Vacuum Moisture Swing

Report 2

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DISCLAIMER

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EXECUTIVE SUMMARY

The goal of this project is to design and build a direct air capture device that utilizes a vacuum moisture swing process to separate CO2 from ambient air. This process utilizes common sorbent materials to bind to CO2 as air passes through them, and then it leverages a process in which moisture unbinds the CO2 from the sorbents. The intent is to have a scalable design which will be practical and energy-efficient for large-scale deployment near high CO2 areas such as factories.

The project's client is Dr. Wade, who has been developing the vacuum moisture process in NAU's Climate Solutions Lab. It is sponsored by SRP, who is providing the bulk of the funding. The project is being completed under the requirements of the ME476C class.

The project has two primary goals: to design a structured sorbent bed that will be more energy efficient than the standard packed bed, and to build a functioning, lab-scale device which will perform the vacuum moisture swing process. The structured sorbent beds will be designed as CAD models and run through CFD simulations to optimize their structures. The device will be designed to run the full direct air capture cycle, with most aspects automated.

The device will run through a five step cycle: adsorption, evacuation, desorption, final evacuation, and pressurization. During adsorption, ambient air will be pulled through the sorbent bed. The sorbent bed will then be isolated from atmosphere and a vacuum pump will draw down to complete evacuation. A water reservoir will then be exposed, causing the water to vaporize and unbind the CO2 from the sorbents in the desorption stage. The water reservoir will then be isolated and a final draw-down of the sorbent chamber will complete the final evacuation. Finally the sorbent bed will be exposed to ambient pressure, which will pressurize the system. The system can then repeat the cycles.

The new designs of the structured sorbent beds are intended to provide a lower resistance to flow, thereby decreasing the power requirement to run the cycle. A primary intent of this project is as a proof-of-concept that a vacuum moisture swing process can be a viable option for removing CO2 from air in large-scale, real-world applications.

As of writing this document, the design is still in development. Initial CFD simulations have been run, generating pressure drop numbers for monolith, laminate, and packed bed sorbent structures. A full PLC program has been written on run on a PLC emulator, and is prepared for deployment in a physical PLC. Initial sorbent bed designs have been 3D printed using just plastic. The Bill of Materials is nearly complete, and parts purchasing is intended to be the primary next step.

TABLE OF CONTENTS

Contents

Dl	ISCLAIMER		. 1
EΣ	XECUTIVE S	SUMMARY	.2
T/		NTENTS	
1		ROUND	. 1
		et Description	
		erables1	
		ss Metrics	_
2		EMENTS	. 3
		mer Requirements (CRs)	
	_	eering Requirements (ERs)	
_		e of Quality (HoQ)4	_
3		Within Your Design Space	. 5
		marking 6	
	3.2 Litera 3.2.1	ture Review	
	3.2.1	Literature Review: Randy Brierley	
	3.2.2	Literature Review: Elijah Woolridge	
	3.2.3	Literature Review: Justin Patterson 10	
		ematical Modeling	
	3.3.1	Evaporation Rate Based on Mass Flow, Heater, Pressure drop, and Reservoir (Randy	
	Brierley)		
	3.3.2	Pressure Drop and Cooling Power Associated with the Condenser at 1m/s Flow Rate	
		a KF40 Pipe and Varying Pressures. (Eli Woolridge)	
	3.3.3	Surface Area Required to Maintain Condenser Using a Water-Cooled Heat Exchanger.	
		16	
	3.3.4	ANSYS Simulations: Pressure Drop in Monolith and Laminate Structures17	
	3.3.5	Ansys Validation Using Darcy Weisbach21	
4		oncepts2	22
	4.1 Funct	ional Decomposition	
	4.2 Conce	ept Generation	
	4.2.1	Valve Type (Eli Woolridge)	
	4.2.2	Vapor CO2 Separation (Branden Welker)	
	4.2.3	Pipe Diameter (Branden Welker)	
	4.2.4	Control protocol (Randy Brierly)23	
	4.2.5	Sorbent Mesh and Filters (Justin Patterson)	
	4.2.6	Ambient Air and Pump Filters (Justin Patterson)	
	4.2.7	Vacuum Pump (Randy Brierly)	
	4.2.8	Sorbent Structure (Eli Woolridge)	
		tion Criteria	
	4.3.1	Vacuum Pump Selection	
	4.3.2	Heating Element selection	
		ept Selection	
	4.4.1	Valve Type Selection	
	4.4.2	Vapor CO2 Separation Selection 27	
	4.4.3	Filter Selection 27	
	4.4.4 4.4.5	Pressure sensor models and configurations	
	7.7)	1 mai whichth	

5	S	Schedule and Budget	33
	5.1	Schedule	
	5.2	Budget	34
	Bill (of Materials (BoM)	
6		Design Validation and Initial Prototyping	
	6.1		36
	6.2	Initial Prototyping	
	6	5.2.1 Automation Prototype: PLC Program [Randy Brierley]	37
	6	5.2.2 ANSYS prototyping	38
	6.3	Other Engineering Calculations	38
	6.4	Future Testing Potential	38
7	C	CONCLUSIONS	40
8	R	REFERENCES	41
9	A	APPENDICES	46
	9.1	Appendix A: RSLogix500 PLC ladder logic program	46
	9.2	Appendix B: condenserCalcs.m	
	9.3	Appendix C: BOM	
	9.4	Appendix D: ANSYS Simulations	90

1 BACKGROUND

This chapter contains a project description, deliverables, and success metrics. The project description gives an overview of the project, sponsors, and the importance of the project. The deliverables section discusses the deliverables based on the client, the course, and the team's goals. Success metrics are described for the primary aspects of the projects, and the methods of gauging success are discussed.

1.1 Project Description

The goal of this project is to create a direct air capture device which utilizes a vacuum moisture swing technique to extract CO2 from air. The CO2 capture will be achieved by a sorbent bed, with structured sorbent beds developed and tested against the performance of a packed bed. The vacuum moisture swing device will function by pushing air through the sorbent bed, resulting in cleaner air exiting. A vacuum will then be pulled, which will cause a reservoir of water at room temperature to vaporize. The water vapor will be pulled through the sorbent bed, causing the CO2 to unbind from sorbent. The CO2 will be carried downstream and contained. The cycle will then repeat.

The dynamics of the vacuum moisture swing process have already been calculated and simulated by the NAU Climate Solutions Lab, and will inform many of the parameters of the cycle. For this project, the team will focus on optimizing the sorbent bed and designing a functioning and automated vacuum moisture swing direct air capture (DAC) device.

The project's client is Dr. Jennifer Wade. SRP is sponsoring the project, and have promised \$50,000. To satisfy our fundraising requirement, we have applied to the NAU Green Fund for a \$2000 grant and are currently awaiting approval. Based on early budgeting, this total will be more than sufficient for completing the full project.

This project is important as a proof-of-concept of a novel method of removing CO2 from air. CO2 is the largest contributor to global warming and ocean acidification. The client intends for the design to be scaled up in the future to provide a method of extracting CO2 from the air near factories. If the vacuum moisture swing design proves to be effective and energy efficient, it could be deployed near many factories and other CO2-producing facilities and significantly decrease CO2 emissions.

1.2 Deliverables

The two primary deliverables for the client are structured sorbent beds and a vacuum moisture swing device. The structured sorbent beds must perform better than a standard packed sorbent bed. The vacuum moisture swing device must be capable of testing a wide range of sorbent beds while maintaining the temperature and speed conditions that the client has specified. Further deliverables for the device are that it must be automated, maintain a clean lab environment, and output the data to Matlab.

The ME476C course deliverables are to complete three presentations, two reports, several individual learning assignments, and weekly timecards and staff meetings. In addition, the team has set client deliverables of meeting with the mentor every week and the client biweekly.

1.3 Success Metrics

Success for this project will be based on two categories: the structured sorbent beds and the vacuum moisture swing device. Success in structured sorbent beds will be assessed by creating one which performs better than the baseline of a packed sorbent bed. The proposed designs will have computational fluid dynamics performed with ANSYS to simulate airflow through them. Designs successful in

simulation will then be tested in the vacuum moisture swing device. Success of these structures will be analyzed by observing the pressure drop, and the adsorption efficiency, based on pressure transducers and gas analyzers. The pressure drop must be lower than the packed bed, and the adsorption capacity must be reasonably close to the packed bed. Testing will therefore include a packed bed to obtain the baseline numbers which will be used to analyze success of the structured beds. Success in the vacuum moisture swing device will be based on whether it can create and maintain the conditions desired for the vacuum swing process. Calculations will be performed to identify the ideal velocity and pressure during the adsorption and desorption processes. The client has already identified the steps in the cycle (being adsorption, evacuation, desorption, final evacuation, and pressurization). The device must cycle through these steps properly, opening and closing valves, powering on and off pumps and heating elements, and recording data from sensors throughout the process. If the device can perform the full vacuum moisture swing cycle on all of the sorbents that are tested, it will be a success.

2 REQUIREMENTS

After meeting with the client, several customer requirements and corresponding engineering requirements were established. These were then formed into a house of quality to determine the most important aspects of this design.

2.1 Customer Requirements (CRs)

- 1. Capture CO2 as efficiently as possible
 - Capture the most amount of CO2 for the least amount of energy
- 2. Capture as much CO2 as possible
 - Capture as much CO2 as possible from the air pulled through the reactor
- 3. Utilize Vacuum moisture swing
 - Utilize Vacuum pressures that allow water to vaporize with minimal heating to allow for a more efficient moisture swing
- 4. Minimize water use
 - Recycle as much water as possible through the system
- 5. Track the metrics of the apparatus as it runs
 - Position various sensors in critical areas to record pressures, temperatures and evaporation rates
- 6. Variable flow rate, and pressure
 - Allow variation in operational conditions to allow for testing and optimization of various structures
- 7. Maintain clean lab environment to protect experimental equipment
 - Avoid any contaminants such as oil and dust from interfering with sensors, pumps and other equipment
- 8. Keep design compact
 - The design must be a practical scale for small batch tests of experimental sorbents and fit within the available lab space.
- 9. Utilize existing common vacuum parts
 - Majority of components should be selected from commercially available options to keep costs down, save time, and allow for future modifications or scaling.

2.2 Engineering Requirements (ERs)

- 2. Capture CO2 as efficiently as possible
 - Maximize kg CO2 / Watt
- 3. Capture as much CO2 as possible

- Maximize kg CO2 / hour
- 4. Utilize Vacuum moisture swing
 - Operating pressure < saturation pressure
 - At 23°C saturation pressure is 2811Pa
- 5. Minimize water use
 - <1 Liter added per cycle
- 6. Track the metrics of the apparatus as it runs
 - ≥3 Thermocouples
 - ≥3 Pressure Transducers
 - ≥1 mass scale (for water)
- 7. Variable flow rate, and pressure
 - ≥1 Variable frequency drive
 - ≥1 Adjustable valve
 - ≥1 Programmable logic controller
- 8. Maintain clean lab environment to protect experimental equipment
 - 0 oiled components
 - ≥ 1 filter on each inlet
 - ≥1 filter or trap before pump
 - ≥1 filter after sorbent bed
- 9. Keep design compact
 - <1m height and depth
 - <2m width
- 10. Utilize existing common vacuum parts
 - ≤3 fabricated components

2.3 House of Quality (HoQ)

Once the customer and engineering requirements were determined a house of quality was created to set goals and determine the most important design factors. The house of quality can be seen in figure x.

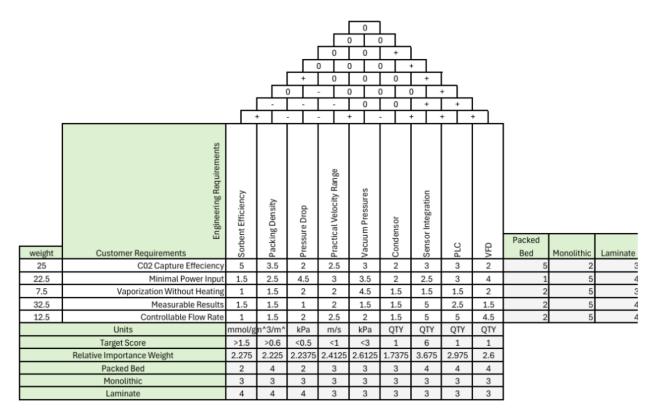


Figure 1: House of Quality

The first step of this process was to assign weights to all customer requirements based on their importance and then rank their correlation to each engineering requirement on a scale of 1 to 5. The weight was then applied to these scores to find the relative importance of each engineering requirement. Next target values were set for each of these engineering requirements. The benchmark sorbent bed designs were then ranked relative to the customer and engineering requirements on the bottom and right side of the diagram. Lastly the correlations between engineering requirements were determined in the roof of the house. This diagram concluded that elements such as sensors, a programmable logic controller, variable frequency drive, and vacuum pressure would be crucial to the design. This diagram is iterative and may change based on updated client needs.

3 Research Within Your Design Space

This chapter contains both team and individual research into the direct air capture realm. Benchmarking is described, in which other existing DAC devices are analyzed. Given that the vacuum moisture swing process has never been performed in the way that this project intends, the benchmarking provides comparisons, but not direct substitutions. Literature reviews into the major subsystems of the design are listed, with individual team members listing and describing literature resources. Mathematical modeling is described in detail, showing calculations, software simulations, and Matlab programming that investigated the expected or required performance of different subsystems.

3.1 Benchmarking

Most existing DAC systems rely on a thermal moisture swing where water is heated to create vapor for the desorption and stripping processes. For our team design we will be relying on a vacuum moisture swing where vacuum pressures are used to boil water at room temperature. Vacuum pumps typically require less energy than heating elements which will allow for a more energy efficient design. The use of vacuum pumps in the DAC process is a newer concept and little benchmarking is available. Due to this we will use thermal moisture swing data as the best estimate of sub system performance.

The most important subsystem within our DAC system is the Sorbent Bed where the reaction occurs. The most common sorbent structures in existing processes are packed bed, fluidized bed, monolith and laminate. Both packed and fluidized beds consist of an open column full of small sorbent beads. In the packed bed the beads are packed between two screens allowing a flow to pass with great contact as well as great pressure drop. In a fluidized bed the velocity is fine tuned so that beads are suspended in the air, often described as an indoor skydiving effect. Alternatively, the monolith and laminate structure consist of intricate structures made from sorbents that allow flow to pass. The monolith is like a honey comb structure and the laminate is composed of many sheets layered on top of each other.

