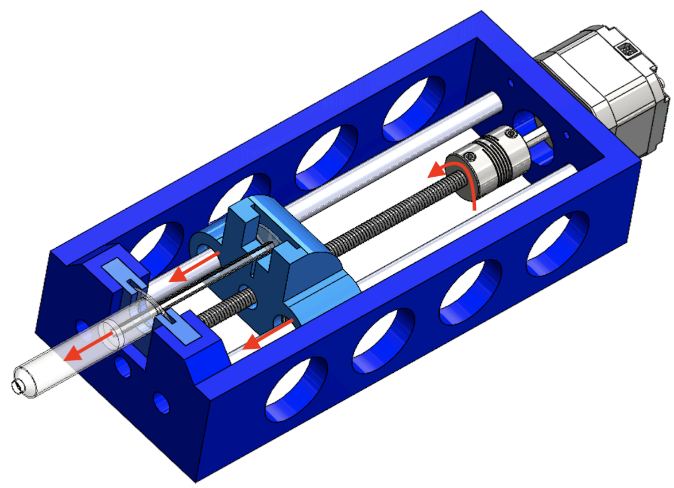


Figure xx. Indication of Motion.

Refill Mechanism

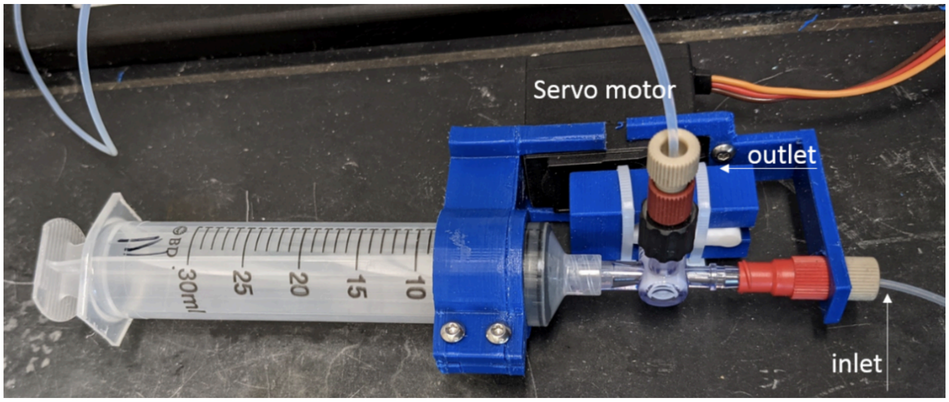


Figure xx. Servo motor-Syringe-Stopcock Connection. [Burkart Laboratory].

The second major component of the flow system is the servo motor - stopcock refill mechanism. The parts for this mechanism include a servo motor, a three-way stopcock, a 5-volt power supply unit to power the servo motors, and 3D printed parts to both mount the servo - stopcock mechanism to the syringe. The stopcock valve is able to control the direction of the flow between the refilling and dispensing stages depending on the position of the stopcock latch. For refilling the syringe the stopcock latch is oriented such that the flow channel from the chemical reservoir is open, but the flow channel into the main tubing where reactions take place is closed. Otherwise, when the is set to dispense fluid, the latch of the stopcock is flipped by the servo motor, allowing chemicals to flow into the main tubing, but restrict flow to the chemical reservoir.

Graphical User Interface (GUI)

The third major component is the graphical user interface that controls all the syringe pump systems. The user interface represents both the hardware that displays the graphics and the software for designing the GUI. The hardware selected for our user interface is the Nextion 7” Intelligent Series touchscreen display because it includes easily programmable software for graphical user interface design and is compatible with Arduino. The key functionality of the graphical user interface is that it has an intuitive layout where the user can easily set up one or more syringe pumps to perform flow chemistry experiments. In order to perform these experiments the user interface is able to receive and collect user input on syringe pump parameters when the user presses these specific buttons on the touchscreen display which can be seen in both figure () and (). These parameters include pump mode, syringe inner diameter, volume, syringe size, flow rate and either the dispense/withdraw option.

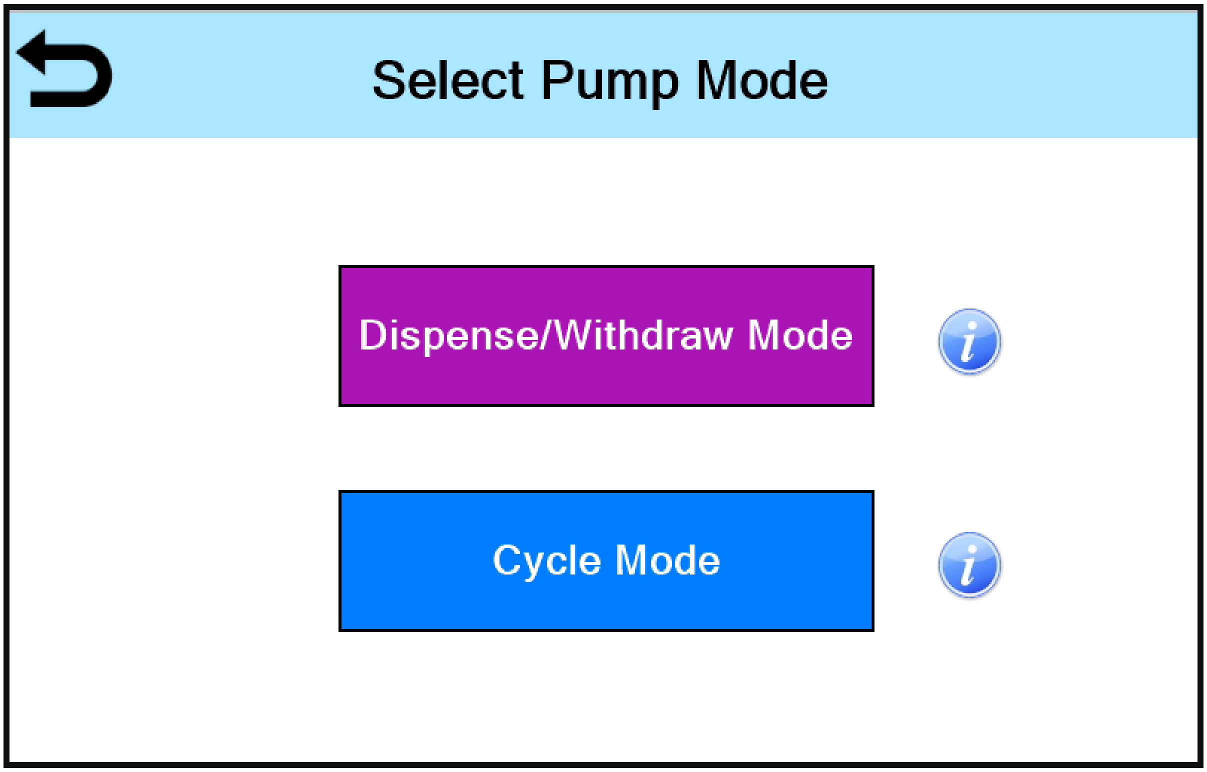


Figure xx. The *Select Pump Mode* page of the user interface.

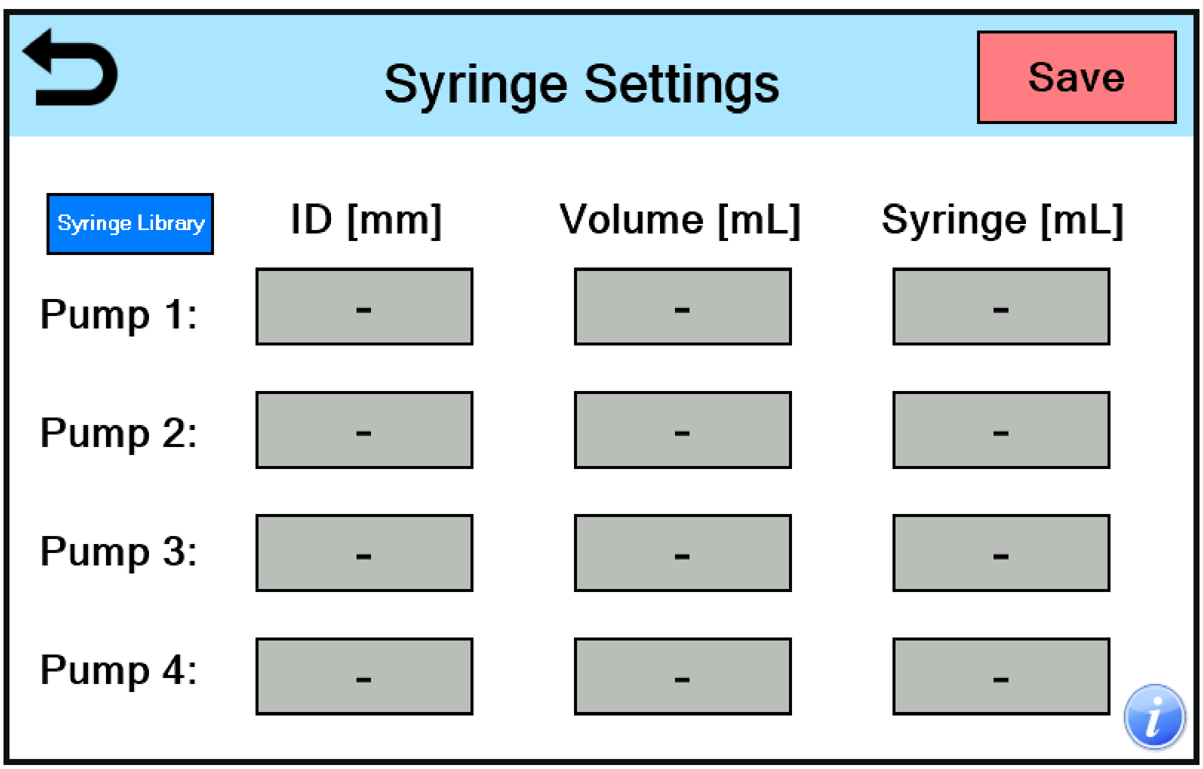


Figure xx. The *Syringe Settings* page of the user interface.

Once the pump parameters are defined by the user, the pump(s) is able to be run using the user interface as well as be paused or resumed during the entirety of the operation. Its volume output progress is continuously tracked on the run status page of the display which can be seen in figure (). In order for this to occur, the Nextion display is able to communicate with Arduino. This includes sending data from the Nextion display to the Arduino serial monitor to set the syringe pump parameters and to start the operation. Also, data is able to be sent from Arduino to the Nextion display in order to track the progress of the syringe pump. The Arduino Mega 2560 microcontroller board is what is used to control the syringe pump system directly and is the fourth major element of the design solution.