A vacuum pump is needed to bring the system to the pressures needed. The most common types of vacuum pumps are rotary vane, diaphragm, scroll, and liquid ring pumps. Choosing a pump type depends primarily on the target pumping speed, pressure, and pump-down time. Each of those types of pumps are ideal for different ranges of target parameters. It was found that rotary vane and scroll pumps are designed to pump within the target parameters of the vacuum moisture swing (about 1m/s and 1kpa).

Given that the system needs to be automated, an automations control is necessary. For control architecture, three options were considered: OPC UA, Matlab, and Matlab with Modbus. All three could work for the project, but have varying levels of complexity and reliability. Using a PC with Matlab to communicate with a PLC communicating over Modbus was chosen due to it's simplicity and reliability.

Standard KF vacuum fittings will be used to build the system, these are available in various shapes, sizes and connection types. Filters will also be placed at various locations in the system, these are available in many different mesh sizes. Lastly the water vapor must be separated from the CO2 before capture. This can be achieved through condensation from cooling or repressurizing, It can also be achieved using additional sorbents with different properties.

3.2 Literature Review

3.2.1 Literature Review: Randy Brierley

"Flanges and Fittings" [1]:

This resources is a catalogue from a major manufacturer, Oerlikon Leybold, lists the standard ISO-KF fittings. This serves as a reference of what standard KF rated vacuum fitting parts are available along with their dimensions and tolerances.

"Fundamentals of Vacuum Technology" [2]:

This resource, also from Leybold Vacuum, covers the fundamental physics and engineering of vacuum systems. It covers the equations and physical parameters, the types of pump, flow regimes, and pumping

methods. It also covers how to troubleshoot and maintain vacuum systems. Essentially, it provides a full guide for an engineer and a technician to become familiar with all major aspects of vacuum systems.

"Introduction to Vacuum Technology" [3]:

This resource is a textbook, introducing the basic physics and engineering for vacuum systems. It goes over vacuum gauges, pumping systems, lines, conductance, valves, and fittings. It also gives an overview of troubleshooting common issues in vacuum systems.

"Sizing Vacuum Pumps" [4]:

This resource presents a guide to sizing vacuum pumps. It gives a concise checklist, as well as detailed explanations of the physical parameters that determine vacuum pump size. It covers important numbers such as conductance, pump-down time, target pressure, and gas load.

"Handbook of Mechanical Engineering Calculations" [5]:

This handbook covers mechanical engineering broadly, but Chapter 9 covers vacuum systems. It includes sections on calculating conductance, pressure drops, target pressures, and pump-down times, and also delves into methods to size vacuum pumps.

"Conductance and Throughput in Vacuum Pipelines" [6]:

This resource covers specifically the impact of line conductance on vacuum pump throughput. It gives equations for finding and summing up the line conductance with different fittings, and how to calculate the throughput of a vacuum pump after ting into account total conductance.

"Evaporation of Water with Emphasis on Applications and Measurements" [7]:

This resource gives a detailed overview of the physics of water evaporation in different circumstances. It gives equations used to find upper limits of evaporation based on different limiting mechanisms, and discusses how to derate the theoretical maximums to approximate real-world evaporation rates. It gives examples of calculations compared to empirical data with specific experiments in both lab settings and open ponds.

"Kinetics of Evaporation: Statistical Rate Theory Approach" [8]

This journal article covers a certain type of approach to modeling evaporation. This approach is statistical rate theory, which claims to be a more accurate approach to predicting real-world evaporation rates. It uses a statistical approach to modelling the kinetics of evaporation at the gas-liquid interface.

"RSLogix Getting Results Guide" [9]:

This resource, from Rockwell Automation, gives a detailed guide on setting up, programming, and running PLCs. It documents user interface conventions, how to set up the appropriate parameters for specific types of devices, and workflow practices to make them run efficiently.

"Evaporation and Condensation at Liquid/Vapor Interface" [10]:

This article, from NASA, discusses the physics of a liquid vaporizing and condensing at the surface of the liquid. It discusses the Hertz-Knudsen equation which calculates the upper limit of evaporative flux due to kinetics, and then discusses how this result can be derated by the fraction of vaporized molecules that recondense while still near the liquid-vapor interface.

3.2.2 Literature Review: Elijah Woolridge

"Flow Through Packed Beds" [11]

Describes the pressure drop across a packed bed and the use of the Ergun equation.

"50 years of Geldart classification – ScienceDirect" [12]

This is a state-of-the-art article describing the Geldart classification of fluidization behavior as well as key characteristics of each region. In the case of IRA900, the bed should exhibit type B fluidization as a sand like particle with bubbling, a low fluidization height, and immediate de-fluidization.

"Fluid Mechanics for Fluidized Beds" [13]

Describes the pressure drop and critical velocities for fluidized beds. Provides equations for the terminal velocity of particles and the weight of a bed of particles.

"Aeration, fluidization, permeability of powders" [14]

Defines the key behavior of a fluidized bed, namely the constant pressure drop and the expansion of the bed. It also provides visuals for pressure and volume at varying speeds.

"Comparison of Attrition Test Methods: ASTM standard fluidized bed vs jet cup | Industrial & Engineering Chemistry Research" [15]

Describes the increased wear on particles present in fluidized bed experiments and attempts at building current endurance testing standards of particles. This will be a major deciding factor for the suitability of IRA 900 in fluidized beds.

"Systems design and economic analysis of direct air capture of CO2 through temperature vacuum swing adsorption using MIL-101(CR)-PEI-800 and mmen-mg2(dobpdc) MOF adsorbents | Industrial & Engineering Chemistry Research:" [16]

Describes the efficiency, cost, and performance of laminate and monolith structures for temperature swing sorbents. Much of the analysis holds for moisture swing processes.

"Friction modeling of flood flow simulations | Journal of Hydraulic Engineering | Vol 144, no 12" [17]

Defines a general approximation for the darcy friction factor for use in all flow regimes with a high degree of accuracy.

"Properties of Water and Steam" [18]

Steam table and calculator. This standard provides all required information to perform for flow or energy calculations by hand, down to very low pressures.

"Saturated Ice and Steam" [19]

Provides the necessary enthalpy information for ice required for both hand and computer simulated condenser calculations. These are necessary to determine the feasibility and size of condenser systems.

"Eazao Bio" [20]

The printer we intend to buy provides core limitations for the fabrication of structured sorbents. This in turn informs all designs and simulations.

3.2.3 Literature Review: Branden Welker

Throughout the design process, CFD will be used to simulate fluid flow through the sorbent structure. To better understand the modeling process a literature review was performed on the topic of CFD simulation and validation.

1. Flow Through Sorbent Beds

- [21] [22] [23] These first three sources are very similar with slight differences in parameters geometry and sorbent type. All three sources are an overview of using ANSYS to model the capture of C02 passing through a sorbent bed. These sources provide boundary conditions and user defined functions that can be applied to our simulations. These sources also validated their data using experimental data. These sources will help to setup any CFD simulations performed
- [24] This source provides some similar information to the previous sources with the addition of sorbent expansion. This includes the user defined function used to model the sorbent expansion as well as the variance in results it caused.

2. Flow Through Complex 3D printed Structures

- [25] This source is an overview and comparison of modeling flow through packed beds and 3D printed structures. Some validation is provided for these 3D printed structures
- [26] This source is a review of pressure drops across various sorbent structures based on CFD simulations. This provides a rough structure for performing these simulations and a process for optimizing this data.

3. CFD Validation

- [27] This source is an overview of validation and verification of CFD simulations. This source introduced the standard (AIAA G-077-1998) which provides framework for validation and verification of CFD. The information is more related to aerospace, but many concepts can be applied to any simulation.
- [28] This Source provided experimental constants used to apply fluid dynamic equations to various geometries such as square ducts

4. General Equations and Properties

[29] Provided basic fluid dynamic equations, constants and properties needed throughout the design process

[18] Used for majority of steam properties applied to CFD simulations

3.2.4 Literature Review: Justin Patterson

"AmberLiteTM IRA900 Cl Ion Exchange Resin" [30]

This source was very helpful in describing the conditions that our sorbents will operate under. This includes temperature and pH ranges. Physical properties of the sorbents were also described, such as the density, swelling, range of size distribution, and approximate expansion of a bed of the sorbents when introduced to air flow that creates a fluidized bed structure.

"Moisture-Driven CO2 Pump for Direct Air Capture" [31]

This source is a paper published by Professor Wade, who is our customer. It describes the governing chemical equations relating to the operation of our DAC reactor. These equations helped the team understand the reactions and define the basic steps of our reactor. It also provided experimental data that described the amount of time it took for relative concentrations of CO2 and water to get absorbed by the sorbents which will be very useful in determining the amount of time each state needs when we are testing the rig after construction.

"CO₂ Capture From Air in a Radial Flow Contactor: Batch or Continuous Operation?" [32]

This research paper highlights the CO2 concentration profiles for absorption experiments, which will help in learning the optimum run time. In addition, it showed acceptable velocity ranges for the input air/water vapor and how the reaction output changes because of it.

"Analysis of direct capture of CO2 from ambient air via steam-assisted temperature-vacuum swing adsorption" [33]

This paper includes schematics for basic reactor design and specific electrical/thermal energy compared to CO2 production graphs. The equations they used we will likely need to calculate our parameters for our reactor in the future. Temperature, humidity, pressure, concentration of CO2/H2O graphs were provided that correspond to each step of the cycle that are completed throughout the reaction.

"Scaling up 3D printed hybrid sorbents towards (cost) effective post-combustion CO2 capture: A multiscale study" [34]

For this source, I mainly focused on how they made their sorbent paste so that they could print it using a 3D printer that will be very similar to ours. They used, "polyethyleneimine (PEI) and multiwalled carbon nanotubes (MWCNT) as the main components, and in addition, minor amounts of dispersant (UBE, and methylcellulose (MC) as a binder to make the paste printable." They are using a carbon-based sorbent just like the activated charcoal that we will use so this should be a great help. It also talks about the ratio they

used for each ingredient and how to mix them to ensure the correct properties.

"Investigating The Performance Of 3-D Printed Sorbents For Direct Air Capture Of CO2" [35]

This research paper describes the full set up needed to accurately print structures with these experimental materials, pump pressure for nozzle control, ratios for the slurry and test results. We will use this as a guide for when we are putting our system together, and optimizing the sorbent mixture and print quality.

"3D-Printing of Adsorbents for Increased Productivity in Carbon Capture Applications (3D-CAPS)" [36]

This source is very similar to the source above, however, it focuses on silica based sorbents which is what our IRA900 sorbents are made of. This will be helpful if we want to either grind the sorbents up into powders and make a paste or integrate the beads into the 3D printing material. Isoreticular shapes were produced that are another way of porous structure that we may want to experiment with.

ANSYS Fluent Tutorials Guide: Fluid Flow in an Exhaust Manifold," [37]

This tutorial details the setup and solution of a steady-state fluid flow simulation within an exhaust manifold geometry, covering steps like meshing, setting boundary conditions, and running the calculation.

"ANSYS Fluent Tutorials Guide: Fluent Postprocessing: Exhaust Manifold," [38]

This tutorial focuses on visualization and reporting techniques using the solution data from the previous case, covering topics such as creating contours, velocity vectors, animations, and generating integral reports.

"ANSYS Fluent Tutorials Guide: Modeling Flow Through Porous Media," [39]

This tutorial demonstrates how to set up and solve a simulation that incorporates the porous media model, a feature often used to represent pressure loss in devices like filters or packed beds.

3.3 Mathematical Modeling

3.3.1 Evaporation Rate Based on Mass Flow, Heater, Pressure drop, and Reservoir (Randy Brierley)

During the vapor stripping phase of the VMS cycle, water will be evaporated from the surface of the water reservoir and pulled through the sorbent bed by the vacuum pump. The water reservoir will have a heater which will keep the water at a constant room temperature, counteracting the cooling effect of evaporation. The customer has specified a certain velocity, pressure, and temperature to keep the system at. The following calculations define the relationships between flow rates, heat input, flow restriction, evaporative interface area, and evaporative kinetics to help size the vacuum pump, the heating element, and the reservoir.

Assumptions and known values

• Uniform conditions at gas-liquid interface

- T_{ν} Temperature of the water reservoir is isotheral at 300 K
- P_{ν} Pressure of the chamber will be kept constant at 1000 Pa
- D_i The inner diameter of the chamber and sorbent bed is 0.04 m
- $M_{\rm w}$ The molar weight of water is 0.018 kg/mol
- R The ideal gas constant is 8.314 J/mol*K
- P_{sat} The saturation pressure of water at 300 K is 3600 Pa
- μ The dynamic viscosity of water vapor at 300 K is $9x10^{-6}$ Pa*s
- h_{fg} The latent heat of vaporization of water at 300 K is $2.43x10^6$ J/kg
- α The evaporation accommodation coefficient is 0.1
- ϵ The void fraction of a packed bed is 0.5
- d_s The average diameter of the sorbent beads is $5.68x10^{-4}$ m
- L The length of the sorbent bed is 0.254 m
- q The heat flux of the heating element is $1x10^4 W/m^2$

Equations

Ideal gas law: This is the density form of the equation

$$\rho = \frac{PM_w}{RT}$$

Equation 1

Where ρ is density, M_w is molar weight, R is ideal gas constant, and T is temperature.

<u>Continuity equation (mass flow)</u>: This equation relates mass flow rate to the density and velocity of a gas, along the cross-sectional area it travels through.

$$\dot{m} = \rho v A$$

Equation 2

Where \dot{m} is the mass transfer rate, v is the velocity, and A is the cross-sectional area.

<u>Hertz-Knudsen</u>: This equation calculates the mass flux of evaporation due to the kinetic limit at the gasliquid interface. The α is a multiplier to derate the idealized kinetic limit of evaporation to a real-world number, between 0 and 1.

$$\dot{m}$$
 " = $\alpha \sqrt{\frac{M_w}{2\pi RT}} \Delta P$

Equation 3

Where \dot{m}'' is the mass flux, α is the condensation coefficient, M_w is the molar weight of water, R is the ideal gas constant, T is the liquid temperature, and ΔP is the difference between the saturation and the environment pressure.

<u>Kozeny-Carman Equation</u>: This equation gives the permeability of a packed bed based on the void fraction and the diameter of the beads.

$$k = \frac{\varepsilon^3 d^2}{180(1 - \varepsilon)^2}$$

Equation 4

Where k is permeability, ε is the void fraction, and d is the bead diameter.

<u>Darcy's Law:</u> The equation used here is a version of Darcy's law, converted to calculate mass flux based on the pressure drop through a chamber, related to viscosity and permeability.

$$\dot{m}'' = \rho_v \frac{k}{\mu} \frac{\Delta P}{L}$$
 Equation 5

Where k is the permeability given by the Kozeny-Carman equation below, μ is the viscosity, and L is the length of the sorbent bed.

Latent heat evaporation energy balance:

$$\dot{m}$$
 " $= \frac{q}{h_{fg}}$ Equation 6

Where q is the heat flux and h_{fg} is the latent heat of evaporation

<u>Mass flux equivalence</u>: This equation is the definition of mass flux, which is the mass transfer rate divided by the area.

$$\dot{m}$$
 " $=\frac{\dot{m}}{A}$

Equation 7

Pumping speed relation:

$$\dot{m} = \rho S_{eff}$$

Equation 8

Where S_{eff} is the effective pumping speed.

Solving for this system of equations yields the following results:

- 1. water $\rho = 7.2167 \times 10^{-3} \ kg/m^3$
- 2. required $\dot{m} = 9.0688 \times 10^{-6} \text{ kg/s}$
- 3. kinetic $\dot{m}'' = 0.2786 \ kg/m^2 s$
- 4. packed-bed $k = 8.9618 \times 10^{-10} m^2$
- 5. flow $\dot{m}^{"} = 7.3558x10^{-3} kg/m^2s$
- 6. heat $\dot{m}'' = 4.1152x10^{-3} kg/m^2 s$
- 7. limiting $\dot{m}^{"} = 4.1152x10^{-3} kg/m^2s$
- 8. water surface A = $2.2037x10^{-3} m^2$
- 9. reservoir diameter D = 0.0530 m

10. required pumping speed $S_{eff} = 1.26 \text{ l/s}$

These results, coupled with the customer-specified parameters, give the results needed to size an appropriate heater, reservoir, and vacuum pump. This system of equations also provides the relation of those three primary parts on the evaporation process, allowing the team to optimize the device by altering one of those parts and seeing what the needed change for the others will be. In this way, the team can choose the optimal combination of heater, reservoir size, and vacuum pump size to efficiently run the vapor stripping process at the parameters that the customer has requested.

3.3.2 Pressure Drop and Cooling Power Associated with the Condenser at 1m/s Flow Rate Through a KF40 Pipe and Varying Pressures. (Eli Woolridge)

A condenser is required to protect the pump and purify the CO2. In order to size the condenser, the required cooling power was calculated at the absolute worst case flow speed and varying pressures. Using this same data, the decrease in pressure across the condenser caused by rapid is calculated. This allows us to determine how much the condenser contributes to the flow rate and decreases pressure within the system. A MATLAB script called condenserCalcs.m was written for this purpose, it can be found in appendix B.

The program works in two phases, It first relies on mass flow and conservation of energy to calculate the cooling power then calculates the partial pressures of various gasses in the chamber to find the decrease if steam were replaced by liquid water and the mixture were slightly cooled. As one would imagine, this relies heavily on the ideal gas law. In these calculations, the steam entering is assumed to be five degrees above saturation to adjust for exothermal reactions in the sorbent and heat transfer through the walls. The pressure ranges from 1 KPa to 30 KPa to capture the saturation pressure of water between 6.5 degrees and 70 degrees C . Mass flow in is calculated for various pressures as follows:

$$mdot = u * A * p = (1) * (\pi * \left(\frac{20}{1000}\right)^2) * \left(\frac{P}{Rspecific * T}\right)$$
 Equation 9

This can then be used to find the amount of cooling power required to keep up with the mass flow rate using energy balance.

$$Qdot\ condense = mdot*(h_{steam} - h_{water})$$
 Equation 10
$$Qdot\ freeze = mdot*(h_{steam} - h_{ice})$$
 Equation 11

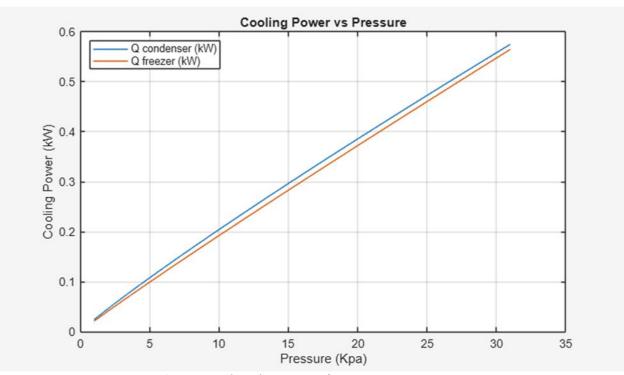


Figure 2: Required cooling power for steam at varying pressures.

This graph shows a nonlinear but increasing curve of the power requirement to condense steam at the given pressure and flow rate. Because of the proximity to its tripple point the enthalpy of ice is not distinctly different from the enthalpy of saturated water and as such caution must be taken to prevent freezing. With that said the actual required cooling power is not impractically large, so a condenser is a viable option.

As for the pressure drop, it can be assumed that all partial pressure due to steam is removed and a portion of the volume of the chamber becomes liquid water. Assuming .4 moles of CO2, the quantity released by 200g of sorbent, and an arbritrary chamber size of 1/8 m^3 the partial pressure of CO2 by the ideal gas law must be around 9 KPa depending on the temperature. All remaining pressure must then be caused by steam, all of which is removed by the condenser. The pressure drop across the condenser is then almost exactly equal to the partial pressure of the steam. The pressure of the CO2 adjusted for temperature and volume on condensate can be found below.

$$P_{after} = (P - P_{steam}) * \left(\frac{T_{sat}}{T_{Inlet}}\right) * \left(\frac{V}{V - \left(\frac{m}{p}\right)}\right)$$
 Equation 12

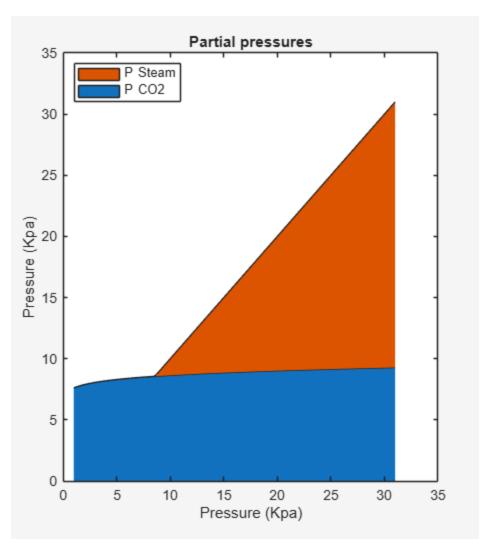


Figure 3: Partial pressures within the condenser.

The mismatch between total pressures on the X and Y axis of this graph indicates that the condenser is incapable of balancing pressures below the partial pressure of non-steam gases within the mix. Because of this, if allowed to run in a sealed chamber of steam, the condenser will rapidly decrease the pressure until only non-steam gases and liquid water or ice remain. Because of the low power requirement and peculiarities of the cycle, vapor flow through the sorbent can be entirely driven by this effect if it is needed.

3.3.3 Surface Area Required to Maintain Condenser Using a Water-Cooled Heat Exchanger.

An inexpensive option for a heat exchanger that cannot freeze is a water cooled brazed plate heat exchanger. Hand calcs to estimate the feasibility of this were performed using an energy balance. The heat exchanger forces the fluid through many thin channels with a total area far larger than our kf40 pipe. Additionally, the plates are designed to mix the fluids so they are assumed to be at a constant temperature.

The phase change also supports the assumption that there is a constant temperature. The cooling fluid has a relatively high heat capacity and will be flowing quickly so it also can be assumed to be a constant temperature. For this estimate the problem is then reduced to the heat flow through a 2mm copper plate with constant temperature bounds.

Two configurations were tested, room temperature or 21deg C and 1kpa saturated steam at 6.67 degrees C. The same 1m/s was assumed. The k value for copper is 413 W/mk and the heat exchanger examined is 300 mm long. Power was calculated as before resulting in 55 watts for 22 deg C and 24 watts for 6.67 deg C. The linear conduction equations was rewritten for area and solved for each. Interestingly the temperature change decreases far more rapidly than the power required to condense the steam to the greatest required area was actually the one with the lower energy requirement.

A min @ 21 deg C =
$$q*L/(k(dT)) = .00001789 \text{ m}^2 = 17.89 \text{ mm}^2$$

Equation 13

A min @ 6.67 deg C= $q*L/(k(dT)) = .0001805 \text{ m}^2 = 180.5 \text{ mm}^2$

Both of these values are orders of magnitude smaller than the surface area of most brazed plate condensers, so a water-cooled system could be an incredibly promising option for condensers that condense and freeze water separately.

3.3.4 ANSYS Simulations: Pressure Drop in Monolith and Laminate Structures

Various ANSYS simulations have been performed to better understand the factors that affect pressure drops in a monolith and laminate structure. 9 simulations were performed for each structure to determine how pressure drop varies as saturation pressure and velocity are adjusted. These simulations are all specific to the vapor stripping stage as this will have the most interesting behavior once the mass transfer is incorporated. This will also provide a minimum expected pressure drop to begin selecting a suitable pressure transducer. The monolith and laminate structures tested can be seen below. A poly-hexacore mesh pattern was used to mesh these structures with a single boundary layer. The monolith had to be broken into sections with a symmetry plane due to limited computational power. Both resulting meshes were well above the minimum quality.





These simulations were performed using several assumptions listed in the table below.

Assumption	Explanation
Steady State	Constant flow rate
Fluid passing through reactors will be assumed as	Our Advisor will help us integrate a mass transfer
water vapor with constant density and viscosity	coefficient corresponding to the sorbent
	absorption process
The system is isothermal, and no heat transfer	A heat generator will be added with the mass
occurs	transfer coefficient
No slip condition	Standard for surface flow
Smooth surface	Smooth surface will be assumed until more
	knowledge of final surface roughness is obtained
Laminar flow	Laminar flow can be assumed if Reynolds are
	found to be below 2300

Table 1: Assumptions used for ANSYS CFD simulations

The following equation can be used to determine Reynolds number in a square channel for the laminar assumption [29].

$$Re = \frac{\rho Vs}{\mu}$$
 Equation 14

Where Re is Reynolds number, ρ is fluid density, V is the fluid velocity, s is the side length of the channel, and μ is the dynamic viscosity of the fluid

The simulation can then be set up in ANSYS using the following tools and boundary conditions

Boundary Condition	Input	Reasoning
Pressure Inlet	Saturation Pressure	Water will be saturated before
		the reactor so inlet pressure will
		be very close to saturation
		pressure
Mass Flow Outlet	Desired mass flow for velocity	Mass flow can be controlled
		using a pump at the outlet
Wall / No Slip	All sorbent surfaces	Allows the no slip condition or
		future surface roughness to be
		applied
Symmetry	N/A	Used on faces where monolith
		was cut to reduce cell count
Turbulence Model	Laminar	Assumed based on Re
Operating Pressure	Saturation Pressure	Inlet can then be set to 0
		gauge pressure to represent
		saturation pressure
Fluid Material	Vapor density and viscosity at	Allow ANSYS to properly
	selected saturation pressure	model fluid behavior

Table 2: Simulation Boundary Conditions

After performing all simulations the resulting data is as follows

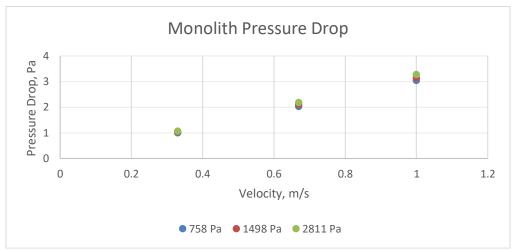


Figure 6: Monolith Pressure Drop From ANSYS CFD

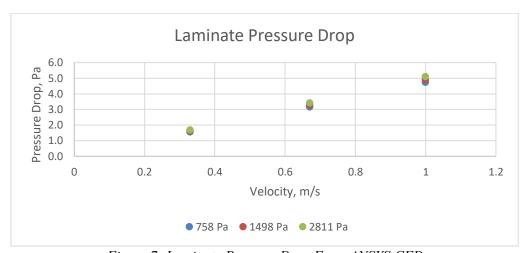


Figure 7: Laminate Pressure Drop From ANSYS CFD

The resulting data showed a linear relationship where pressure drop increases significantly with velocity and that pressure insignificantly increases with saturation pressure (inlet pressure). It was also found that the laminate had higher pressure drop, however it has tighter channels and more surface area.

Pressure Across Monolith (2811 Pa, 1 m/s)

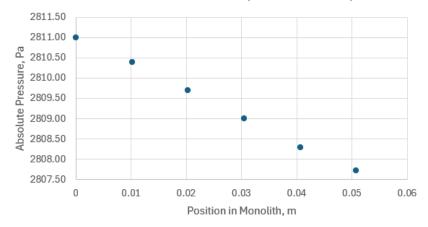


Figure 8: Pressure Drop Across Monolith at 2811 Pa, 1 m/s

This next figure shows that pressure drop also has a linear relationship with length, this will likely change after the mass transfer coefficient is added as fluid properties will change with length. Lastly we can view velocity profiles and streamlines to determine how the flow is actually moving through the channels

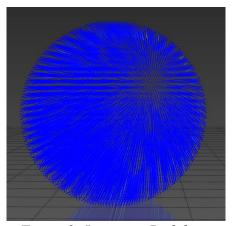


Figure 9: Laminate Path lines

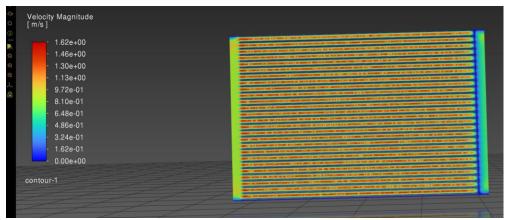


Figure 10: Velocity Profile in Laminate Structure

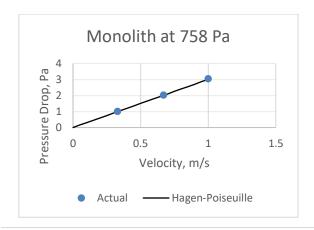
3.3.5 Ansys Validation Using Darcy Weisbach

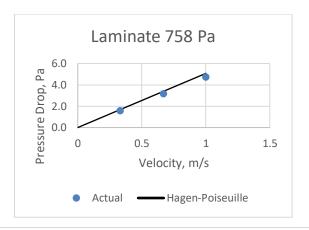
Once The ANSYS simulations had been performed, A modified form of the Darcy-Weisbach was used to find pressure drop for the same conditions. This was done to validate both the ANSYS simulations and the approximation equations. Both Equations were derived from the Darcy-Weisbach [29] and modified based on experimentally tested friction factors [28].

$$\Delta P_{square} = \frac{28.45 \mu LV}{s^2}$$

$$\Delta P_{slot} = \frac{12\mu LV}{h^2}$$

Where, ΔP is pressure drop, μ is dynamic viscosity, L is channel length, V is fluid velocity, s is the side length of the square and h is the height of the channel. The resulting pressure drops were very similar to the ANSYS data. The Monolith was underestimated by 1.2% and the laminate was underestimated by 6.7%. The comparison of data at 578 Pa can be seen below.