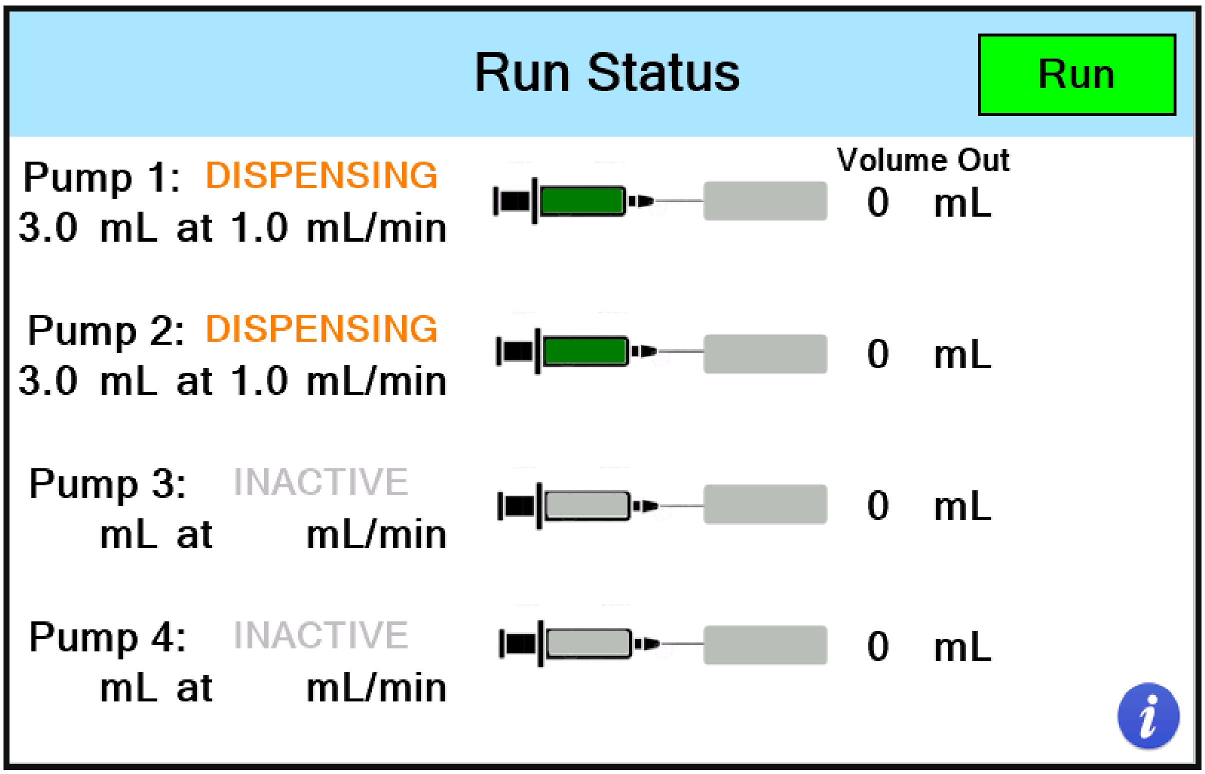


Figure xx. The *Run Status* page of the user interface.

Electronics and Code

The fourth major element of the design is the electronics and code. The electronics feature an Arduino Mega 2560 and one motor driver for every stepper motor in the system. The code to control the system was written using the Arduino software. The only external library used in the code is the AccelStepper library. We chose to use this Arduino library to control the stepper motors because it allows for multiple stepper motors to be controlled simultaneously. Serial communication is used for communication between the Arduino and Nextion touchscreen. A schematic of the electronics wiring for the entire system can be seen in Figure XX.

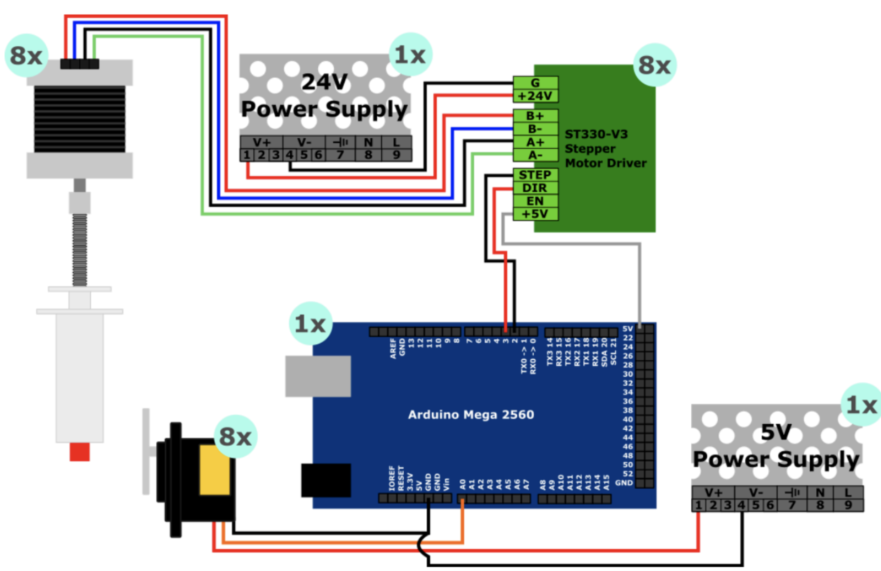


Figure xx. Electronics Schematic [3].

Each of these four components come together to make up the flow chemistry system. The user interface sends commands to the Arduino, which in turn controls the motors and functionality of the syringe pump. As the syringe pump is operating, the stopcock valve ensures that the flow of chemicals is in a singular direction. Figure XX. displays a simple schematic of how each component operates within the flow system as a whole.

Functional Requirements

The system must accurately pump chemicals out at a specified flow rate. While this accuracy is important, it is even more important for multiple syringe pumps to be consistent with each other. That is, they all need to be precise with respect to each other because, in chemistry, it is more important to have the ratio of chemicals in a reaction to be correct than to have the actual amount correct. Thus, it is acceptable to have a bias in the system as long as all pump systems have the same bias. In order to achieve the flow rates desired, the speed of the stepper motor must be adjusted accordingly, depending on the dimensions of the syringe and the number of motor steps needed per volume amount. Provided that there is little friction in the system, the stepper motor will be able to reliably rotate at the desired speed controlled by the pulse signals from the Arduino.

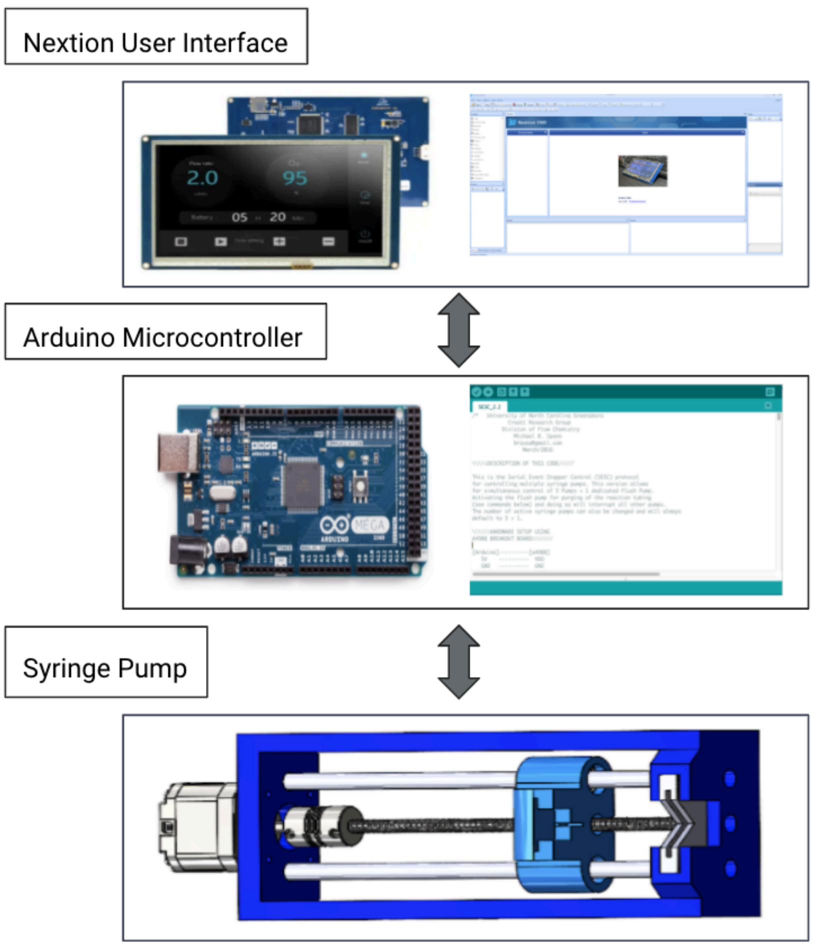


Figure xx. Schematic of System Connections.

Performance Results

(TBD - describe performance results quantitatively)

Chapter 3 : Design of Key Components

Major components:

- Graphical User Interface (GUI)
- Microcontroller
- Modular Syringe Holder
- Electronics Containment Box
- Lead Screw Actuator

Graphical User Interface (GUI)

An important aspect of this system is having a suitable user interface that is easy to understand and use. The system is to be used by students and others looking to get into chemistry, and this audience might not have much experience handling electronics and programming. As such, it is essential to have an interface that can be operated by anyone.

Initially, there were a variety of different options that could be used for this interface. The existing design from the Croatt Research group utilized a bluetooth app as a way to control the syringe pump. While this is a valid solution, it requires an Android phone and users may be resistant to the idea of having an app for work or school installed on their personal devices. One could buy a low-cost Android phone specifically for the purpose of this system, but even the lowest prices range around $100. In addition, the app that the Croatt Research group developed was unavailable, so any app would have to be fabricated from scratch.

Another possibility was having an LCD screen with a physical control panel of knobs and sliders that can be used to adjust the settings of the syringe pump system. While it is feasible, a touchscreen interface is generally easier to work with and integrate into the system. The touchscreen greatly reduces the amount of wiring needed because it only requires a single cable connection, versus the multitude of connections needed to implement in a physical control panel. In addition, LCD displays generally come in smaller sizes, so to display all the wanted data, multiple screens or one large screen would be necessary. Though, with a larger screen, it is not much of a leap to simply go with a touchscreen LCD display. The price point is quite similar and any additional settings and options can be handily developed for the touchscreen device. Any such updates and changes to the UI to improve the function of the system would just need to be downloaded onto the device. With the non-touchscreen display and the control panel, more physical buttons and such would need to be bought and integrated into the control panel for any additional changes and options. In the end, under the guidance of this project's sponsor, a touchscreen device was chosen to be the user interface as it is very adaptable and is easy to use.

Functional Requirements

The user interface must be able to send commands to the microcontroller in order to control the servo and stepper motors. It must also be able to receive data regarding the current position of the stepper motors from the microcontroller. Also, as the setting for this system will be in a chemistry lab, it would be important that the touchscreen is suitable for this environment. The touchscreen will have to be a resistive type as those types of touchscreens can be operated when wearing a glove or with a stylus. Capacitive touchscreens are the other common type of screen, but these touchscreens rely on the conductive properties of the human body. So, this would require that users use their bare fingertips when using the touchscreen, which can be quite dangerous in a lab full of chemicals. Furthermore, since chemicals could accidentally come in contact with the screen, a stylus would be used as well as a suitable screen protector to prevent damage.

Comparison of Designs Considered

	Nextion 7” Intelligent Display	Adafruit Touchscreen	Touchscreen with Arduino shield
Screen Dimensions	7” x 3.4”	4.7” x 3”	7” x 4”
Screen Type	Resistive	Resistive	Resistive
GUI Design Software	Nextion Editor	None, code from Arduino	None, code from Arduino
Cost	$90	$40	$70

Table XX. Comparison of GUI Design Considerations

Final Choice

The Nextion Intelligent HMI Display touchscreen was selected as the user interface in the final design. The Nextion touch screen has a lower learning curve when compared to other user interface software design due to its free Nextion Editor Software which features drag-and-drop components. The touchscreen is resistive which means that it will be able to be used even when the user is wearing gloves.

The Nextion touch screen is a little more expensive than all the other options considered, but its software allows developers to easily design a GUI by dragging in components such as buttons and sliders. Touch events can be coded in the software with simple commands and the Nextion can output data via serial communication, perfect for communicating with the Arduino.

This saves a lot of time for developing the GUI as elements do not need to be coded in by hand, and it is easier to work on the display if you can see what is going on as you edit the screen.

The advantage of touchscreen has been thoroughly discussed earlier, no need to repeat

Figure xx. Nextion Basic Series 7" touchscreen display

Software and Programming

The Nextion Editor Software allows buttons and text to be programmed according to one's needs. It can also print information over Serial to a microcontroller. Essentially, this is the method of communication currently being used between the touchscreen and Arduino. Once the data is done printing over to the Arduino, it is just a simple matter of processing the string and changing the parameters of the system accordingly. This software provides a significant advantage as opposed to designing the user interface from scratch, and was therefore a key factor in the decision of the user interface selection.