4 Design Concepts

4.1 Functional Decomposition

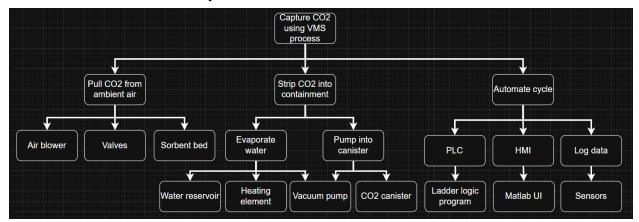


Figure 12: Functional Decomposition of DAC System

Figure 12 shows the functional decomposition of the full VMS device. Under the overarching requirement of utilizing the vacuum moisture swing process to capture CO2, there are three main requirements: Capture the CO2 from the air, strip the CO2 into containment, and have the device automatically perform the cycle. This functional decomposition is important for this project because it breaks down the core functions of the device visually, in a way which the physical diagram does not. The physical design of the system overlaps in function, with multiple parts participating in different phases. This functional decomposition delineates the main functions so that they can be analyzed separately. This has become representative of the way the work has been divided up among the team: focusing on either CO2 adsorption, vapor stripping, or automation. These three fields cover all tasks that the project must achieve. We can see that further down the decomposition, the functions umbrella into actual parts. Utilizing this, the team can maintain a focus on what the primary purpose of each part is for.

4.2 Concept Generation

4.2.1 Valve Type (Eli Woolridge)

The type of valve used to isolate sections of the test rig plays a key role in the efficiency, safety, effectiveness, and ease of automation of the system. To minimize complexity, the valves should also interface with KF fittings and be electronically actuated. For this application, there are several types of valves that are commonly used and fit these characteristics. These being needle or gas dosing valves, butterfly valves, gate valves, globe valves, solenoid valves and ball valves. Each provide a unique combination of benefits and limitations.

4.2.2 Vapor CO2 Separation (Branden Welker)

During the vapor stripping stage of the cycle a mixture of water vapor and CO2 gas will leave the sorbent bed heading to the pump. To capture close to pure C02 this water must be separated from the C02 and recycled to the water reservoir. This separation can be achieved through pressurization, absorption, or cooling. For pressurization the water vapor would have to pass through the pump back to atmospheric pressure where it would condensate at room temp requiring no extra process. If absorption is chosen an additional sorbent bed featuring different sorbents must be added after the bed where the main reaction occurs. This would also require an additional process to then remove the water from these sorbents. Lastly for cooling, a refrigeration element would be required which would use additional energy, however, the water can then be knocked out before the pump. Since vacuum pressures are used it should be considered that liquid water does not exist below 0.6 kPa.

4.2.3 Pipe Diameter (Branden Welker)

Standard KF vacuum fittings and tubing will be used to construct most of the DAC system. These tubes will be used for their commercial availability and ability to withstand pressures significantly lower than the expected operating pressure. These tubes come in a large variety of diameters. The available options in our expected size range are KF16, KF25, KF40 and KF50 where the number represents the inner diameter in mm. These fittings and tubes can be attached using clamps and have a spot for a seal or filter between sections. There are many available fittings and adapters to connect valves, sensors and pumps. All components will be made of 3/16 stainless steel due to its corrosion resistance.

4.2.4 Control protocol (Randy Brierly)

A number of different control protocols would function for this project. The ones considered were OPC UA, a central PLC, and Modbus via Matlab. OPC UA was ruled out due to it's complexity and having no one on the team with enough experience. OPC UA would be suitable for reliability and future expansion. Matlab alone would be too basic for future expansion, and less reliable. Modbus over a PLC to Matlab on a PC was chosen for this project. It will provide a reliable and relatively simple setup with the ability to expand.

Which control protocol to use to control the powered equipment and read the sensors was considered. A number of different control protocols would function for this project. The ones considered were OPC UA, a central PLC, and Modbus via Matlab, due to them being common setups. The pros and cons of each setup is shown in the table below.

	OPC UA	Central PLC	Modbus via Matlab
Pros	 Can handle nearly any type of sensor Designed to be easily scalable Intended to generate metadata 	 Deterministic control All logic centralized in one program Modular card slots to accept variety of sensors Medium learning curve 	 Simple learning curve Inherent integration with Matlab as the native lab software Quick to modify and deploy

Cons	More complex to program	Future expansion more limited than OPCUA	Particularly non- deterministic on PC
	Higher energy usage	More vendor-specific software	 Grows complex when scaling up
	Steeper learning curve		• Smaller choice of sensors and
	Non-deterministic		equipment

Table 3: Pros and Cons of Control Systems

4.2.5 Sorbent Mesh and Filters (Justin Patterson)

Our smallest measured particle size has a diameter of .35mm. To be safe, we want our mesh to be near .2mm in case for any other smaller particles, this corresponds to a mesh size of 70 (.21mm). We will use a centering ring with this mesh integrated into it to keep the sorbent beads from leaving the reactor column.

4.2.6 Ambient Air and Pump Filters (Justin Patterson)

The inlet ambient air filtration system will need 3 stages, with each one making the next filter in line more efficient and last longer. The pump filtration system doesn't need the largest filter due to the large filter on the ambient air. The HEPA filters are the industry standard for protecting sensitive equipment such as sensors. ULPA filters were decided against due to their vastly restricted airflow.

4.2.7 Vacuum Pump (Randy Brierly)

The vacuum pump is a critical component of the VMS device, with the vacuum ability being at the heart of the VMS process. The vacuum pump has to be able to pull down to 1kPa and maintain a flow speed of 1 m/s, as per customer requirements. The customer also specified that the pump has to be oil-less to maintain a clean lab environment. After researching vacuum pumps (see section 3.2 for literature references), three primary vacuum pump types were determined to be options: turbo-molecular, roots pump plus backing stage, and a dry scroll pump. The pros and cons of each are compared in the table below:

	Turbo-molecular vacuum pump		
Pros	Easily reaches high	High throughput	• Compact
	vacuum	• Fine with vapor and some	• Quiet
	Virtually no leakage	particulate	• Cheaper
	High pumping speed	• Fast pump-down rates	• Can handle vapor

Con	ıs	•	Sensitive to any particulate	•	Requires the extra backing stage to	•	Lower pumping speeds
		•	More powerful than required	•	compress to atmosphere Extra cost of extra pump	•	Sensitive to particulate
		•	Expensive				

Table 4: Pros and Cons of Vacuum Pumps

4.2.8 Sorbent Structure (Eli Woolridge)

There are two major types of sorbent structure, these being structured and unstructured. The structured category is generally made of sheets or extruded ceramic and is defined by its ability to hold a distinct shape. The most common types to be considered are laminar and monolith type structures. A laminate structure is composed of parallel sheets of sorbent which the fluid passes between. Monolith structures contain many even channels through a block. Other shapes are possible but not common and difficult to simulate or fabricate. Unstructured sorbents often take the form of beads or powders. The standard bed configuration is a packed bed, though in rare cases a fluidized bed may be employed.

4.3 Selection Criteria

4.3.1 Vacuum Pump Selection

To size the vacuum pump, the primary parameters needed are typically the pressure range, the throughput, and the draw-down time. The customer specified a lowest pressure of 1kPa, a max velocity of 1 m/s, and specified that draw-down time is not a concern. This left throughput as the primary calculation needed to size the vacuum pump.

To find the throughput, the customer required speed of 1 m/s and the chosen fitting diameter of 40mm were plugged into the equation:

$$Q = v\pi D^2/4$$

This came out to 1.26 liters/second. This results in the selection criteria for the vacuum pump being: able to maintain 1kPa pressure, able to maintain a 1.26 l/s throughput, and be oil-free.

4.3.2 Heating Element selection

The heating element in the water reservoir needs to generate enough heat to maintain the water at room temperature while the evaporation process at it's surface attempts to cool the water down due to it's endothermic process. To find this required value, the equation below can be used:

$$\dot{m}^{\prime\prime}=q/h_{fg}$$

To solve this, the water vapor density is required. Using the parameters of 1 kPa and 300K in the below equation:

$$\rho = PM_w/RT$$

The density is found to be $7.2167x10^{-3} kg/m^3$. Plugging this into the following equation:

$$\dot{m} = \rho S_{eff}$$

Where S_{eff} is the pumping speed found in the previous section, it yields $\dot{m} = 9.0688 \times 10^{-6}$ kg/s. Converting this mass transfer rate to a mass flux using the equivalence:

$$\dot{m}^{\prime\prime} = \dot{m}/A$$

This gives a mass flux of $7.2167x10^{-3} kg/m^2s$. Finally, plugging that along with the latent heat of vaporization of water into the equation:

$$\dot{m}^{\prime\prime} = q/h_{f,g}$$

This yields a heating flux of $17536 J/m^2 s$. This heat flux is the primary number used for concept selection of the heating element.

4.4 Concept Selection

4.4.1 Valve Type Selection

Valve types were evaluated on a scale of -5 to 5 against relevant customer and engineering requirements with critical failures of -5, highlighted in red, eliminating a design.

Engineering Requirements	2a. Minimize pressure drop	2b. Keep air velocity within 1m/s	3a. Vacuum pressure below 3 Kpa	6b. Incorporate control logic	Customer Requirement: Low Cost	Customer Requirement: Corrosion and abrasive resistance	
Ball Valve	5	2	5	3	4	4	23
Butterfly Valve	5	5	-5	5	5	-2	13
Globe Valve	0	5	5	4	0	2	16
Needle	-5	4	5	5	5	1	19

Solenoid	5	2	5	3	3	3	21
Gate	5	2	5	4	-2	-1	13

Table 5: valve choice

This chart reveals that butterfly valves and needle valves are not suitable due to pressure requirements and pressure drop requirements, respectively. The best valve for our use case is ball valves. These are common in fluid applications but not often electronically actuated in vacuum systems. They are more often used as manual shutoff valves. As such, solenoid or globe valves may be necessary to use due to part availability.

4.4.2 Vapor CO2 Separation Selection

To determine the best way to separate water vapor from CO2 a pro-con list was created and assessed. This information can be seen below.

	Pros	Cons
		Water vapor may ruin pump
	No additional systems required	
	Water knockout before pump	May require additional cycles
Absorption		May require additional energy
		Additional components required
	Water knockout before pump	Additional energy required
Cooling	Easier freeze thaw to ensure maximum	Additional components required
-	separation	

Table 6: Pros and Cons of water separation

Based on this data a final selection could not be made for the separation process. Absorption has been ruled out due to the extensive cons and minimal pros. If a pump can be found that allows water to pass through, pressurization will be selected. If a pump cannot be found, Cooling will be selected at the best option

4.4.3 Filter Selection

Selected Filters can be seen in the table below

Filter Stage		 Purpose for Pump Air Filtration

Stage 1: Mesh Screens	50 to 100+ microns	1–4	Captures the largest particles such as sand or coarse debris	Not needed
Stage 2: Polyester or Cartridge Filter	1 to 10 microns	8–11	Captures dust, pollen and mold. Key for protecting lifespan of the final, more expensive filter	Will capture larger sorbent particles. These will be from possible breakdown due to water absorption.
Stage 3: HEPA Filter	0.3 microns	17–20	Removes 99.97% of particles with diameters of .3 microns. Crucial for protecting sensors and the vacuum pump	Will capture the finest particles generated by the rubbing of the sorbents in a fluidized bed

Table 7: Filter Selection

4.4.4 Pressure sensor models and configurations

High precision pressure sensors with incredibly fine precision and broad ranges are required for the core functionality of the device. These characteristics are in direct opposition to each other and as such sensors that can achieve this come from hyperspecialized distributors at a high cost. As recommended from wade we searched Validyne and DwyerOmega for sensors that could measure on the absolute scale from zero to 15 Kpa and still register pressure differences of 8 less than pascal between chambers. We found three sensors that could work for this application. These are the DwyerOmega PX490 absolute sensor, the Validyne DP45 Low Pressure Variable Reluctance differential sensor with swapable ranges, and the P895 Test and Measurement Pressure Transducer which is also from Validyne, has swappable ranges, and measure differential, gage, or absolute pressure. A chart containing six ranked configurations of these sensors is below. The final decision is awaiting the client's approval.

P1 resolution & cost	9pa for \$1500 or	35 pa for \$1000
sensor	PX490	p895

P2	PX490	PX490	PX490	p895	p895	P895
dif	DP45	P895		DP450	P895	
P3	PX490	PX490	PX490	p895	P895	P895
cost	\$4,200	\$4,000	\$3,000	\$3,200	\$3,000	\$2,000

additional costs	.+4 dia	.+2 dia		.+7 dia	.+4 dia	
resolution (pa)	0.35	2.15	12	0.35	2.15	50
	1st	2nd	3rd	4th	5th	6th

Table 8: Ranked Sensor Configurations

4.4.5 Final concept

Below is a Piping and Instrumentation Diagram of the final design of the VMS device:

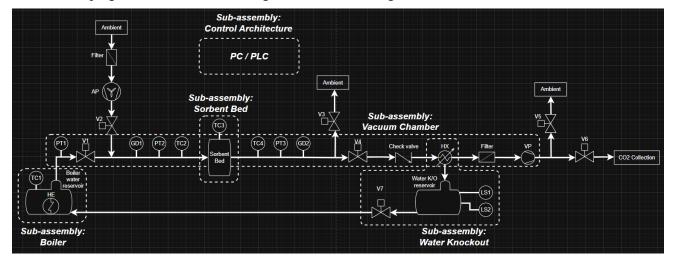


Figure 13: Final Design P&ID

This diagram represents all major powered parts, sensors, and chambers in the final design. The subsystems are highlighted, showing the boiler water reservoir, the sorbent bed, the vacuum chamber, and the water knockout as the main subassemblies. These sub-assemblies combined perform all the functions required by the customer to run a vacuum moisture swing CO2 capture process. Below is a diagram of the physical final design, including all parts and fittings such as piping elbows and thread adapters:

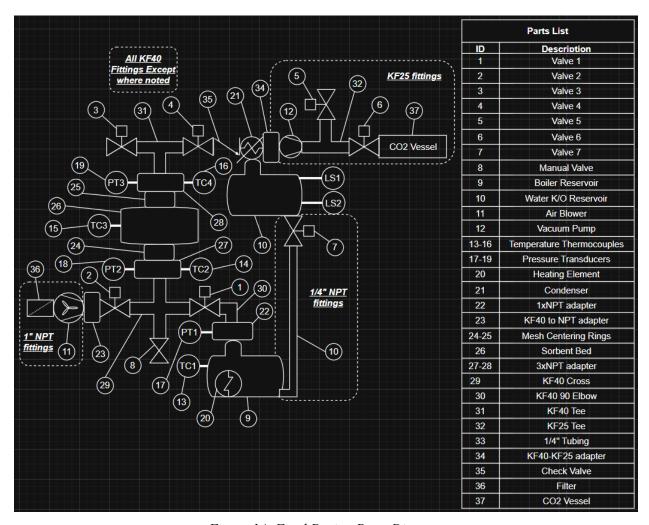


Figure 14: Final Design Parts Diagram

This diagram gives a two dimensional view of the physical structure of the final design. It was decided that the device will be built vertically to match this view. Scaffolding and the lab table it will be attached to are the only parts not shown in this diagram. This physical build keeps the device compact and structurally stable, to match the customer requirements of being compact and lab-safe.

The Control System Block Diagram, which illustrates the final design for the automation and control architecture, is shown below:

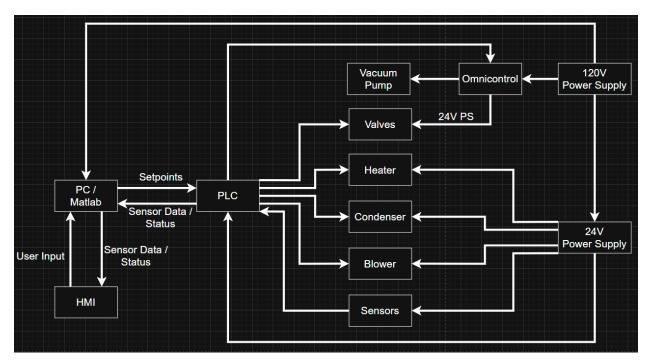


Figure 15: Control Block Diagram

This control block diagram shows all of the parts that are electrically powered and controlled in the final design. The PLC is the centralized control center, being able to write to all of the electrical parts and the HMI. The 120V and the 24V power supplies will be the only parts not controlled by the PLC, as they simply need to output constant power. This control architecture is the physical embodiment of the control and automation system for the final design; the control logic, which was created as a ladder logic program for the PLC, can be seen as Prototype 1 in Appendix A of this report.

Below are the subsystem block diagrams for PID controlled subsystems:

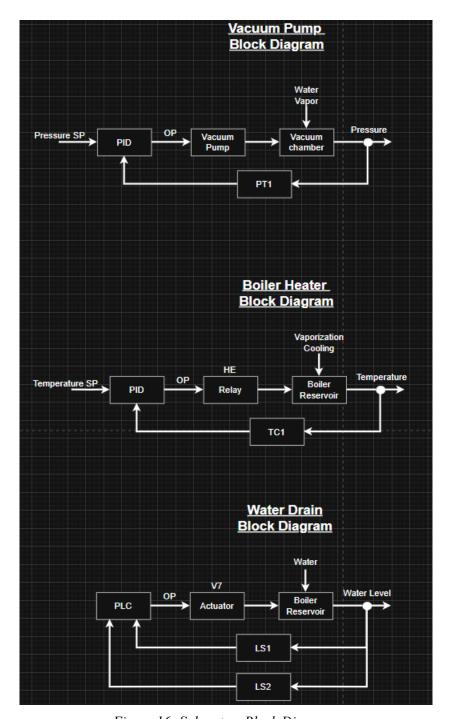


Figure 16: Subsystem Block Diagrams

These block diagrams illustrate how the PLC will control the vacuum pump, heater, and water drain during operation of the device. For the vacuum pump, during the vapor stripping phase a constant pressure needs to be maintained. This PID loop based on pressure sensor feedback will control the vacuum pump for the entirety of the vapor stripping phase. Also during the vapor stripping phase, the heating element will be required to maintain a constant temperature in the water reservoir. This will be

accomplished similarly by a PID loop with the PLC based on feedback from a thermocouple in the water reservoir. For the water drain subsystem, the control will be a simpler logic loop. In this, the water drain will be opened if the high level sensor is triggered, and the water drain will be closed if the low level sensor is triggered. These subsystems represent the only parts of the final design that require monitored automated control; all other parts are simply triggered off or on.

5 Schedule and Budget

5.1 Schedule

The schedule for this semester can be seen in the Gant chart below. The top set of tasks are project related tasks that must be completed to stay on task with the design and testing process. The bottom set is the required deliverables for the capstone class. As it is currently week 14 many tasks have been completed, however few are still to be completed in the coming week. Upcoming tasks are described below the figure.

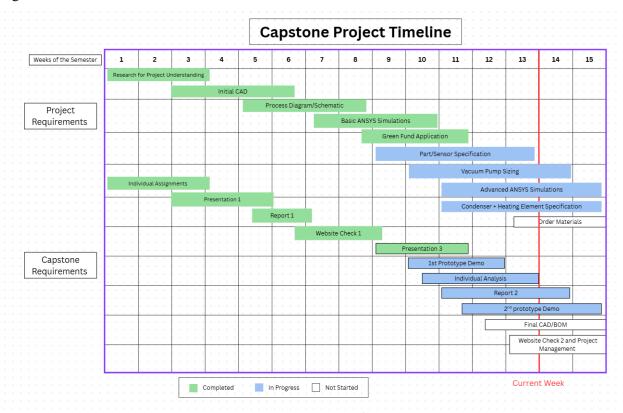


Figure 17: Vacuum Moisture Swing 1st Semester Gant Chart

Vacuum pump sizing: As theoretical pressure drops and required flowrate are dialed in, the final vaccum pump will be specified and selected

Advanced ANSYS simulations: More complex ANSYS simulations will be performed with minimal assumptions for high accuracy predictions, mass transfer will also be added to represent the reaction caused by the sorbents

Condenser + **heating element specifications:** Final heating and cooling requirements will be determined and final condenser and heating element will be selected

Order Materials: BOM will be finalized, and all parts will be ordered

Prototype 2: 2 working prototypes must be developed and shared to answer a question relative to design, will be further discussed in section 6

Final CAD/BOM: A final BOM must be submitted, and any custom parts must be modeled using CAD software.

Website Check 2: Website must be up to date with prototype and CAD

Project Management: A project management plan for the following semester must be submitted

A rough draft of a project schedule for semester 2 can be seen below. Capstone deliverables have not yet been established. Due dates may change based on capstone deliverables, and shipping times.

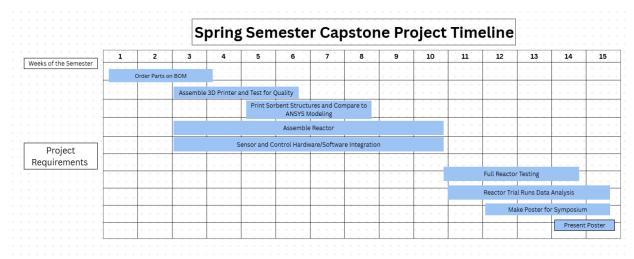


Figure 18: Rough Draft of Vacuum Moisture Swing 2nd Semester Gant Chart

5.2 Budget

For The design and assembly of the DAC apparatus we have been provided \$50,000 by the Arizona Salt River Project. The rough cost estimate used to obtain this budget can be seen below.

Item	Purpose	Cost Estimate			
		Lov	V	Hig	h
Oil free vacuum pump (1	Drives vacuum				
mbar, 10 LPM)	evaporation of water to				
	generate a vapor sweep				
	of variable flow rates	\$	6,000	\$	15,000
Variable Frequency Drive	Operates pump at				
	controlable flow rates	\$	500	\$	1,000
Cold Trap & Chiller	condense water vapor				
	downstream of sorbent,				
	upstream of vacuum	\$	2,500	\$	5,000
Water Vessel w/ thermal	Reservoir of water that				
jacket and temperature	will be vacuum				
control	evaporated to water				
	vapor/steam	\$	3,000	\$	5,000
KF40 vessel	cylindrical vessel that				
	contains sorbent beds				
	and adapts to vacuum				
	fittings	\$	100	\$	200
KF25/40 Adapters /	clamps, o-rings,				
sorbent bet supports	adapters to sensor ports	\$	5,000	\$	10,000
Instrumentation	pressure transducers,				
	thermocouples and data				
	logging with vacuum				
	adapters/feedthroughs	\$	4,000	\$	12,000
Shop Welding (10-20 hrs)	316 Stainless steel				
	welding of components				
	(~\$150/hr)	\$	1,500	\$	3,000
Contingency (10%)		\$	2,260	\$	5,120
Total		\$	22,600	\$	51,200

Table 9: Theoretical Budget for DAC apparatus

Bill of Materials (BoM)

This project is particularly unique in that the client has specifically asked that no parts are fabricated. Additionally, they have put constraints that require extremely costly components. Because of this there can be very little iterative prototyping, and all items purchased must work together on the first try at the risk of hundreds of dollars and several weeks of shipping time. Because of this, almost the entire BOM must be completed before anything can be purchased. Our BOM notes purpose, description, manufacturer, link, individual cost, quantity, and total cost. We do not have lead times as of yet because many suppliers require special orders, so it is difficult to predict without quotes. We have also sorted into distinct subsystems which require particular coordination. These include plumbing, sensors, automation, and miscellaneous which includes mounts and wiring. We are waiting on feedback from Dr Wade to finalize sensors and the cold trap. The pump sizing is nearly complete, and the current ball valves may be replaced with Pfeiffer brand valves depending on their quote. The PLC is also being finalized but needs to wait on the sensor inputs to be fully specked. We hope to order all parts before the end of the semester.

6 Design Validation and Initial Prototyping

6.1 Failure Modes and Effects Analysis (FMEA)

To mitigate risks with our experimental apparatus a failure modes and effects analysis was performed. All potential risks associated with the components, processes, and conditions, have been looked at and compiled into the table below

Part # and Functions	Potential Failure Mode	Potential Effect(s) of Failure	Severity (S)	•	
Control hardware	Malfunction	Unable to control pump, heating, etc.	10	Poor Monitoring/Calibration	Medium
1-8, Valves	Corrosion/Wear	Unable to control cycle steps	5	Poor Maintenance	Low
9, Bolier Reservoir	Overheating	High Pressure (possible explosion)	8	Poor Maintenance	Low
10, Water K/O reservoir	Carbonic Acid Buildup	Corrosion in entire system as water flows	5	Poor Maintenance	Low
12, Vacuum Pump	Overheating	Pump breaks, pressure rises	7	Poor Maintenance	Low
20, Heating Element	Control Malfunction	Overheats Boiler Reservoir	8	Poor Maintenance	Low
21, Condenser	Over-freezing	Pipes freeze or vapor contamination	5	Poor Monitoring/Calibration	Low
26, Sorbent Bed	Sorbent Rubbing/Reaction	Heating and Microparticle infiltration	6	Poor Maintenance	Medium
36, Filter	Particle Wear	Vacuum pump and sensor damage	7	Poor Maintenance	Low
37, CO2 Vessel	Over pressurization	Explosion/Concentrated CO2 leaking	9	Poor Maintenance/Safety	Medium
KF25/40 tubing and adapters	Corrosion/Wear	Leaking and ruined experiment	5	Poor Maintenance	Low

Table 10: Failure Modes and Effects Analysis

The resulting data from this analysis is that with regular maintenance and monitoring there is very little risk of harm or even failure. This includes, monitoring pressures and temperatures, checking seals, and regular cleaning of certain components. It was determined that the largest risk would be CO2 leaking from the system contaminating the air in the lab in which work is done. CO2 sensors can however be placed around the room to watch for this.

6.2 Initial Prototyping

6.2.1 Automation Prototype: PLC Program [Randy Brierley]

One of the initial protypes is a fully functioning PLC program that can automatedly run the VMS device through the full adsorption/desorption cycles. The question it is trying to answer is, what logic is needed to have the device autonomously run through the VMS cycle with predetermined setpoints?

To answer this, a ladder logic program was created in RSLogix500. This was built as the first-pass prototype for the complete PLC program. Below is a photo of the program files ladder structure (the full program is in the Appendix A):



Figure 19: PLC program ladder structure

The program begins with the input and output from the HMI, so that the user con input the setpoints desired during the VMS cycle, and can also control the auto / off mode. Digital inputs and outputs are run through, along with analogue inputs and outputs. After these are processed, the program goes to the "State Control" ladder, which is the overhead control of whether the device is in Manual, Off, or Auto mode. It also handles the transitions from phase to phase as the cycle runs, and determines when the preset number of cycles has been completed and the device should return to it's idle state. Within the five different phase ladders, which handle the individual phases of the VMS cycle, each piece of equipment on the device is set to the unique position needed for that phase. Valves, heaters, and pumps are all controlled, either in an on / off state, or in a PID loop to maintain a setpoint which was determined from the HMI I/O.

So the answer to the question, "what logic is needed to have the device autonomously run through the VMS cycle with predetermined setpoints?", is answered generally by the structure of the fourteen ladders above. These general functions, when combined, allowed the program to run on a PLC emulator, and successfully ran repeated automated cycles through the VMS process based on the user-input setpoints. The detailed logic needed in each ladder was also found, and can be seen in Appendix A.

This prototype informed the design and future iterations by confirming that a single PLC connected to an HMI is capable of automating the full VMS device. This program functioned as desired on an emulator. But, since it was just on an emulator, this means that how the PLC reacts to real-world scenarios is still unsure. Sensor inputs were preset digitally instead of fluctuating with real-world effects. Considering the

potential effects of live testing, such as harmonic fluctuations and run-away PID controls, means that this prototype should be iterated on by first building in safety interlocks and alarms. This will safeguard physical equipment when the PLC is run live, and also help prevent dangers to operators. Additionally, while the automation mode of this PLC prototype worked well, the manual mode did not always engage properly. Specifically, if the program ran an automated cycle and then was switched to manual mode, it would become stuck in the idle phase. This will need to be investigated and rectified for the next prototype.