Microcontroller

The Arduino Mega 2560 was chosen as the microcontroller to be used in the design. This particular Arduino meets all of the functional requirements listed below, and has a number of other positive attributes.

Arduino is an open-source hardware and software company. Arduino products are cost effective and may be interfaced to various other circuits and breadboards. Arduino is one of the most commonly used brands of microcontroller and can be purchased from a number of suppliers for low prices.

After comparing various Arduino and Raspberry Pi microcontrollers, the Arduino Mega 2560 was selected as it is easily accessible and inexpensive.

Functional Requirements

The microcontroller must be able to control four stepper motors and four servo motors. Therefore, it must have eight digital pins (two for each motor driver) and four analog pins (one per servo motor). In addition, the microcontroller should have pins reserved for Serial communication (a TX pin and RX pin). Generally, most Arduinos have these pins on digital pins 0 and 1, so these should be reserved only for Serial communication (not counted with the other eight pins required for the stepper motors). The microcontroller must also have an available 5V pin and the ability to connect to a power supply or wall outlet. This enables the user to use the system without an external power supply which would reduce the total cost of the system.

The microcontroller must also be able to interface with the GUI. It must be able to receive commands from the GUI over Serial and receive position data from the motor (from the AccelStepper Library).

Comparison of Designs Considered

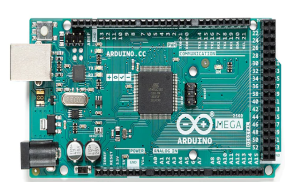
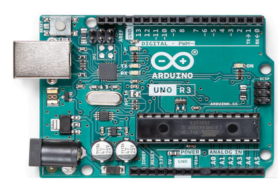
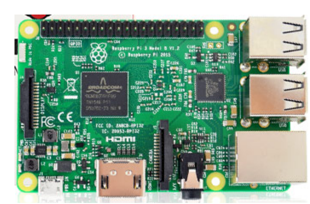
	Arduino Mega 2560 	Arduino Uno Rev3 	Raspberry Pi 3 Model B 
Operating Voltage	5V	5V	5V
Input Voltage (recommended)	7-12V	7-12V	4.75-5.25V
Input Voltage (limit)	6-20V	6-20V	4.75-5.25V
Digital I/O pins	54	14	26
Analog Input pins	16	6	14

Table XX. Comparison of Microcontroller Design Considerations

Justification of Final Design Choice

The Arduino Mega 2560 was ultimately selected to be used in the final design. The choice of microcontroller was first narrowed down to an Arduino due to its compatibility with the code provided by both the Croatt Research Group as well as the Burkart Laboratory. The Arduino Mega 2560 was selected due to its greater number of digital I/O pins which will allow for additional syringe pumps to be added to the system if desired. However, any Arduino model with a sufficient amount of pins will suffice for this system.

Electronics Containment Box

The electronics containment box is intended to house all of the electrical components excluding the power supplies. It also serves as a mount for the user interface.

Functional Requirements

The electronics containment box must provide an enclosure for the electronics and have multiple points of exit for the wires to extrude from. It is important that there is sufficient room for the wires to protrude from each of the components so that the bend radius of each wire is not exceeded. Easy access to the wires and electrical components should be maintained at all times, therefore there should be no permanent sealing of the box.

The electronics containment box must:

- Fits four motor drivers, one Arduino Mega 2560, one breadboard.
- Mount the user interface.
- Provide easy access to all connections and electrical components.
- Provide necessary cooling to all components.

The containment had to be designed to be properly ventilated to reduce heating of the motor drives and the controllers. The (12V?) power supply including the additional 5V power supply for the servo motors remain outside the containment inorder to reduce complications with cooling.

Comparison of Designs Considered

The first design featured a single solid structure with openings to place the components and the touch screen. However this design faced numerous complications:

- 3D printing the singular solid structure was not possible as the dimensions exceeded the limit of the 3D printer.
- Tight fitting of all the components resulted in wires disconnecting and causing issues with the functioning of the system.

- Once assembled, the interior electronics are not easily accessible in order to make corrections or changes.

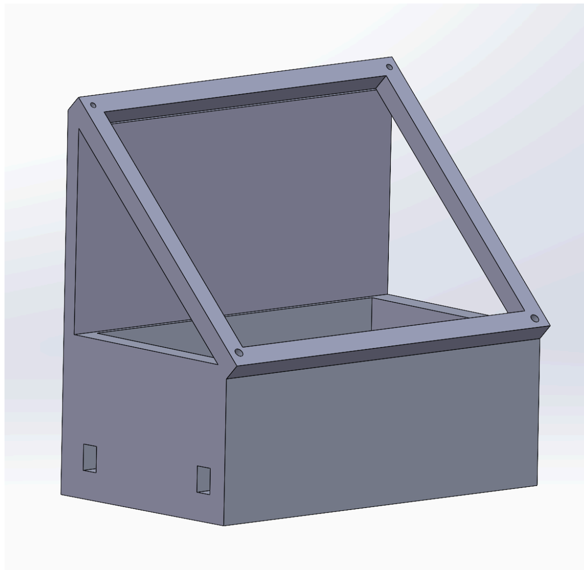


Figure xx. Electronics Containment Preliminary Design

The second design was then modeled where the entire enclosure would be made out of two parts to fix the issues with the first design. The top lid and the bottom container would fit using snaps. However, the design considered was not made with respect to the limitations of the 3D printer bed. Therefore, it had to be scaled down and the layout of the components inside the box had to be rethought in order to reduce the footprint of the box. Also, 3D printing snaps were not efficient as they were not accurate after the print.

The third design fixed these constraints. The two parts were scaled down in order to be easily printed on a 3D printer. The lid was fitted using a rail mechanism. This made it easier to access and assemble the electronics. There was a slot and a rest made on the lid for the placement of the stylus.

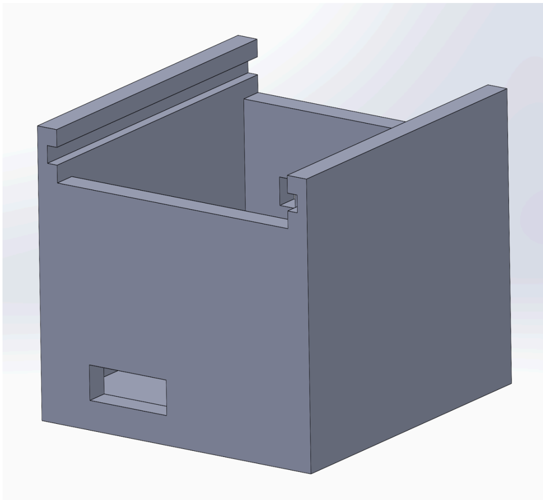


Figure xx. Electronics Containment Box (resized and edited to support the new orientation)

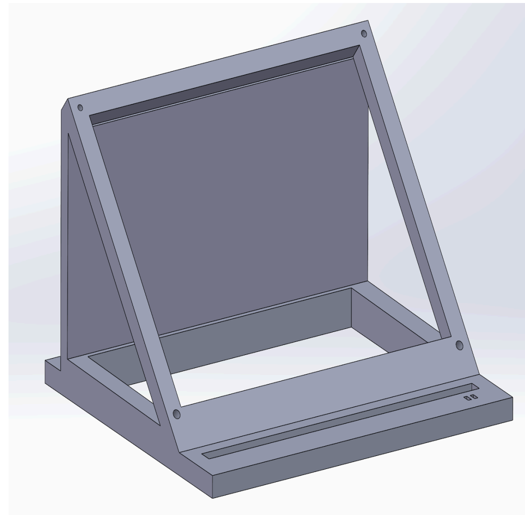


Figure xx. Electronics Containment Box Lid

The final design considered was a purchased electronics case with circular cutouts for the wires to come out from. This design circumvented all of the 3D printing issues and is only marginally more expensive than it would have been to 3D print the electronics box, accounting for the cost of filament used. Additionally, this design enhances the ease of manufacturing of the design because users do not have to struggle with 3D printing and print multiple iterations of the electronics box in order to get satisfactory results. Therefore, this design takes into consideration the potential novice of the iser when it comes to 3D printing, and drastically reduces the manufacturing time needed to assemble the system. Two versions of this electronics box were considered. The larger option was considered due to its ability to contain the power supply and protect it from any potential chemicals on the laboratory work bench. However, the smaller option was ultimately chosen due to concerns about heat generation front he power supply. In general, it is not recommended to store heat generating components in closed spaces along with other electrical components. It was determined that the risk of potential spills on the workbench were of lesser concern than heat generation within the electronics box.

Figure XX. Large Electronics case with Innterface

Figure XX. Large Electronics case (10 x 7.9 x 3.1”).

Designs Considered	**Pros**	**Cons**
Single 3D printed box	● None	● Difficult to reach wires ● Difficulties with 3D

		printing ● Does not fit on 3D printer bed ● 20 hours + of printing time ● Unprotected power supply
Two part 3D printed box	● Ability to access electrical components with ease ● Customizable	● 18 hours+ of printing time ● Unprotected power supply
Electronics case (Extra Large)	● No printing time needed ● No manufacturing errors need to be considered ● Increased waterproofing and protection of interior electronics, including power supply	● Less customizable ● Cost: $24 ● Internal heat generation of power supply
Electronics case (Large)	● No printing time needed ● No manufacturing errors need to be considered ● Increased waterproofing and protection of interior electronics, excluding power supply	● Less customizable ● Cost: $21 ● Unprotected power supply

Lid Design

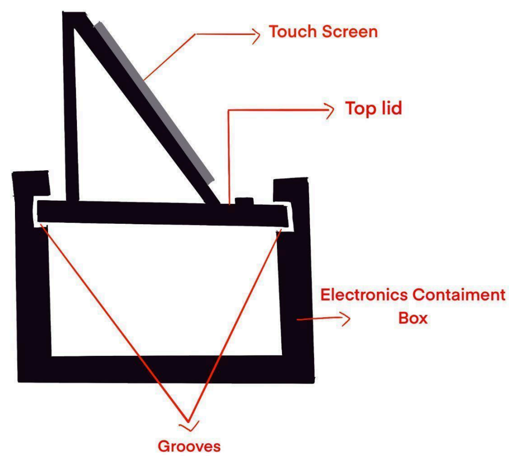


Figure xx. Lid fitment with the electronics containment

User Interface Mounting Design

With the Nextion 7inch display with enclosure, the top lid design was changed in order to support the new fitment of the interface. The approach was shifted to an out-front fitment instead of a slit from the back of the lid. This makes it easier to fit the interface and reduces potential for human error or breakage. The overall size of the angled support was increased to support the enclosure and cut outs were made on the side to feed the interface wires into the electronics containment.

Modular Syringe Holder

The modular syringe holder is one of the high priority objectives in the project proposal. The syringe holder is intended to be capable of holding syringes of 1, 3, 5 and 10 mL capacity without any alterations being made to the system.

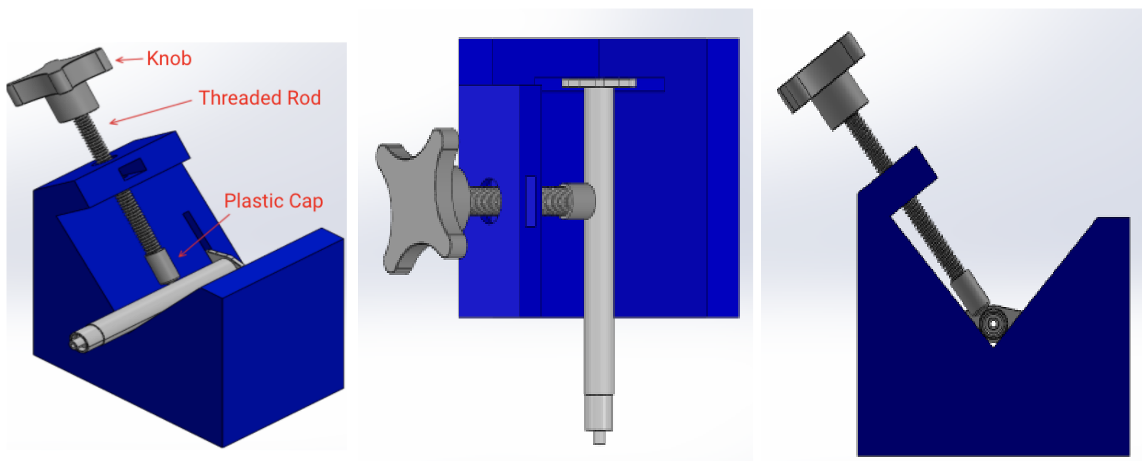
Functional Requirements

The syringe holder must:

- Be capable of securely holding syringes of 1,3,5 and 10 mL capacity.

Comparison of Designs Considered

The first design under consideration utilized a screw with a hex nut embedded into a slot that is inside the ledge of the chassis in order to hold the syringe securely in place as can be seen in figure xx. The barrel of the syringe rests on the triangular shaped chassis design which provides the advantage of being able to fit any size syringe. The flange of the syringe (refer to figure xx in appendix for syringe anatomy) is captured within a thin slot so that the syringe is fixed in place when force from the carriage is applied to it. A screw with a knob on one end and a plastic cap on the other would be used to tighten down on the barrel of the syringe to provide extra resistance to motion. In order to avoid the issue of not being able to tap 3D printed material, this design includes a nut inserted into a cavity in the 3D print so that the screw has threads to properly rotate within. Another solution to this issue is a heat set insert, however this was avoided due to extra manufacturing steps that it would create.



(a) Isometric (b) Top (c) Front

Figure xx. Set Screw Modular Syringe Holder

The second design considered was the syringe holder designed by the Mass Spectrometry Research Group with the Analytical Chemistry Division in the Chemistry Department of Moscow State University as seen in Figure xx [4].

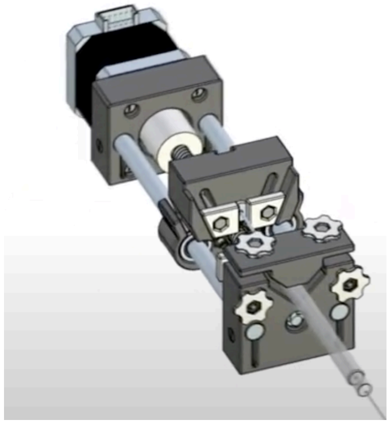


Figure xx. Full syringe pump model [4].

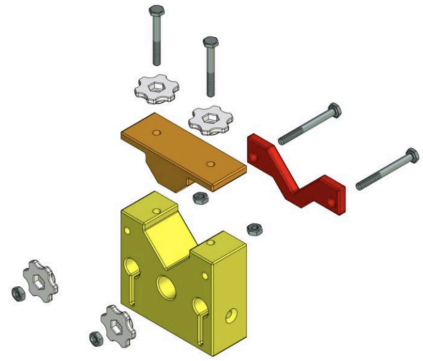


Figure xx. Assembly instructions for syringe holder [4].

While this design has its merits and fultils the functional requirements of the syringe holder, it also has a number of the same disadvantages as the previous design. The need to tighten screws to secure the syringe allows for the possibility of overtightening. This design also requires additional hardware and assembly as seen in Figure xx. Therefore, a third design was developed.

The third design considered is pictured in Figure xx. The v-shape allows the syringe to sit at any height within the syringe holder. Syringes of smaller diameter will rest closer to the crux of the v-shape whereas the larger diameter syringes will be supported closer to the top of the v as shown in Figure XX. The flange of the syringe is held in place by the slot in the syringe holder. Because there is some variance in the width of the flange for each syringe size and model, some syringes will be more tightly held between the gap in the holder than others. However, this will not create a large issue because the only force being applied on the syringe holder is that from the syringe. The forces applied by the syringe are applied only along the horizontal axis because the force from the motor is transmitted to linear, horizontal motion which acts on the carriage and in turn the syringe.

slot still provides the necessary horizontal force to counteract the force applied by the carriage. Since the carriage only applies force along the horizontal axis, there is minimal concern of the syringe escaping from the holder.

This design has a number of advantages over the previous two designs, such as no additional hardware being needed. This decreases cost, complexity, and potential manufacturing errors. Another advantage of this design is that it can be inserted into the original chassis so that no extra filament or components are needed to create the design.

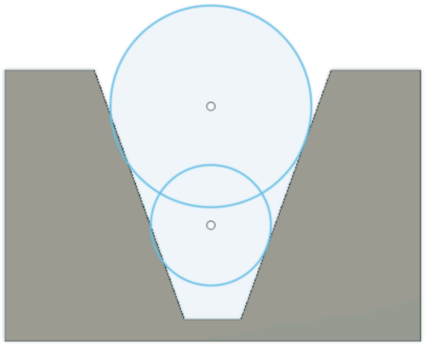


Figure xx. Syringe holder model with circles to indicate fit of various syringe sizes.

Figure xx. Syringe holder with 1mL and 5mL syringes.

One disadvantage of this design is that it provides minimal clamping support to keep the syringe in place which may be a safety concern. The clamping support provided depends on the tolerance between the flange of the syringe and the slot it is inserted in. This tolerance will vary depending on the specific syringe in use as different manufactures use different geometry and thicknesses of the flange. It is possible to modify the design of the syringe holder so that the specific syringe in use will fit within the slot with a press fit rather than a clearance fit and therefore provide sufficient clamping. However, this will require some modification to the CAD files, which may not be in some user's area of expertise. Therefore, the syringe holder in this design allows for some clearance so that multiple types of syringes will fit in the system, and the possibility of altering the design to provide more accurate tolerancing is available to the user. Despite these minor disadvantages, this design was selected as the final syringe holder design due to its fulfillment of the functional requirements of the syringe holder and the overarching project objectives of minimal assembly and cost.

A future design consideration is to embed the syringe holder in the chassis to combine them into a single 3D printed component. Therefore, only one file would need to be configured for 3D printing, and any potential tolerancing issues between the two components would be eliminated. This would also benefit with respect to alignment and accuracy because there would be no potential for the syringe holder to be inserted off center or to not be completely seated in the chassis.

It may also be noted that when the syringe holder is printed laying down on its side, minor post-processing is required to remove the remaining support materials from the interior slot. This was done using tools on hand such as pliers and a small screwdriver to scrape out remaining unwanted filament. Tweezers may also be useful for this task. However, the need for post processing can be eliminated if the syringe holder is printed upright rather than laying on its side. With the proper build plate adhesion type selected, the print will be stable enough

Designs Considered	**Pros**	**Cons**
V-shape with knob	• Fills functional requirements • Provides vertical resistance which adds safety • Easy to assemble, minimal components	• Additional hardware • Increased cost • Additional manufacturing steps • Possibility of overtightening the knob leading to inaccurate volume/fracturing the barrel of the syringe • No mechanism to prevent loosening of screw.
Mass Spectrometry Research Group, Open Source Syringe Pump	• Fills functional requirements • Equal force applied to syringe	• Additional hardware • Increased cost • Additional manufacturing steps • Possibility of overtightening the knob leading to inaccurate volume/fracturing the barrel of the syringe
3D printed v-shape	• Fills functional requirements • No additional hardware • No additional manufacturing steps • No additional purchases required	• No additional securing mechanism. • Clamping force depends on the specific syringe dimensions which vary depending on syringe size and model.

Table XX. Summary of Syringe Holder Designs Considered

Modular Carriage Design

The selected syringe holder design allows for syringes to sit at different heights within the holder. In order to accommodate for the variance in height of each different syringe size, the carriage must also allow the syringe plunger to sit at different heights so that the syringe remains horizontal. The Croat Group's design included a single rectangular slot which didn't allow for the plungers to sit low enough to match the height that the smaller diameter syringes sit in the syringe holder. Therefore, a simple modification to the carriage was made by adding a triangular cutout. Like with the syringe holder, this triangular geometry allows for the syringe to sit at varying heights depending on the syringe's diameter.

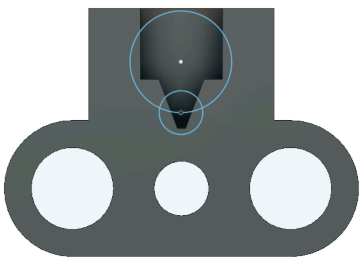


Figure xx. Carriage model with circles to indicate fit of various syringe sizes.

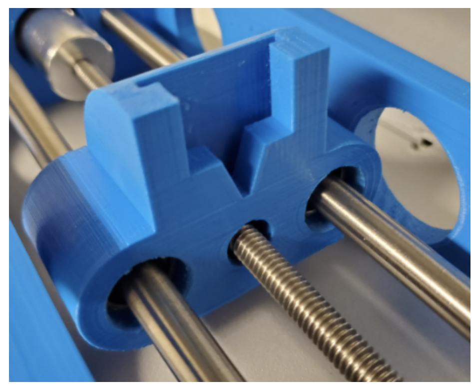


Figure xx. 3D printed Carriage.

After 3D printing the third design of the modular syringe holder and the modified carriage, it was verified that this combination is a viable design. The syringe holder fits syringe sizes of 1,3,5, and 10 mL as outlined in the functional requirements and the syringe is held horizontal due to the modifications made in the carriage.

Lead Screw Actuator

Single handedly the most important component of the syringe pump system which will determine the performance of it, the lead screw actuator is the mechanism which provides the force to move the syringe plunger and it refers to the system that includes the Nema-17 stepper motor, threaded rod and hex nut.

Functional Requirements

The functional requirements of the lead screw actuator is that it must allow for the accurate linear positioning of the carriage which in turn allows for the control of the flow rate of the syringe pump system based on the velocity of the stepper motor as well as other parameters.

Comparison of Designs Considered

1. **Threaded rod (screw) with nut**
2. **Ball screw**
3. **Pre-coupled Lead Screw w/ stepper motor**

Designs Considered	Pros	Cons
Threaded Rod with Nut	● Already bought ● Easily accessible ● Low cost ● Accurate ● Corrosion resistant	● Low screw efficiency
Ball Screw with Nut	● More accurate	● More expensive ● Not as easily accessible
Pre-Coupled Lead Screw with Stepper Motor	● No coupling required	● Expensive ($67.64) ● Higher step resolution (0.024383 mm/step) ● Lower maximum linear force (250 N) ● Not as easily accessible

Justification of Final Design Choice

From the lead screw analysis it was found that the maximum theoretical linear force that is provided by the motor is 593.3 N. This result is significant because it provides a conservative maximum baseline for the output linear force of the motor. To see the magnitude of forces that would be present during the operation of the syringe pump system, an analysis to estimate the theoretical pushing forces needed to get a specific flow rate from a syringe was done. The results received for a 2 mL/min flow rate were that forces between 1.47 N and 16.9 N would need to be provided for syringe sizes ranging from 1 mL to 10 mL. These results therefore show us that the motor we have chosen provides more than enough linear force to operate the syringe pump system effectively.

Chapter 4 : Prototype Performance

Theoretical Predictions

Theoretical predictions regarding the performance of the flow chemistry system were determined through experimentation as follows:

- The theoretical maximum pushing force that the motor is capable of producing was determined to be 593.3 N (or 133.3 lbf) and the analysis performed to get this value can be viewed in *Lead Screw Analysis* on page xx.
- The theoretical forces required to push syringes at a specific flow rate can be seen in the *Pushing Force Required Analysis* on page xx.
- The maximum flow rates that the syringe pump at which the syringe pump will be able to reliably operate for a variety of syringe sizes are listed in the table below:

Syringe Size	Dispense Resolution [μL/step]	Max Flow Rate [mL/sec]	Max Flow Rate [mL/min]
1 mL	0.0922	0.1844	11.064
3 mL	0.3862	0.772	46.32
5 mL	0.7062	1.412	84.72
10 mL	1.063	2.126	127.56

Table xx: Maximum Flow Rates for given Syringe Sizes

- The calculations to determine these flow rates can be found in *Flow Rate Calculations* on page xx.
- The flow rates of each syringe pump will be within ±(##) of the programmed flow rate. (Maybe separate accuracy by syringe size/ flow rate if they're different and add another table).