6.2.2 ANSYS prototyping

The Ansys Simulations performed in section 3.3.4 was meant to act as initial virtual prototype. The questions we wanted to answer with this prototype are as follows

- 1. How does pressure drop change relative to factors such as length velocity, operating pressure, geometry and channel size?
- 2. How does a fluid act as it moves through a sorbent bed structure?
- 3. What is the minimum pressure drop that the pressure transducer must accurately read?

We learned that for constant fluid properties, pressure drop has a linear relationship with velocity operating pressure and length, so we have some freedom with operating pressure. Velocity, geometry and length seemed to have the largest effect on pressure drop. It was also examined that the square channel had a lot of stagnant areas in the corner, so a circular or hexagonal monolith may perform better. The pressure drops were also found to be lower than what can be easily recorded so a longer test section may be used for a more measurable pressure drop. In the future, a mass transfer coefficient will be added to accurately update the fluid properties the reaction would be occurring. More structures will also be tested varying variables such as surface area and void fraction.

6.3 Other Engineering Calculations

All calculations performed thus far have been included in selection processes and have therefore been placed previously in the report

6.4 Future Testing Potential

There are many potential tests to run in the future as the device is developed. Each subsystem could be tested verify that the PID loops function, and would also provide a useful testing grounds to dial in the PID parameters. These would be running the vacuum pump on a simple throttled chamber to maintain a constant pressure. The reservoir heater PID control could be tested in a simple reservoir, trying to maintain a constant temperature above ambient temperature. The water knockout system can also be tested by pulling water vapor through it with the vacuum pump and using a scale on both reservoirs to measure the efficiency of water recapture.

Pressure drops in the different designs of sorbent beds could also be tested in the future. A simple setup that can pull both air and water vapor through a sorbent bed could be built, with the sorbent bed easily swapped out. This would allow empirical testing of the pressure drops caused by the flow restrictions of the sorbent structures, which could then be compared to the values obtained in CFD simulations to ensure they match.

Once the full build of the device is assembled, testing can begin on the cycles. Each phase of the VMS cycle can be run individually, while collecting data from sensors to ensure it is operating as intended. A

power meter could be hooked up for these trials, allowing testing of the power draw of each phase. This would allow the team to see where the most power draw is, and take steps to optimize those parameters to minimize power usage. Long-term durability testing could also be conducted, where the device would be set to run many cycles consecutively, while the team monitors for any failures or compounding issues that could cause failures.

7 CONCLUSIONS

This project is working towards creating a direct air capture device that utilizes a vacuum moisture swing process to remove CO2 from air. Critical requirements of this project are to design efficient structured sorbent beds, create a functioning vacuum moisture swing device, and gather data from testing. The efficiency of the structured sorbent beds will be based on their performance compared the baseline of a packed sorbent bed. The structures will need to have a lower pressure drop than the packed bed, and ideally have comparable adsorption efficiency. The vacuum moisture swing device will need to be built with lab-grade parts and be fully automated, to allow long-term testing the Climate Solutions Lab. The device is required to function during testing of a variety of sorbent bed styles.

The proposed final solution is to build a device utilizing primarily KF40 vacuum fittings, electrically actuated valves, and a vacuum pump for the vacuum chamber. Ambient air will be pushed in by a blower fan. The water vapor will be knocked out by a condenser, and a water capture reservoir with level sensors will trigger a water drain to refill the vaporization reservoir. Pressure transducers, thermocouples, and gas detectors, will provide data from testing. A control architecture of a PLC connected to a PC with Matlab, communicating over Modbus, will allow the system to be automated.

A special ceramic 3D printer will be used to print different structured sorbent beds. Utilizing ANSYS software, different structure designs will be evaluated and optimized. Once structures are selected, they will be 3D printed and used in testing in the vacuum moisture swing device. The VMS device will be designed so that the sorbent beds are quick and easy to replace, allowing accessible testing of the multiple sorbent bed designs.

The status of the design is a structured diagram with many final components selected. Several parts such as sensors, the condenser and the vacuum pump are undergoing their final selection process to soon be ordered for assembly, A 3D printer has also been selected and is currently being proposed to green fund to acquire the necessary funding. ANSYS simulations have been performed to begin optimizing sorbent structures for final testing. Soon all parts will be ordered, and the rig will be assembled to begin testing and dial in the PLC loop. ANSYS simulations will become more detailed to find the best structures to physically test. Lastly the printer will hopefully be funded so these optimized structures can be printed out and physically tested.

8 REFERENCES

- [1] Oerlikon Leybold Vacuum, Flanges and Fittings CP_080 Fittings Catalogue, Oerlikon Leybold Vacuum, 2016. [Online]. Available:
- https://www.leyboldproducts.com/media/pdf/8e/c6/3f/CP_080_Fittings_EN57beb2d4b36d0.pdf. [Accessed: Nov. 26, 2025].
- [2] Oerlikon Leybold Vacuum, Fundamentals of Vacuum Technology, Oerlikon Leybold Vacuum, 2016. [Online]. Available: https://www3.nd.edu/~wzech/Resources_LEYBOLD_FUNDAMENTALS.pdf. [Accessed: Nov. 26, 2025].
- [3] D. J. Mathewson, Introduction to Vacuum Technology, Milne Publishing, Geneseo, NY, 2018. [Online]. Available: https://milnepublishing.geneseo.edu/introtovacuumtech/. [Accessed: Nov. 26, 2025].
- [4] ThomasNet, Sizing Vacuum Pumps, Thomas Publishing Company, 2019. [Online]. Available: https://cdn.thomasnet.com/ccp/20106502/32516.pdf. [Accessed: Nov. 26, 2025].
- [5] T. Mekonnen, "Vacuum and Evacuation Systems," in Handbook of Mechanical Engineering Calculations, 3rd ed., New York, NY, USA: McGraw-Hill, 2006, ch. 9. [Online]. Available: https://www.accessengineeringlibrary.com/content/book/9780071458863/toc-chapter/chapter9/section/section20. [Accessed: Nov. 26, 2025].
- [6] VAC AERO Group, "Conductance and Throughput in Vacuum Pipelines," Vacuum Technology & Heat Treating Resources, 2015. [Online]. Available: https://vacaero.com/information-resources/vacuum-pump-technology-education-and-training/9365-conductance-and-throughput-in-vacuum-pipelines.html. [Accessed: Nov. 26, 2025].
- [7] J. J. Marciano, Evaporation of Water With Emphasis on Applications and Measurements, Universidad de Valparaíso, 2012. [Online]. Available: https://construccion.uv.cl/docs/textos/coleccion03/TEXTO.03.EvaporationofWater.pdf. [Accessed: Nov. 26, 2025].
- [8] B. W. Ninham and P. A. Thorne, "Kinetics of Evaporation: Statistical Rate Theory Approach," J. Phys. Chem., vol. 113, no. 12, pp. 4432–4440, 2009. [Online]. Available: https://doi.org/10.1021/jp810152j. [Accessed: Nov. 26, 2025].
- [9] Rockwell Automation, RSLogix 500 Getting Results Guide, Publication LG500-GR002, Rockwell Automation, 2012. [Online]. Available: https://literature.rockwellautomation.com/idc/groups/literature/documents/gr/lg500-gr002 -en-e.pdf.

[Accessed: Nov. 26, 2025].

- [10] L. Woods and H. Kassemi, "Evaporation and Condensation at a Liquid/Vapor Interface," NASA Technical Report 20170008827, NASA Glenn Research Center, Cleveland, OH, USA, 2017. [Online]. Available: https://ntrs.nasa.gov/api/citations/20170008827/downloads/20170008827.pdf. [Accessed: Nov. 26, 2025].
- [11] D. Thornhill, "Flow Through Packed Beds," Packed beds, https://faculty.washington.edu/finlayso/Fluidized_Bed/FBR_Fluid_Mech/packed_beds_fbr.htm#ergun (accessed Oct. 9, 2025).
- [12] R. Cocco and J. W. Chew, "50 years of Geldart classification sciencedirect," 50 years of Geldart classification, https://www.sciencedirect.com/science/article/pii/S0032591023006459 (accessed Oct. 9, 2025).
- [13] D. Thornhill, "Fluid Mechanics for Fluidized Beds," FBR Fluid Mechanics, https://faculty.washington.edu/finlayso/Fluidized_Bed/FBR_Fluid_Mech/fluid_bed_scroll.htm (accessed Oct. 9, 2025).
- [14] <u>Www.powderprocess.net</u>, "Aeration, fluidization, permeability of powders," Fluidization, Aeration, Permeability of powders: An overview, https://powderprocess.net/Powder Flow/Aeration Permeability.html (accessed Oct. 21, 2025).
- [15] R. Zhao, J. G. Goodwin, K. Jothimurugesan, J. Spivey, and S. K. Gangwal, "Comparison of Attrition Test Methods: ASTM standard fluidized bed vs jet cup | Industrial & Engineering Chemistry Research," Comparison of Attrition Test Methods: ASTM Standard Fluidized Bed vs Jet Cup, https://pubs.acs.org/doi/10.1021/ie990730j (accessed Oct. 22, 2025).
- [16] A. Sinha, L. Darunte, C. Jones, M. Realff, and Y. Kawajiri, "Systems design and economic analysis of direct air capture of CO2 through temperature vacuum swing adsorption using MIL-101(CR)-PEI-800 and mmen-mg2(dobpdc) MOF adsorbents | Industrial & Engineering Chemistry Research," Systems Design and Economic Analysis of Direct Air Capture of CO2 through Temperature Vacuum Swing Adsorption Using MIL-101(Cr)-PEI-800 and mmen-Mg2(dobpdc) MOF Adsorbents, https://pubs.acs.org/doi/10.1021/acs.iecr.6b03887 (accessed Oct. 9, 2025).
- [17] V. Bellos, I. Nalbantis, and G. Tsakiris, "Friction modeling of flood flow simulations | Journal of Engineering | Vol 144, no 12," ASCE library, https://ascelibrary.org/doi/10.1061/%28ASCE%29HY.1943-7900.0001540 (accessed Oct. 9, 2025)
- [18] "Properties of Water and Steam." Ski App Durchflussrechner. Accessed November 26, 2025. https://www.ski-gmbh.com/swa/tools/steam.

- [19] The Engineering ToolBox (2005). Saturated Ice and Steam Thermodynamic Properties. [online] Available at: https://www.engineeringtoolbox.com/saturated-ice-steam-d_970.html [Accessed 22/11/25].
- [20] "Eazao Bio," Eazao, https://www.eazao.com/product/eazao-bio/ (accessed Oct. 9, 2025).
- [21] N. A. A. Qasem and R. Ben-Mansour, "Energy and productivity efficient vacuum pressure swing adsorption process to separate CO₂ from CO₂/N₂ mixture using Mg-MOF-74: A CFD simulation," Applied Energy, vol. 209, pp. 190-202, Jan. 2018.
- [22] Q. Chen, F. Rosner, A. Rao, S. Samuelsen, A. Jayaraman, and G. Alptekin, "Simulation of elevated temperature solid sorbent CO2 capture for pre-combustion applications using computational fluid dynamics," *Applied Energy*, vol. 239, pp. 374–387, Apr. 2019. doi: 10.1016/j.apenergy.2019.01.179
- [23] E. S. Mogire, A. J. Mboya, E. E. Bakit, P. M. Musembi, M. Bwondera, D. K. Githinji, and V. V. Barasa, "Simulation and airflow experimentation of a multi-layer adsorbent chamber for enhanced direct air capture efficiency," in *Proc. 2024 Sustainable Research and Innovation Conf.*, JKUAT Main Campus, Kenya, Oct. 2–3, 2024, pp. 14–17
- [24] E. Abbasi, A. Hassanzadeh, and J. Abbasian, <u>"Regenerable MgO-based sorbent for high temperature CO₂ removal from syngas: 2. Two-zone variable diffusivity shrinking core model with expanding product layer," *Fuel*, vol. 105, pp. 128–134, Jan. 2013, doi: 10.1016/j.fuel.2012.06.005.</u>
- [25] A. M. Elkissi, F. Rezaei, and R. Smith, "<u>Vacuum swing adsorption process for post-combustion carbon capture with 3D printed sorbents: Quantifying the improvement in productivity and specific energy over a packed bed system through process simulation and optimization," *Chemical Engineering Science*, vol. 253, p. 117585, May 2022. doi: 10.1016/j.ces.2022.117585</u>
- [26] S. Sluijter, J. Boon, J. James, S. Krishnamurthy, A. Lind, R. Blom, K. Andreassen, A. Cormos, V. Sandu and R. de Boer, "3D-printing of adsorbents for increased productivity in carbon capture applications (3D-CAPS)," *International Journal of Greenhouse Gas Control*, vol. 112, p. 103512, 2021. doi: 10.1016/j.ijggc.2021.103512.
- [27] F. Stern, R. Wilson, and J. Shao, "Quantitative V&V of CFD simulations and certification of CFD codes," *International Journal for Numerical Methods in Fluids*, vol. 50, no. 11, pp. 1335-1355, 2006.

- [28] R. K. Shah and A. L. London, *Laminar Forced Convection in Ducts*. New York, NY, USA: Academic Press, 1978.
- [29] M. J. Moran, H. N. Shapiro, D. D. Boettner, and M. B. Bailey, Fundamentals of Engineering Thermodynamics, 8th ed. Hoboken, NJ, USA: Wiley, 2015
- [30] The Dow Chemical Company, "AmberLiteTM IRA900 Cl Ion Exchange Resin Gaussian, Macroporous, Strong Base Anion Exchange Resin for Industrial Demineralization Applications," 2019.

Online. Available: https://www.thebricks.com/resources/guide-how-to-make-a-data-sheet-in-excel. Accessed: Nov. 26, 2025.

- [31] J. L. Wade, H. Lopez Marques, W. Wang, J. Flory, and B. Freeman, "Moisture-driven CO2 pump for Direct Air Capture," *Journal of Membrane Science*, vol. 685, p. 121954, 2023. doi: 10.1016/j.memsci.2023.121954.
- [32] M. Schellevis, T. Jacobs, and W. Brilman, "CO2 capture from air in a radial flow contactor: Batch or continuous operation?," *Frontiers in Chemical Engineering*, vol. 2, 2020. doi: 10.3389/fceng.2020.573155.
- [33] V. Stampi-Bombelli, M. van der Spek, and M. Mazzotti, "Analysis of direct capture of CO2 from ambient air via steam-assisted temperature–vacuum swing adsorption," *Adsorption*, vol. 26, no. 7, pp. 1183–1197, 2020. doi: 10.1007/s10450-020-00222-7.
- [34] S. Krishnamurthy, R. Roelant, R. Blom, B. Arstad, Z. Li, M. Rombouts, V. Middelkoop, A. B. Borras, and L. Naldoni, "Scaling up 3D printed hybrid sorbents towards (cost) effective post-combustion CO2 Capture: A multiscale study," *International Journal of Greenhouse Gas Control*, vol. 132, p. 104069, 2024. doi: 10.1016/j.ijggc.2024.104069.
- [35] T. Obeng-Ampomah, "Investigating The Performance Of 3-D Printed Sorbents For Direct Air Capture Of CO2," M.S. thesis, Dept. Civil and Environmental Engineering, Carnegie Mellon University, Pittsburgh, PA, 2020. Online. Available: https://builtin.com/software-engineering-perspectives/repository. Accessed: Nov. 26, 2025.
- [36] S. Sluijter, J. Boon, J. James, S. Krishnamurthy, A. Lind, K. A. Andreassen, R. Blom, A. M. Cormos, V. Sandu, and R. de Boer, "3D-printing of adsorbents for increased productivity in carbon capture applications (3D-caps)," *SSRN Electronic Journal*, 2021. doi: 10.2139/ssrn.3970258.

[37] ANSYS, Inc., "ANSYS Fluent Tutorials Guide: Fluid Flow in an Exhaust Manifold," (Release 2024 R2). Online. Available:

https://ansyshelp.ansys.com/public/Views/Secured/corp/v242/en/flu_tg/flu_tg.html
Accessed: Nov. 1, 2025

[38] ANSYS, Inc., "ANSYS Fluent Tutorials Guide: Fluent Postprocessing: Exhaust Manifold," (Release 2024 R2). Online. Available:

 $\underline{https://ansyshelp.ansys.com/public/Views/Secured/corp/v242/en/flu_tg/flu_tg.html}.\ Accessed:\ Nov.\ 1,\\ 2025$

[39] ANSYS, Inc., "ANSYS Fluent Tutorials Guide: Modeling Flow Through Porous Media," (Release 2024 R2). Online. Available:

https://ansyshelp.ansys.com/public/Views/Secured/corp/v242/en/flu_tg/flu_tg.html. Accessed: Nov. 1, 2025

9 APPENDICES

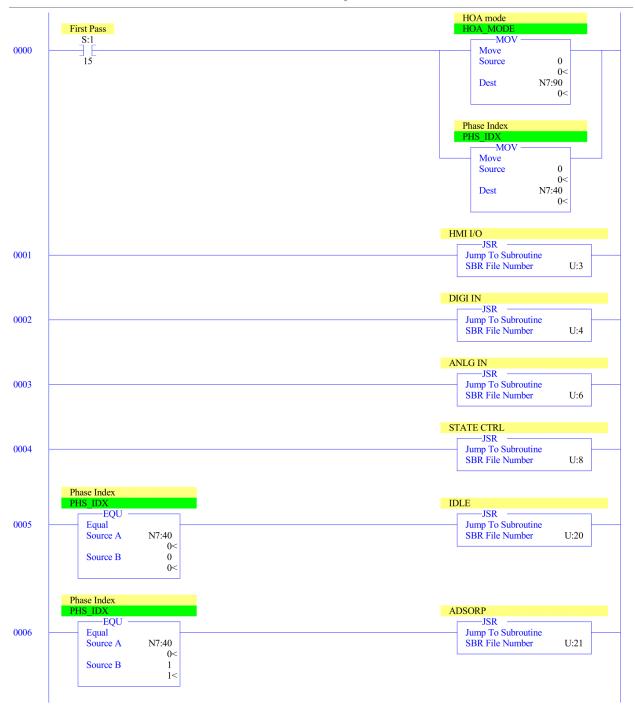
9.1 Appendix A: RSLogix500 PLC ladder logic program

VMS_PROTOTYPE1_3

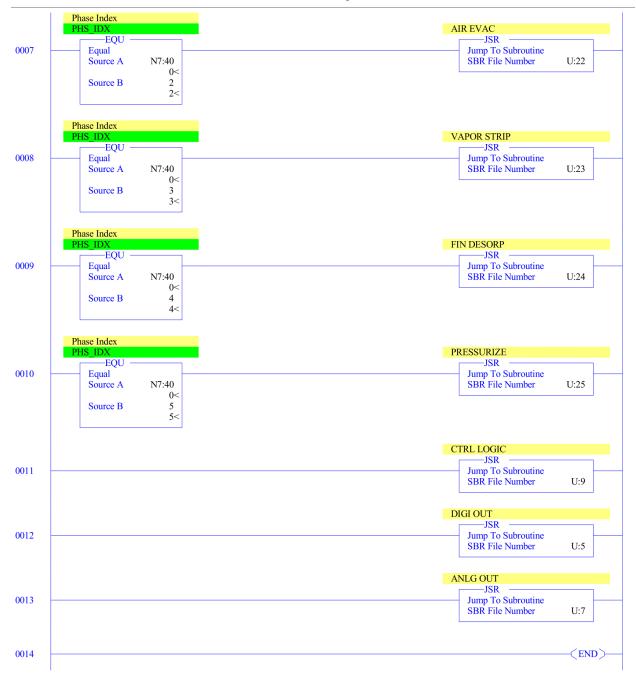
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-	1	SYS	0	No	0	
	2	LADDER	15	No	239	
HMI I/O	3	LADDER	22	No	318	
DIGI IN	4	LADDER	5	No	67	
DIGI OUT	5	LADDER	12	No	179	
ANLG IN	6	LADDER	9	No	467	
ANLG OUT	7	LADDER	4	No	126	
STATE CTRL	8	LADDER	18	No	919	
CTRL LOGIC	9	LADDER	14	No	229	
IDLE	20	LADDER	11	No	93	
ADSORP	21	LADDER	15	No	155	
AIR EVAC	22	LADDER	15	No	168	
VAP STRIP	23	LADDER	16	No	183	
FIN DESORP	24	LADDER	15	No	168	
PRESSURIZE	25	LADDER	15	No	155	

LAD 2 - --- Total Rungs in File = 15



LAD 2 - --- Total Rungs in File = 15

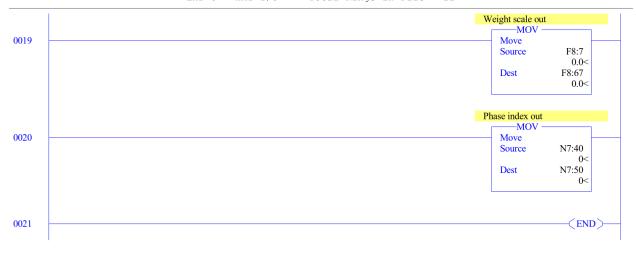






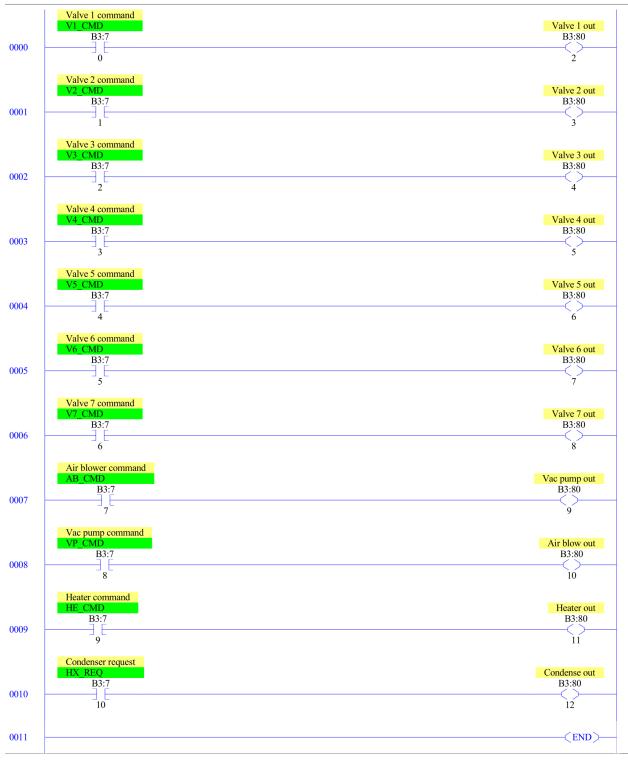


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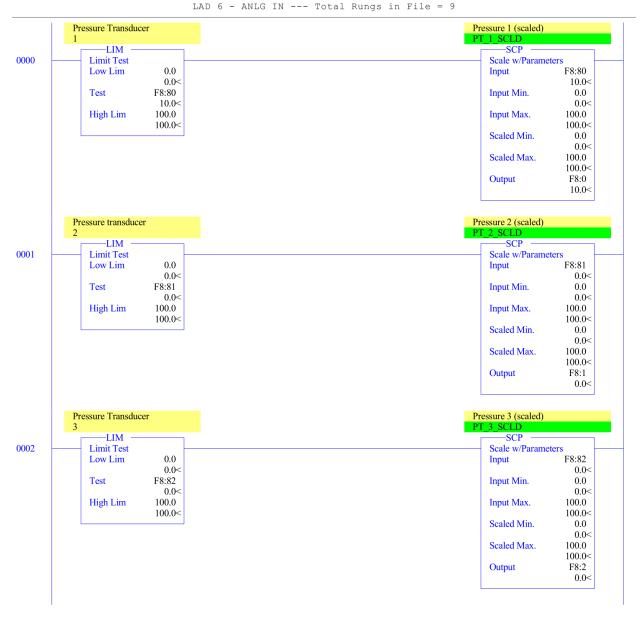
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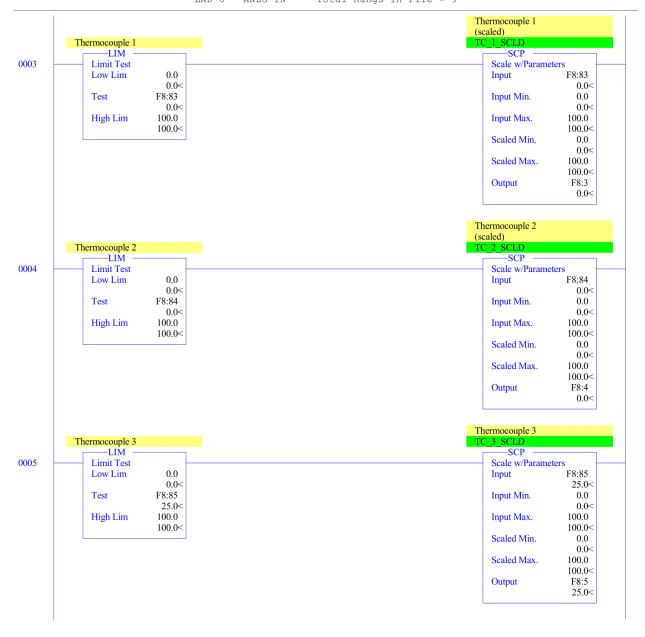


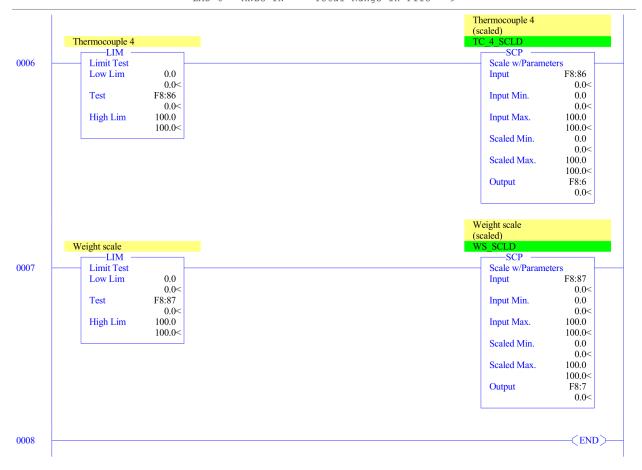


Page 1

Wednesday, November 26, 2025 - 11:54:56



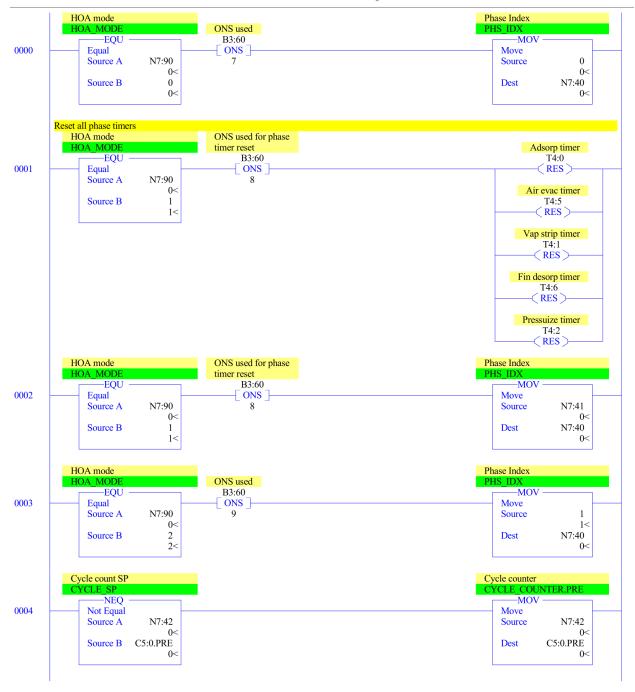




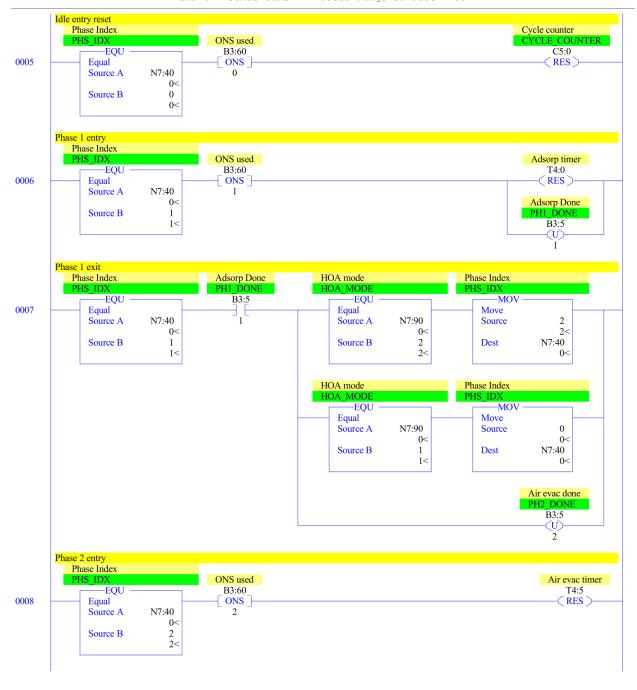
LAD 7 - ANLG OUT --- Total Rungs in File = 4