Test Conditions

Maximum Syringe Size

In order to verify the maximum syringe size that the syringe pusher is capable of pushing reliably, syringes of increasing size were inserted into the syringe pump and the stepper motor was initiated at a specific flow rate. Reliable operation of the stepper motor was determined by measuring the output flow rate. If the stepper motor reaches a point where it is not capable of providing sufficient torque output to overcome the force needed to advance the carriage and push the plunger of the syringe, it will skip steps in its rotation. When this occurs, the flowrate will be lower than expected due to the decreased aggregate rotation of the motor.

First, a baseline flow rate was recorded with a 1 mL syringe. This baseline was recorded with a syringe that the motor is assuredly capable of pushing because every syringe pump will have slight inconsistencies which lead to a flow rate slightly different than the programmed flow rate. Therefore, by comparing the measured flow rate with increasing syringe sizes to the baseline flow rate, it was evident when the flow rate no longer matched the baseline flow rate, indicating that the stepper motor did not have sufficient torque to push the syringe.

After the baseline flow rate was recorded, syringes of increasing size were placed in the system and the flow rate was recorded and compared with the baseline.

Maximum Flow Rate

The maximum flow rate that the syringe pump can operate at is determined by the maximum speed of the stepper motor. In order to verify the accuracy of the analysis performed, increasing flow rates were programmed and the measured flow rate was recorded. The maximum flow rate was determined when the increasing speed no longer increased the measured flow rate.

Quantitative data - TBD

Flow Rate Accuracy

The accuracy of the flow rate was determined by running multiple experiments with various syringe sizes and recording the measured flow rate. These experiments were performed with the two flow systems on hand which were both manufactured with the same 3D printer. Therefore, these accuracy ranges unfortunately do not include the accuracy of systems manufactured with different printers. However, these measurements may provide a baseline to which flow rate deviations in other syringe pumps can be compared.

Potential factors that may affect the accuracy of the system include both the physical components of the system and the coding used to control the pump. For the physical component side of the system, any small gap between the carriage pusher block contact surface and the syringe plunger can lead to inaccuracies. The code is programmed such that it assumes once the motor starts, the syringe plunger will be pushed or pulled at the first step the motor rotates. However, if there is a gap between the carriage and the plunger, then the motor will have to move a given amount of steps so that the carriage is contacting the syringe plunger and begin to push/pull the plunger. Therefore, the calculated volume dispensed will be wrong since it is assumed that the amount of steps turned by the motor from the start and thus the distance moved by the carriage is equal to the distance that the syringe plunger travels. However, in these tests it was ensured that the syringes fit tightly within the carriage in order to minimize these potential errors.

It was found in the risk reduction that large amounts of friction can interfere with the accuracy of the syringe pumps. With too much friction on the linear shafts guiding the carriage, the stepper motor may skip steps due to being unable to overcome friction. After correcting manufacturing errors with the syringe pump chassis, this problem appears to have been resolved. However, if a potential user wanted to manufacture a new system, manufacturing errors may occur and introduce friction to the system. In this case, the output flow rate of the system would be lower than desired. This effect is more noticeable at higher speeds, so running the system at lower speeds would be recommended.

In the Arduino code, the stepper motor runs the required number of steps per second, and the number of steps is calculated based on parameters such as the thread density of the lead screw and the diameter of the syringe being used. As such, minor changes in the diameter may change the actual required steps that the motor must turn. Consequently, there may be minor changes in the flow rate due to small changes in the diameter of the syringe or improper measurement of this diameter. Finally, because of the library used for this system, the Arduino must constantly update and tell the motor that it needs to spin. As a result, slow communication from the Arduino to stepper motor, due to causes like long execution time for certain lines of code or an insufficient baud rate, may slow the rotation of the motor.

Results

(TBD)

Comparison of Results to Initial Performance Requirements

(TBD)

Chapter 5 : Design Recommendations and Conclusions

Design Recommendations for the Future

Incorporate Real-time Flow Rate Sensing Capability

Due to the DIY nature of the project it is impossible to attain uniform results. Variations in the model of 3D printer used, 3D printing settings and conditions, tolerances of the hardware, as well as variations in the brand and model of syringes used all contribute to discrepancies between any two given systems. As such, the flow rate dispensed by each syringe pump may differ slightly from the programmed flow rate as well as from the other syringe pumps being used with the system. This is an issue due to the stoichiometric ratios not being maintained. Without proper stoichiometric ratios, reactions will not take place as intended and losses of supplies, time, and money may occur.

In order to avoid these discrepancies each syringe pump must be calibrated before usage. As the system currently stands, this calibration entails measuring the volume extruded from the syringe pump for a recorded amount of time, then manually calculating the flow rate from these results. Once the actual flow rate is known for a range of programmed flow rates, values can be entered to create equal flow between the syringe pumps to maintain proper stoichiometry.

This calibration process could be streamlined by implementing real-time flow rate sensing capabilities. By adding a flow-rate sensor to the output valve from each syringe pump and displaying the flow rates to the user interface, users would be able to see the flow rates in real-time. This would significantly reduce the effort required in the calibration process and make accurate, real-time adjustment of the flow rates possible.

Leak Detection System

In some cases it may be desirable to run reactions over extended periods of time. In these cases it would be convenient to leave the system unattended as the reaction is carried out. However, extreme care must be taken to ensure that no chemical spillages occur when the system is unattended.

This device is currently not suitable for unsupervised use due to its lack of automated monitoring and emergency shut off controls. A chemist is needed to supervise the system in the case a blockage or leak in the system occurs. If such an issue occurs, the chemist supervising the experiment must detect the issue and manually shut off the system to avoid chemical spillage.

Ensuing implementation of real-time flow rate sensing as previously mentioned, autonomous detection of leaks or blockages in the system would be possible. If the flow rate is much higher than expected a leak may be present in the system. If the flow rate is lower than the expected, this would be an indication that there is a blockage obstructing the flow. Therefore, the ability to detect flow rates would allow for the implementation of an automatic shut off command which shuts off the system if the measured flow rate indicates that a leak or blockage has occurred. The addition of an automatic shut off command would enhance the overall safety of the system and allow for a flow system that is safe to leave unattended for extended periods of time.

Safety Considerations

Safety considerations for this project relate to the use of chemicals within the flow system, electrical wiring, and 3D printing protocols.

When designing the system, care was taken to account for the safety of the individuals operating the system. Therefore, an automated refill option has been included to minimize the handling of chemicals by allowing users to command the system to refill the syringes using the user interface. Without this option, the syringes must be detached from the system, refilled by hand, and repositioned within the syringe pump. This process may lead to accidental chemical spills and the chance of chemicals coming into contact with the operator's skin.

When dealing with chemicals proper laboratory protocols should be followed at all times. Experiments should be conducted with the flow pump system within a closed fume hood. If a leak or blockage is detected the system should be shut off immediately. As the design currently stands, the flow system should never be left unattended.

With respect to the electrical components in the system, it is important that the wiring diagrams be followed so that no short circuits are created. A short circuit may produce sparks, smoke, or fire. This may result in personal injury, as well as permanent damage to the electrical components in the system.

Operation of the 3D printer is another area of potential risk. To mitigate this risk, it is important to follow the operating instructions of the specific 3D printer being used. 3D printers are generally safe machines, although care must be taken to avoid touching the heated components of the printer. The nozzle of the printer is generally heated to 210 - 250ºC and the bed to 60 - 110ºC. If contact with the skin occurs, a burn may result. Additionally, when removing supports from the finished 3D printed components, care must be taken to not to scratch oneself on the jagged support material.

Although this flow system does not require syringe needles, these needles are sometimes included when ordering syringes. These needles pose a safety hazard and must be disposed of properly. The California Department of Social Services has guidelines regarding proper disposal of syringe needles [5]. It is currently illegal to dispose of syringes in trash, recycling, or composting bins. To properly dispose of needles they must be discarded in an approved disposal container and later disposed of at a proper disposal facility.

Engineering Standards

Restriction of Hazardous Substances (RoHS)

The Restriction of Hazardous Substances (RoHS) Directive (2002/95/EC) regulates the use of hazardous substances in electronic devices[1]. The RoHS Directive was adopted by the European Union in 2003. California adopted the directive in 2003 as well but under a limited scope. The hazardous substances limited by California Senate Bills 20 and 50 include four of the ten substances limited by the RoHS Directive, those being lead, mercury, cadmium, and hexavalent chromium. Another directive which sets standards for electronic equipment is the Electromagnetic Directive (EMC) (2014/30/EU). A device is EMC compatible if it is able to function acceptably in its electromagnetic environment. This includes limiting the unintentional generation, propagation and reception of electromagnetic energy, all of which may cause unwanted effects such as electromagnetic interference (EMI) or physical damage in operational equipment[2]. The electronics in this design were selected to be compliant with the RoHS and EMC directives. Specifically, the Nextion 7" Basic Series Display and Arduino Mega 2560 are both RoHS and EMC compliant.

ASME Y14.5 Dimensioning and Tolerancing

The ASME Y14.5 Dimensioning and Tolerancing standard is applicable to this project due to the use of CAD files in order to design the 3D printed components. This standard creates a common technical drawing language for standardized drawing practices and has been revised over the years to be compatible with electronic systems, such as Computer Aided Design (CAD). This standard was therefore applied when creating the CAD files for the 3D printed components of the system.

ANSI Internal and External Thread Classes

ANSI Internal and External Thread Classes is a widely adopted standard for thread screw classes which specifies the degree of tightness between threaded components[3]. Thread screw classes specified in the ANSI Thread Classes represent manufacturing tolerances that specify minimum and maximum pitch diameters for both internal and external threads. The stainless steel threaded rod used as the linear actuator in the syringe pump system is sized with ANSI

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[1] *RoHS Directive*. Environment. (n.d.). Retrieved January 29, 2022, from https://ec.europa.eu/environment/topics/waste-and-recycling/rohs-directive_en

[2] *EMC Directive 2014/30/EU*. cemarking.net. (2022, January 3). Retrieved January 29, 2022, from https://cemarking.net/eu-ce-marking-directives/emc-directive/

[3] Edge, Engineers. "ANSI Internal and External Thread Classes: Engineers Edge." *Engineers Edge - Engineering, Design and Manufacturing Solutions*, www.engineersedge.com/thread_strength/thread_classes.htm#:~:text=There%20are%20three%20classes%20of,play%20or%20clearance%20in%20assembly.

class 2A external threads. This class is intended to maximize the strength of the threads, and is therefore an advisable choice for this design since the threaded rod and nut are used to translate rotational force to linear force acting on the syringe. The tolerance allowed for a class 2A lead screw is a minimum pitch diameter of 0.2127 inches and a maximum pitch diameter of 0.2164 inches. The threaded rod in the system is paired with an ANSI class 2B steel hex nut which has an allowed pitch diameter ranging from a minimum of 0.2175 inches to a maximum diameter of 0.2248 inches.

Chemical Hazards and Toxic Substances

OSHA (Occupational Safety and Health Information) has standards regarding Chemical Hazards and Toxic Substances. Controlling Exposure is a section of these standards which includes controls such as Elimination/Substitution, Engineering Controls, Administrative and Work Practice Controls, as well as Personal Protective Equipment. The Engineering Controls involve implementing physical change to the work environment which reduces or eliminates the hazard on the job. Examples of such controls include changing processes to minimize contact with hazardous chemicals, isolating or enclosing the process, use of wet methods to reduce generation of dust or other particles, general dilution ventilation, and the use of fume hoods[4]. This flow system has been designed to adhere to these standards. Specifically, the automatic refill option was designed to minimize contact with hazardous materials. In the Croatt Research Group's original design, the chemist is required to fill a syringe by hand, install it in the syringe pump, and refill the syringe when necessary. With the automatic refill, the need for contact with and transportation of a syringe full of hazardous materials is eliminated by automating the process once the syringe has already been placed in the syringe pump. Additionally, the design of this flow system was made to control exposure by accommodating the use of fume hoods. Extended wires between the syringe pump and the GUI allow for the syringe pump to be placed in an enclosed fume hood while the GUI and electronics sit on a nearby surface. Therefore, the portion of the system in contact with chemicals and hazardous substances can be enclosed in a fume hood while the electronics remain operable at a safe distance away. These design choices have been made to act in accordance with OSHA's Chemical Hazards and Toxic Substances standards.

Impact on Society

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[4] *Chemical Hazardous and Toxic Substances*. Chemical Hazards and Toxic Substances - Controlling Exposure | Occupational Safety and Health Administration. (n.d.). Retrieved January 29, 2022, from https://www.osha.gov/chemical-hazards/controlling-exposure

Green chemistry (or sustainable chemistry) refers to the development of efficient chemical processes that reduce or eliminate the generation of hazardous substances[5]. It takes into consideration the environmental impact of every step in the process of chemical synthesis, from the waste created during the reaction to the lasting effects that the chemicals created will have on the environment. It also concerns safety, aiming to minimize potential hazards to laboratory personnel. As environmental concerns have come to a head over the past half-century, government, academia, and industry alike have begun to look towards green chemistry as a necessary scientific advancement in order to promote a more sustainable civilization[6].

Flow chemistry has made valuable contributions towards the practice of green chemistry. By allowing for strict control of reaction parameters, the efficiency of reactions is increased, waste is reduced, and safety is enhanced. However, one important consideration when it comes to green chemistry initiatives is the economic impact of the processes being implemented. Governments, industries, and research institutions desire both environmental and economic sustainability. Practices must therefore be cost effective in order to gain acceptance and widespread use. Currently, chemistry flow systems are prohibitively expensive and therefore largely impractical for large-scale implementation. By greatly reducing the price of flow systems, use of these systems will become more commonplace as institutions no longer have to choose between environmental and economic sustainability. This creates opportunity for a larger portion of chemical synthesis to be conducted in a sustainable manner.

This design will have valuable social implications in addition to its environmental ones. Cost-effective, DIY flow systems have already been developed, however these systems are non-intuitive and not user friendly. The user-friendly nature of this flow system will allow for increased prevalence of flow systems in undergraduate laboratories because students will not require significant training and expertise to operate the system. Therefore, a greater number of students will have the opportunity to conduct experiments using this equipment, leading to a workforce of adept chemists. Furthermore, by removing unnecessary obstacles associated with operating the system, students will be inspired rather than discouraged when using this flow system. This inspiration will encourage students to persevere through difficult courses, and enhance the retention of students from underrepresented groups in STEM fields.

Professional Responsibility

While the use of this design advances sustainable chemistry initiatives and therefore addresses environmental concerns, the environmental implications of the production of this system must also be taken into consideration. The majority of the design is 3D printed, and is

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[5] Environmental Protection Agency. (n.d.). *Basics of Green Chemistry*. EPA. Retrieved January 17, 2022, from https://www.epa.gov/greenchemistry/basics-green-chemistry#definition
[6] Vaccaro, L., Lanari, D., Marrocchi, A., & Strappaveccia, G. (2014). Flow approaches towards Sustainability. *Green Chem.*, *16*(8), 3680–3704. https://doi.org/10.1039/c4gc00410h

therefore not intended for long-term use. Replication of this design will therefore lead to the creation of plastic waste once the system has reached the end of its lifespan. Most common types of 3D printing filament are classified as Type 7, or “Other” by the ASTM International Resin Identifier Codes[7]. Type 7 plastics are not recycled by most curbside municipal recycling programs and consequently often end up in landfills. However, independent plastic recycling and processing companies exist which process plastics not typically handled by municipal recycling programs. It is also possible to melt down old 3D printed components and re-extrude them as usbale filament[8]. Additionally, PLA (Polylactic Acid), one of the most commonly used 3D printing filaments, is a biodegradable material which means that it can be broken down over time. As 3D printing gains popularity, there is discussion regarding the introduction of more comprehensive recycling codes in order to include common 3D printing filament polymers.[9] Therefore, there are options for recycling the 3D printed components created for the purpose of this flow chemistry system.

Lessoned Learned

(TBD)

Conclusions

(TBD)

Acknowledgements

(tbd)

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[7] *3D Print Recycling*. Iowa State University Computation and Construction Lab. (n.d.). Retrieved January 17, 2022, from https://ccl.design.iastate.edu/3d-print-recycling/#:~:text=One%20of%20the%20common%20types,typically%20processed%20by%20municipal%20programs.

[8] *3D Print Recycling*. Iowa State University Computation and Construction Lab. (n.d.). Retrieved January 17, 2022, from https://ccl.design.iastate.edu/3d-print-recycling/#:~:text=One%20of%20the%20common%20types,typically%20processed%20by%20municipal%20programs.

[9] Emily J. Hunt, Chenlong Zhang, Nick Anzalone, Joshua M. Pearce, Polymer recycling codes for distributed manufacturing with 3-D printers,Resources, Conservation and Recycling, Volume 97, 2015. Pages 24-30. ISSN 0921-3449. https://www.sciencedirect.com/science/article/pii/S0921344915000269.

References (still need to add proper formatting)

[1] Croatt Research Group.

[2] Zaiput Flow Technologies.

[3] Burkart Laboratory, UCSD Department of Chemistry and Biochemistry.

[4] Mass Spectrometry Research Group, Open Source Syringe Pump. Samokhin, Andrey. "Open-Source Syringe Pump." *Группа Масс-Спектрометрии*, www.mass-spec.ru/projects/diy/syringe_pump/eng/.

[5]
https://cdss.ca.gov/agedblinddisabled/res/VPTC2/6%20Universal%20Precautions/Guide_to_Syringe_Disposal.pdf

Appendix

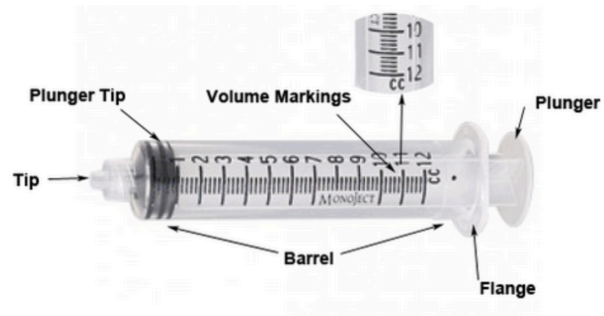


Figure XX. Anatomy of a Syringe. [Vitality Medical].

Users/Maintenance/Safety/Operation Manual

(TBD)

Fabrication Instructions

(TBD)

(3D printing the individual parts

- Electronics casing top lid
- Electronics casing box
- System Chassis (integrated with the syringe holder)
- Syringe Carriage)

Drawings/Layouts/Parts Listing

(TBD)

Bill of Materials

Stepper Motor	2
Linear Coupler (4 pc)	2
Ball Bearing Bushings (4 pc)	2
8 mm Linear Rods (2 pc)	1
Fully Threaded Rod	1
Stepper Motor Driver	2
Bluetooth Transiever	1
M3 0.5x14mm Flathead Screws	1
Nextion Touchscreen	1
12V 30A Power Supply	1
Tubing	
3D printing filiment	
3 Wire power cord	1
File	1
8 mm Linear Rods (2 pc)	2
Fully Threaded Rod	1
Servo Motor (4 pc)	1
5V 5A Power Supply	1
3 Wire power cord	1
Digital Caliper	1
Stylus Pen	1
Electronics Box (Size Large)	1
Zip Ties	1
4-40 Phillips Screws-Hex Nuts A	1
6-32 Phillips Machine Screws	1
4-40 Threaded Heat-Set Inserts	1

Table xx. Bill of Materials (Not Finalized)

Specification Sheets for Parts Purchased

Product information

Product Dimensions	1.6 x 0.78 x 1.69 inches
Item Weight	7.8 ounces
ASIN	B07GRMRH1Q
Item model number	0510U1J2GPSINM53091A89
Manufacturer recommended age	12 years and up
Best Sellers Rank	#37,221 in Toys & Games (See Top 100 in Toys & Games) #15 in RC Servos
Customer Reviews	442 ratings 4.2 out of 5 stars
Is Discontinued By Manufacturer	No
Mfg Recommended age	12 year and up
Manufacturer	Seamuing

Table XX. Seamuing Micro Servo Motor, MG995 RC Servo, 20kg Metal Gear Servo for RC Robot Arm Helicopter Airplane Remote Control Product Information.

Additional information

Display Size	*7.0"*
Resolution	*800*480*
Touch Panel	*RTP*
MCU	*48 MHz*
Flash	*16 MB*
SRAM	*3584 Byte*
Input Power	*DC 5V 500mA*
USART Port	*XH2.54 4P*
Storage Temperature	*-30 ~ 85 °C*
Working Temperature	*-20 ~ 70 °C*
Nextion Editor Components	*Text, Scrolling Text, Number, Xfloat, Button, Progress Bar, Picture, Crop, Hotspot, TouchCap, Gauge, Waveform, Slider, Timer, Variable, Dual-state Button, Checkbox, Radio, QRcode*
Character Encoding	*ascii, utf-8, iso-8859-1~15, gb2312, ks_c_5601-1987, big5, windows-874/1255/1256/1257/1258, koi8-r, shift-jis*
Anti-aliasing font	*Yes*
Product Dimensions	*https://cdn.nextion.tech/wp-content/uploads/2017/09/7.0_Nextion_Dimension.pdf*

Table xx. Nextion 7” Basic Series Touch Display Specifications

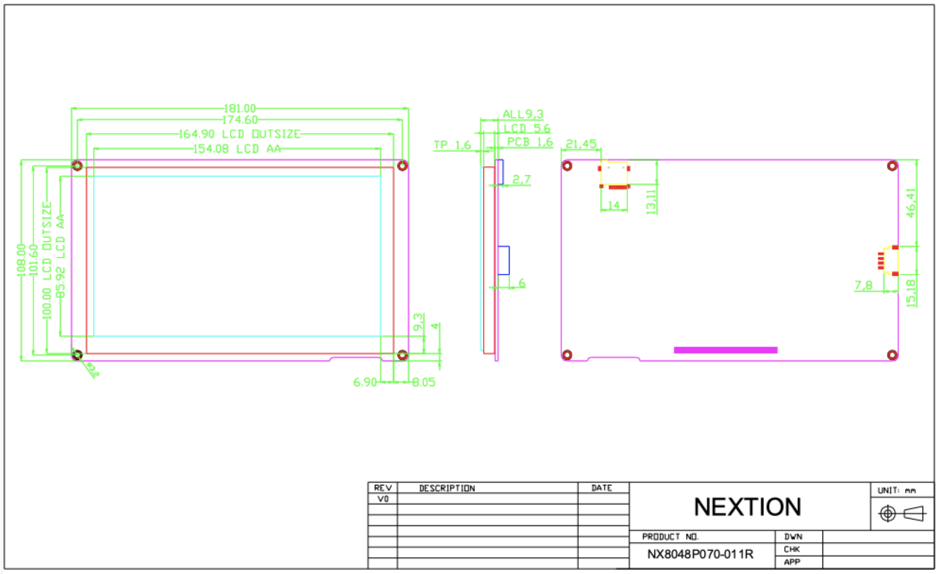


Figure xx. Nextion 7" Basic Series Touch Display Dimensions.

Nema 17 Stepper Motor

Rev: A
Date:

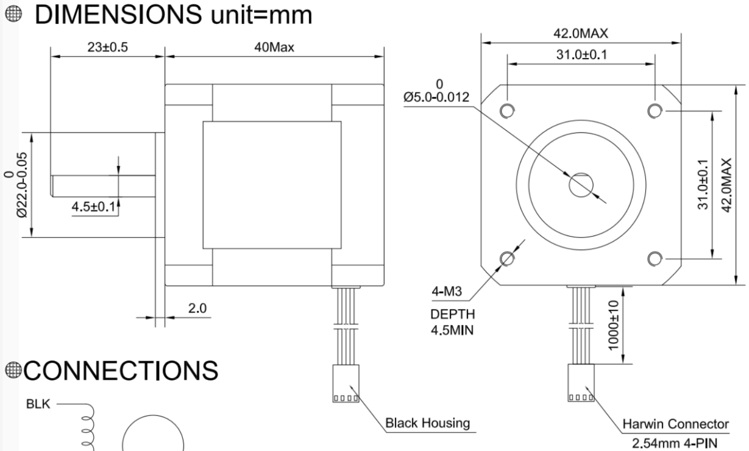
COMMON RATINGS

Step angle :	1.8°	Dielectric strength :	500VAC
Positional accuracy :	±5%	Insulation resistance :	100Mohm(500VDC)
Number of Phase :	2	Ambient Temperature :	-10℃~50℃
Temperature rise :	80℃MAX	Insulation class :	B
Rotor Inertia :	54gcm²	Weight :	0.3Kg

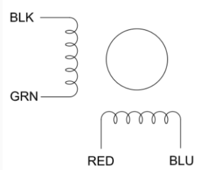
SPECIFICATIONS

Holding Torque (2 phases on) N.m	Rated Current/Phase (Amps DC)	Phase Resistance (ohms) ±10%	Rated Voltage/Phase (V DC)	Phase Inductance (mH)±20%(1KHz) Typical
0.45	2.0	1.1	2.2	2.6

DIMENSIONS unit=mm



CONNECTIONS



标记	处数	分区	更改文件号	签名	日 期	17HS16-2004S1	技术规格书
设计			标准化			阶 段 标 记 / 重量 / 比例	STEPPERONLINE Motors&Electronics
审核							
工艺			批准			共 张 第 张	www.OMC-StepperOnline.com

Table xx. Nema 17 Stepper Motor Specifications and Dimensions

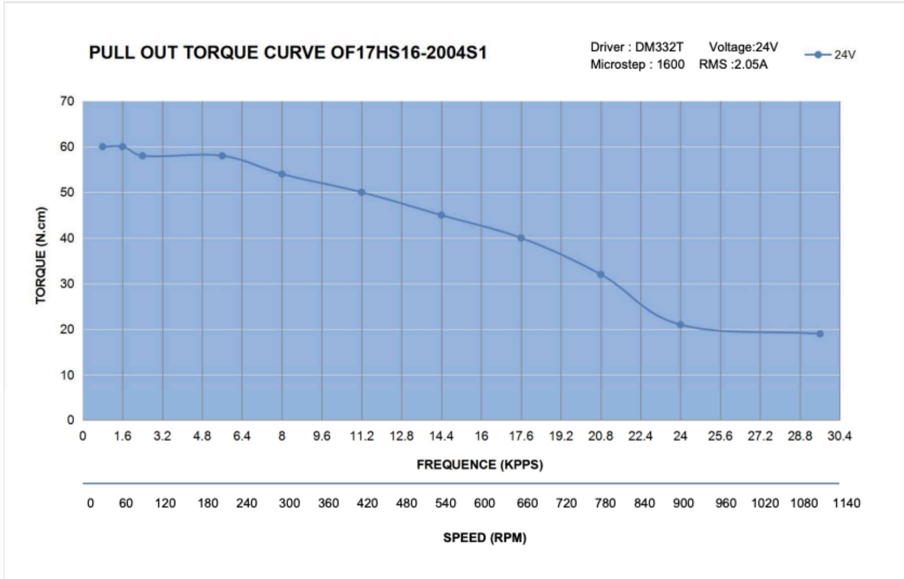
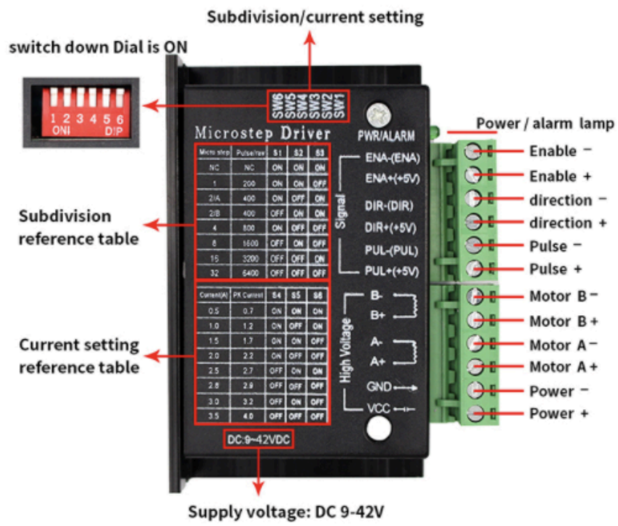


Figure xx. Nema 17 Stepper Motor Torque Speed Curve



Feature:

This driver is an upgraded version of the TB6600
PWM chopper type bipolar stepper motor driver IC

1. 9V-42V DC power supply; H bridge bipolar constant phase flow drive.
2. The maximum 4.0A of the eight kinds of output current.
3. The largest 32 subdivision of the 6 models are optional.
4. Input signal high speed photoelectric isolation.
5. Common-anodestandard single pulse interface. Offline to maintain the function.
6. Built-in temperature protection and over current protection.
7. To provide energy-saving semi-automatic current lock function.
8. Semi closed enclosure can be adapted to a more stringent environment.
9. Only the clock pulse signal can be driven two-phase bipolar stepper motor to achieve low vibration, high efficiency work.
10. Can control 2 phase stepper motor forward and reverse rotation, With 1-2, W1 -2 , 2W1 -2, 4W1 -2 phase excitation mode.

IC parameter:

single chip bipolar sine microstep stepper motor driver
the new BiCD 0.13 nm process
up to 42V , resistance (a +) = 0.4
the forward and reverse rotation control
5 subdivision mode options (1/1, 1/2, 1/4, 1/8, 1/16,1/32)
rated output: IOUT = 3.5 A
output current: IOUT = 4.0A (peak, in 100ms)
package: HZIP25 - 1.00F
input port internal pull-down resistor: 100 K
alarm output pin current:Ialert = 1mA
monitoring output pin (MO): Imo= 1mA
with reset and enable pin,with standby function
Break through the traditional, single power supply
Undervoltage protection, built-in (UVLO) circuit
built in overheating protection (TSD) circuit
built-in overcurrent detection (ISD), circuit

Package Included:

1 x TB6600 stepper motor driver

Figure xx. Usongshine Stepper Motor Driver Specifications

Parameter

- Input: AC110V/220V 50/60Hz
- Output Voltage : DC 12V
- Output Current: 30A max
- Output Wattage: 360W max
- Fix Screw Hole Diameter: 2.5mm (0.1inch)
- Working temperature: -10 to 50 degree Celsius
- Storage temperature: -20 to 60 degree Celsius
- Environmental humidity: 10-95%
- Material: Metal, Electronic Parts
- Safety Compliance: CCC/ FCC / CE

Connection instruction

- L: Live wire
- N: Negative wire
- +V: DC power output "+"
- -V: DC power output "-"
- +V ADJ: Adjust the output voltage (10%)

Kindly note

1. High Voltage inside, do not remove the cover.
2. 110V/220V must be selected by switch before using to avoid damaging. Please change the switch to 110V for USA.
3. It comes without installation instruction, wiring cable, on/off switch and screws. Professional Installation of qualified electrician is highly recommended.

Package included

- 1 x 12V 30A Power Supply Switch

Figure xx. ALITOVE AC 110V/220V to DC 12V 30A 360W Universal Regulated Switching Power Supply Product Specifications

Code Written

(TBD)

Detailed Analysis

Lead Screw Analysis

The purpose of this static analysis was to determine the maximum linear force that the stepper motor coupled with the lead screw could produce. Some assumptions that were made to make this analysis possible was that the maximum torque of the Nema-17 motor, based on the specification sheet, was 0.45 Nm. Another assumption that was made was that the dry friction coefficient between the external threads of the screw and the internal threads of the hex nut was 0.20. Based on these assumptions the motion of the lead screw could now be modeled using static analysis. The way this motion was modeled was that the external threads of the lead screw are supporting a linear load, W, which for this case is the hex nut embedded in the carriage block that provides the linear force to the syringe plunger. The impending motion of the screw as it is supporting a load can be modeled as the 2D free body diagram seen in figure (). Here the green slope represents the external threads of the screw and the black outlined box represents the internal threads of the hex nut. The external threads of the screw are unwrapped to allow them to be modeled in two-dimensions and as a result the length of the base of this slope is equal to the circumference of the screw. The height of the slope represents another important screw dimension which is the screw pitch. Screw pitch is the distance between the threads of a screw and can be found by taking the inverse of the threads per inch. The threaded rod used for the syringe pump system has single-start threads which means that screw pitch is equal to screw lead, which is the linear distance traveled in one revolution by the screw. The particular screw used for the assembly has 20 threads per inch and right-handed threads. Therefore, the lead and pitch is a known value. Another dimension of importance is the mean diameter, or the pitch diameter, of the screw which can be found using a reference table since all screws adhere to standards that manufacturers adhere to and are based on their class, a manufacturer standard as well. With all of this information available the sum of the forces for the free body diagram can be solved for and finally the maximum linear force produced by the lead screw actuator as well.

Calculations:

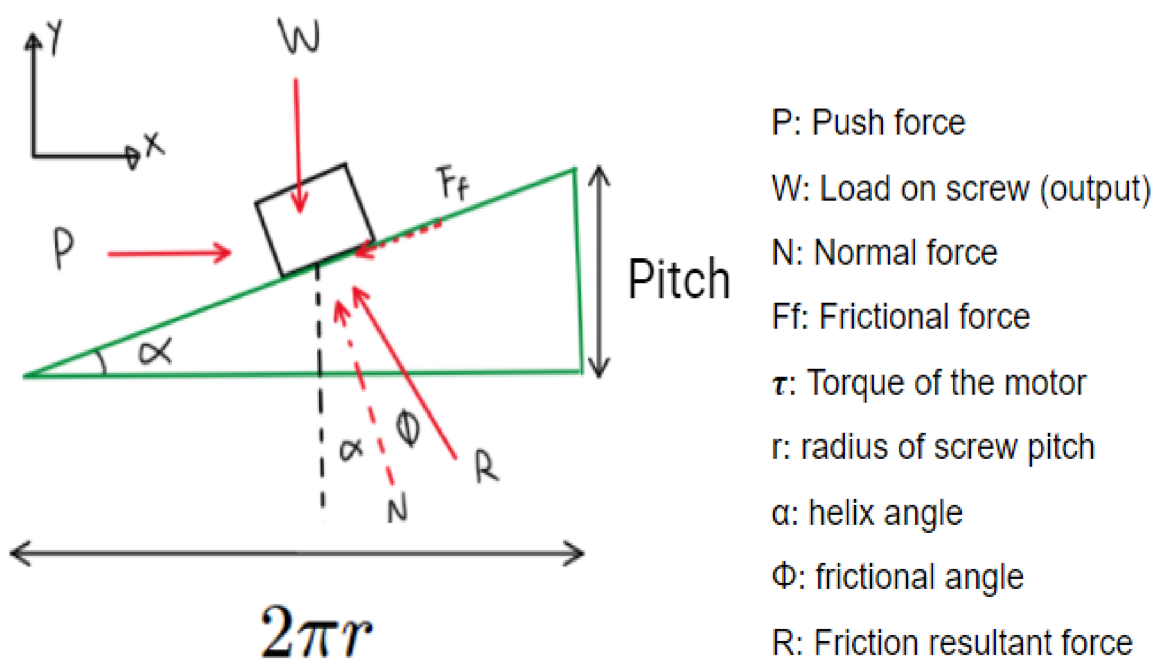


Figure xx. Free body diagram of a linear load (W) on the external threads of a screw at the moment of impending motion.

From summing the forces along the x-axis direction we get the equilibrium equation below.

$$\boxed{\Sigma F_x = 0 \longrightarrow P - Rsin(\alpha + \phi) = 0}$$

It is known that the pushing force is the force produced by the motor and is equal to the torque of the motor over the pitch radius of the screw.

$$\boxed{P = \frac{\tau_m}{r_{pitch}}}$$

Substituting for P, the new equilibrium equation along the x-direction can be found.

$$\boxed{\frac{\tau_m}{r_{pitch}} - Rsin(\alpha + \phi) = 0}$$

Solving for R, the friction resultant force, the new equation is seen below.

$$\boxed{R = \frac{\tau_m}{r_{pitch} \times sin(\alpha + \phi)}}$$

From the summation of the forces along the y-axis the equation below is the result.

$$\boxed{\Sigma F_y = 0 \longrightarrow -W + Rcos(\alpha + \phi) = 0}$$

Solving for R here results in the second equation for the friction resultant force.

$$\boxed{R = \frac{W}{cos(\alpha + \phi)}}$$

The two equations for R that are found from each of the summation of forces are then equal to each other.

$$\boxed{\frac{\tau_m}{r_{pitch} \times sin(\alpha + \phi)} = \frac{W}{cos(\alpha + \phi)}}$$

Finally, the linear load force, W, can be solved for and the resulting equation is shown below.

$$W = \frac{\tau_m}{r_{pitch} \times tan(\alpha + \phi)}$$

The results that were found during this lead screw analysis was that the maximum linear force, W, provided by the lead screw mechanism was 593.3 N or 133.3 lbf. This result is important because it gives the maximum baseline for the linear force produced by the linear actuator. Also, the result is significant because it shows that the motor is more than capable of producing the linear force required to push or pull any syringe size that is compatible with this system. The analysis for the forces required to operate the syringe pump for various syringe sizes can be found in the *Pushing Force Required Analysis*.

(Add references)

Pushing Force Required Analysis

The goal of this analysis was to characterize the forces that would be required during the operation of the syringe pump system for different syringe sizes. This analysis was done using Poiseuille's Law for Laminar Flow which states that the driving force for the flow of a liquid inside of a tube is the pressure difference between each end of a tube. Some assumptions that were made in order to perform this analysis were that the flow inside the syringe was completely laminar and that the friction from inside of the syringe due to the rubber tip of the plunger sliding along the plastic barrel was neglected. Other assumptions that were made were that the pressure at the tip of the syringe was at atmospheric pressure and that the flow rate was set at 2 mL/min. Also, water at 20 celsius was used as the liquid inside of the syringe to determine the value of viscosity. Next, the inner diameter as well as the length of each syringe used for this analysis was measured using digital calipers. The remaining variable left to solve for was the linear force, F, that pushes the plunger of the syringe and creates a pressure on the surface of the water that is directly contacting the plastic tip of the syringe plunger.

Calculations:

Poiseuille's Law for Laminar Flow Equation

$$Q = \frac{P_2 - P_1 \pi r^4}{8\eta l}$$

$$P_1 = \frac{Force}{Area}$$

Q: Flow Rate

P_2: Pressure at outlet

P_1: Pressure at syringe plunger

r: inner radius of syringe

n: viscosity of the liquid

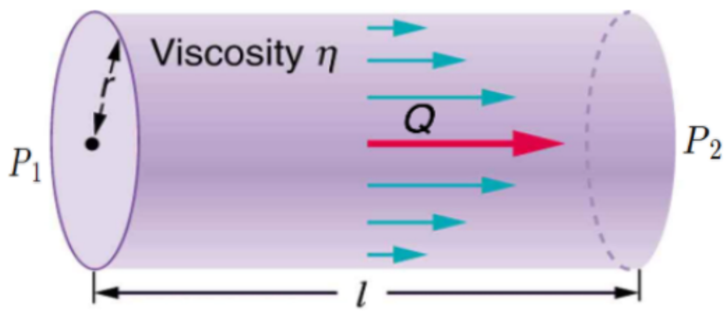


Figure xx. Poiseuille's Law applied to a tube.

The results achieved from this analysis can be seen in the table below.

Syringe Size [mL]	**Force Required [N]**
1	**1.47**
3	**6.16**
5	**12.0**
10	**16.9**

Table xx. Pushing forces that are required on the syringe plunger to get a flow rate of 2 mL/min.

These results are significant because they give a range of forces that would be required to operate the syringe pump for a given flow rate. The results also show that the motor used for the system will be more than adequate to drive the carriage and the syringe plunger for these specific syringe sizes.

(add references)

Flow Rate Calculations:

The purpose of these calculations is to determine the maximum theoretical flow rates and the dispensing resolution for syringe sizes 1 mL, 3 mL, 5 mL, and 10 mL. The maximum flow rates were calculated by using the maximum speed that the stepper motor was limited to in the Arduino code, which was 2000 steps per second (x RPM). Another important parameter that was required to calculate flow rate was the pitch of the screw, or the distance that the carriage would move per one revolution of the motor. This value was found based on the standard dimensions of the threaded rod that was used for the lead screw mechanism. From the specification sheet the stepper motor is known to make 200 steps per revolution. From these values the distance traveled by the carriage per step of the motor can be calculated as follows.

$$\frac{Pitch}{Revolution} \times \frac{Revolution}{Steps} = \frac{Pitch}{Steps} = \frac{1.27[mm]}{200[steps]} = 0.00635[mm/step]$$

The next requirement is to calculate the volume that would be dispensed from the syringe per step of the motor or also known as the dispense resolution. To calculate volume, the equation for the volume of a cylinder is used. The reason for using this equation is that the syringe can be modeled as a tube as seen in the *Pushing Forced Required Analysis.* Therefore, the equation gives the volume in terms of length of the cylinder or distance traveled by the carriage per step of the motor which is also the same as the distance traveled by the syringe plunger. It is found that the distance traveled by the plunger per step of the motor is 0.00635 mm.

$$V = \pi r^2 h$$

r: inner radius of the syringe

h: distance traveled by the plunger

For example, here is the step resolution calculation for a 10 mL syringe with a measured inner radius of 7.3 mm.

$$V = \pi r^2 h = \pi(7.3[mm])^2(0.00635[mm/step]) = 1.063[\mu l/step]$$

To calculate the maximum flow rate the step resolution just needs to be multiplied by the maximum speed of the motor which is given as 2000 steps per second.

$$Q_{max} = V \times w_{max}$$

Using the step resolution calculated for a 10 mL syringe the maximum flow rate can be calculated as:

$$Q_{max} = V \times w_{max} = (1.063[\mu L/step]) \times (2000[steps/sec]) \times (60[sec]/1[min]) = 127.56[mL/min]$$

The results for the rest of the syringe sizes can be seen in the table below.

Syringe	**Maximum Flow Rate [mL/min]**	**Step Resolution [mL/step]**
1 mL	11.064	0.0000922
3 mL	46.32	0.0003862
5 mL	84.72	0.0007062
10 mL	127.56	0.001063

Table xx. Theoretical maximum flow rates and step resolution.

These results are significant because they help define the performance limits of the syringe pump system. Therefore, one can look at these system specifications to see if these maximum flow rates meet their requirements and choose or choose not to use this system.

(add references)

Budget

Name	Quantity	Cost (per quantity)	Cost ($)
Stepper Motor	2	12.99	25.98
Linear Coupler (4 pc)	2	6.66	13.32
Ball Bearing Bushings (4 pc)	2	4.245	8.49
8 mm Linear Rods (2 pc)	1	10.89	10.89
Fully Threaded Rod	1	13.76	13.76
Stepper Motor Driver	2	8.79	17.58
Bluetooth Transiever	1	8.39	8.39
M3 0.5x14mm Flathead Screws	1	4.57	4.57
Nextion Touchscreen	1	112.3	112.3
12V 30A Power Supply	1	27.99	27.99
Tubing		0	0
3D printing filiment		0	0
3 Wire power cord	1	17.25	17.25
File	1	6.45	6.45
8 mm Linear Rods (2 pc)	2	8.99	17.98
Fully Threaded Rod	1	12.98	12.98
Servo Motor (4 pc)	1	23.69	23.69
5V 5A Power Supply	1	10.76	10.76
3 Wire power cord	1	11.31	11.31
Digital Caliper	1	10.99	10.99
Stylus Pen	1	8.81	8.81
Electronics Box (Size Large)	1	17.99	17.99
Zip Ties	1	5.29	5.29
4-40 Phillips Screws-Hex Nuts A	1	15.07	15.07
6-32 Phillips Machine Screws	1	8.37	8.37
4-40 Threaded Heat-Set Inserts	1	11.95	11.95
Total Spent			422.16
Remaining			577.84

Table XX. Budget

Project Management

Task Distribution

Sponsor
Haim Weizman, PhD.
Senior Lecturer
Department of Chemistry and Biochemistry
University of California, San Diego

Sponsor Liaison, Analysis, and GUI Design
Zaivy Gonzales-Valencia

Safety Manager, Syringe Holder and Servo-attachment Design
Eden Detmer

Financial Manager, Electrical Containment and GUI Holder Design, 3D Printing
Shravan Suresh

Website Manager, GUI Design and Programming
Nhat Tang

Intermediate Milestones

Milestone 1: Assemble and test the unmodified Croatt Research Group's chemistry flow system (Risk Reduction).

Milestone 2: Assemble two unmodified Croatt Research Group's chemistry flow systems for future testing.

Milestone 3: Syringe holder design decision.

Milestone 4: Establish communication between the GUI and Arduino.

Milestone 5: Fully functional automated refill option.

Milestone 6: Electronics casing design decision.

Milestone 7: Implement real-time updated syringe position displayed on GUI.

Milestone 8: Implement dispense/withdraw only and continuous output options.

Milestone 8: Finalized GUI layout and design.

Milestone 9: Finalized flow system, including two assembled syringe pumps.

Risk Reduction Efforts

The risk reduction consisted of assembling and testing the unmodified Croatt Research Group's chemistry flow system. This was chosen as the risk reduction effort due to the team's need to be familiar with the existing design in order to make improvements upon it. Through building and testing the flow system, a foundational knowledge of the system was built which allowed for informed decision making going forward. Furthermore, a functional prototype was built which allowed for testing of new modifications to the design and additions to the Arduino code.

Additionally, performing this risk reduction made the team aware of the impacts that increased friction has on the measured flow rate. When assembling the initial system, the wrong diameter or linear rod was delivered. The delivered rod had a 10mm diameter in comparison to the desired 8mm diameter. Due to the time constraints, it was not possible to obtain a replacement for the rods. Therefore, in order to still complete the risk reduction, modifications were made to the 3D printed parts and to the assembly. The holes which the rods fit into were drilled out in order to fit the larger diameter. Additionally, teflon sleeves were used in place of the 8mm inner diameter linear bearings to allow the charriage to glide along the rods. While these changes allowed for a complete syringe pump to be produced and tested, a number of issues resulted from them. The largest issue encountered was excessive amounts of friction introduced by misalignment of the rods due to non-concentric drilling of the holes. With this misalignment of the rods, the carriage was unable to slide along them without significant resistance. This resistance was too much for the stepper motor to overcome and led to inaccurate flow rate measurements upon testing. Once the correct diameter rods were delivered and a new syringe pump assembly was built, these issues were resolved and made no impact on the performance of the system. However, it was useful to be able to observe these effects in order to identify any future problems due to friction.