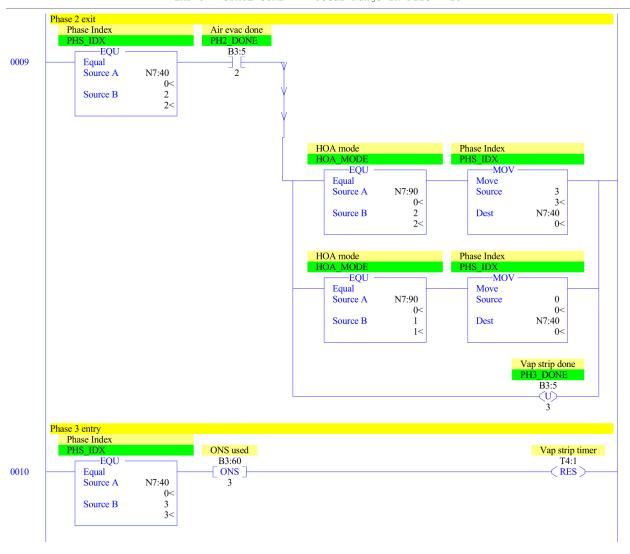


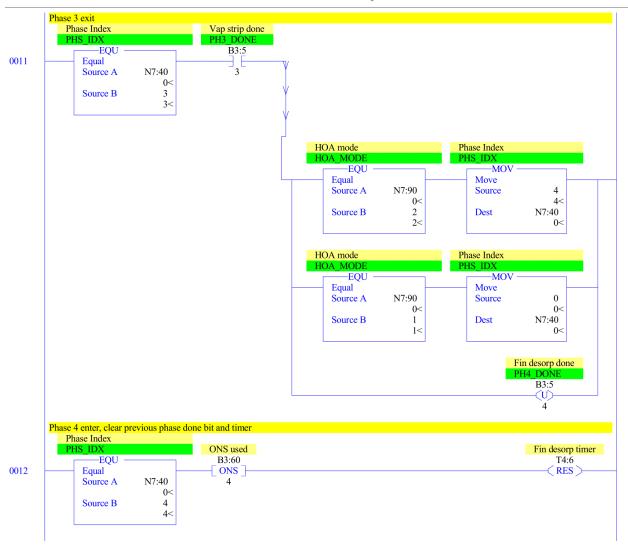
LAD 8 - STATE CTRL --- Total Rungs in File = 18



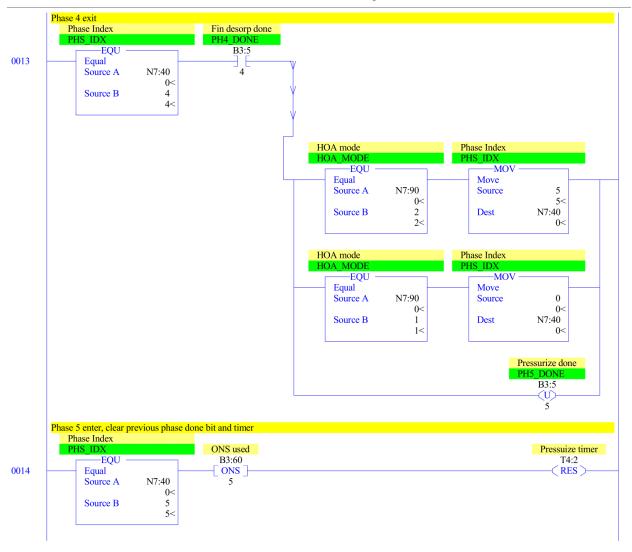
LAD 8 - STATE CTRL --- Total Rungs in File = 18

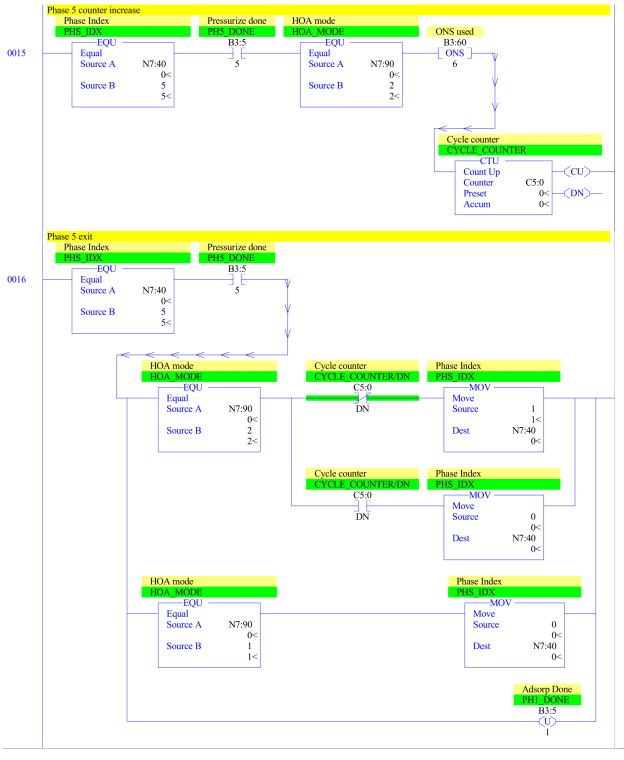






LAD 8 - STATE CTRL --- Total Rungs in File = 18





Page 6

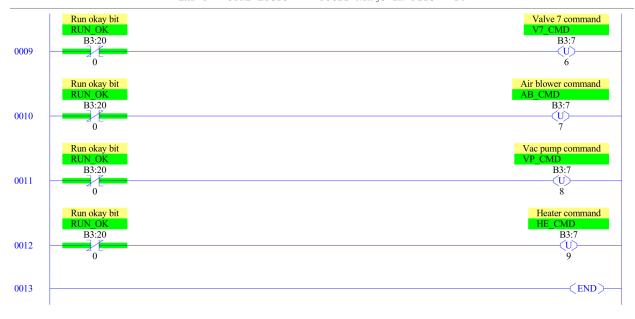
0017 (END)



Page 1

Wednesday, November 26, 2025 - 11:54:58

VMS_PROTOTYPE1_3 LAD 9 - CTRL LOGIC --- Total Rungs in File = 14







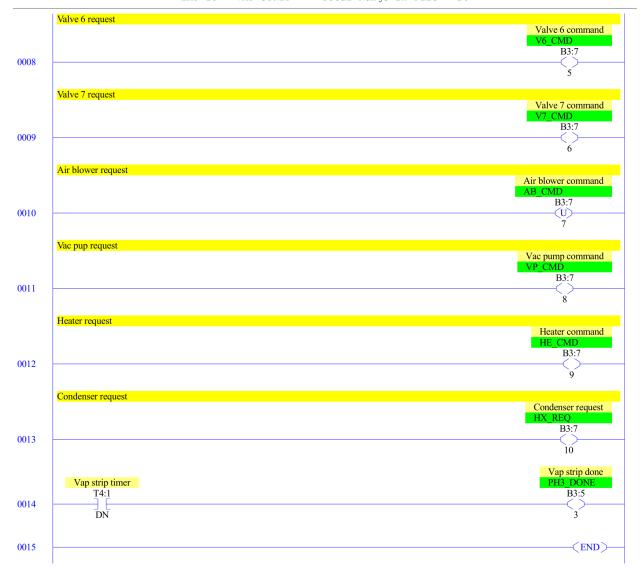


LAD 22 - AIR EVAC --- Total Rungs in File = 15

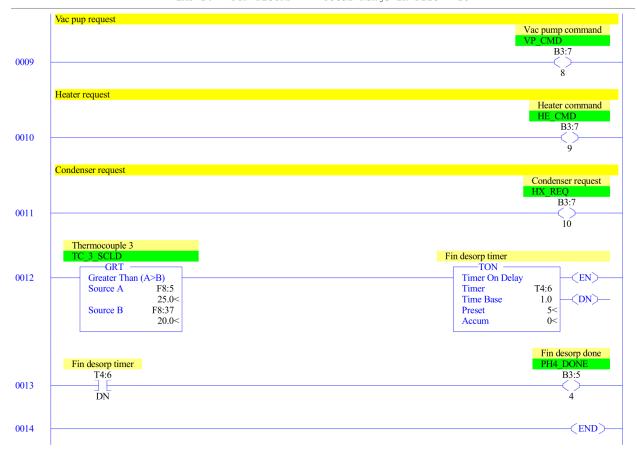
















Data File S2 (hex) -- STATUS

Main

```
Processor Mode S:1/0 - S:1/4 = Remote Program Mode On Power up Go To Run (Mode Behavior) S:1/12 = 0 First Pass S:1/15 = No Free Running Clock S:4 = 0000-0000-0000-0000
```

Proc

```
OS Catalog Number S:57 = 1100 User Program Type S:63 = 8001h
OS Series S:58 = A Compiler Revision Number S:64 =
OS FRS S:59 =
Processor Catalog Number S:60 =
Processor Series S:61 = A
Processor FRN S:62 =
```

Scan Times

```
Maximum (x10 ms) S:22 = 0 Watchdog (x10 ms) S:3 (high byte) = 10 Last 100 uSec Scan Time S:35 = 0 Scan Toggle Bit S:33/9 = 0
```

Math

```
Math Overflow Selected S:2/14=0 Math Register (lo word) S:13=0 Overflow Trap S:5/0=0 Math Register (high word) S:14-S:13=0 Overflow S:0/1=0 Math Register (32 Bit) S:14-S:13=0 Overflow S:0/1=0 Zero Bit S:0/2=0 Sign Bit S:0/3=0
```

Chan (

```
Processor Mode S:1/0- S:1/4 = Remote Program Mode Node Address S:15 (low byte) = 0 Outgoing Msg Cmd Pending S:33/2 = 0 Baud Rate S:15 (high byte) = ? Channel Mode S:33/3 = 0 Comms Active S:33/4 = 0 Incoming Cmd Pending S:33/0 = 0 Msg Reply Pending S:33/1 = 0
```

Debug

Suspend Code S:7 = 0Suspend File S:8 = 0

Errors

Protection

```
Deny Future Access S:1/14 = No
Data File Overwrite Protection Lost S:36/10 = False
```

Mem Module

```
Memory Module Loaded On Boot S:5/8 = 0 Password Mismatch S:5/9 = 0 Load Memory Module On Memory Error S:1/10 = 0 Load Memory Module Always S:1/11 = 0 On Power up Go To Run (Mode Behavior) S:1/12 = 0 Program Compare S:2/9 = 0 Data File Overwrite Protection Lost S:36/10 = 0
```

Address/Symbol Database

ess	Symbol	Scope	Description	Sym Group	Dev. Code	ABV
0						
1 2						
0						
1						
2 3						
3 4						
5						
6						
7 8						
9						
10						
11 12						
13						
14						
15 0						
0	LS 1	Global	Level sensor 1 in bit			
1	LS_2		Level sensor 2 in bit			
0		91 1 1	2.1			
1 2	PH1_DONE PH2_DONE		Adsorp Done Air evac done			
3	PH3 DONE		Vap strip done			
4	PH4_DONE	Global	Fin desorp done			
5 0	PH5_DONE V1 CMD		Pressurize done			
1	V1_CMD V2_CMD		Valve 1 command Valve 2 command			
2	V3_CMD		Valve 3 command			
3	V4_CMD		Valve 4 command			
4 5	V5_CMD V6_CMD		Valve 5 command Valve 6 command			
6	V6_CMD V7_CMD	Global	Valve 7 command			
7	AB_CMD		Air blower command			
8 9	VP_CMD HE CMD		Vac pump command Heater command			
10	HX REQ		Condenser request			
/0			1.1			
/1						
/2 /0	RUN_OK	Global	Run okay bit			
/0		OIODGI	nan ona, bio			
/1						
/2 /3						
/0			ONS used			
/1			ONS used			
/2			ONS used			
/4			ONS used			
/5			ONS used			
/6 /7			ONS used			
/8			ONS used for phase timer reset			
/9			ONS used			
/0			Level sensor 1			
/1 /2			Level sensor 2 Valve 1 out			
/3			Valve 2 out			
/4			Valve 3 out			
/5 /6			Valve 4 out Valve 5 out			
/ o /7			Valve 6 out			
/8			Valve 7 out			
/9 /10			Vac pump out			
/10 /11			Air blow out Heater out			
/12			Condense out			
/13						
/14 /15						
/15						
/1						
/2						
/3 /4						
/4 /0						
/1	QUAL	01.1	Cools and the			
PRE	CYCLE_COUNTER	Global	Cycle counter			
DN						
DIA						

Page 1

Address	Symbol	Scope	Description	Sym Group	Dev. Code ABV
F8:0 F8:1 F8:2 F8:3 F8:4 F8:5 F8:6 F8:7 F8:10 F8:11 F8:12 F8:20 F8:21	PT_1_SCLD PT 2_SCLD PT 3_SCLD PT 3_SCLD TC 1_SCLD TC 2_SCLD TC 3_SCLD TC 4_SCLD WS_SCLD VP_SP AB_SP HE_SP	Global Global Global Global Global Global Global Global	Pressure 1 (scaled) Pressure 2 (scaled) Pressure 3 (scaled) Thermocouple 1 (scaled) Thermocouple 2 (scaled) Thermocouple 3 Thermocouple 4 (scaled) Weight scale (scaled) Vac pump SP Air blower SP Heater SP		
F8:22 F8:30 F8:31 F8:32 F8:33 F8:34 F8:35 F8:36 F8:37 F8:37 F8:55 F8:50 F8:52 F8:55 F8:55 F8:55 F8:55 F8:56 F8:61 F8:61 F8:62 F8:63 F8:61 F8:62 F8:63 F8:64 F8:65 F8:66 F8:67 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:68 F8:88 F8:88 F8:88 F8:89 F8:88 F8:89 F8:89 F8:88 F8:89 F8:89 F8:89 F8:80 F8:81 F8:81 F8:81 F8:83 F8:84 F8:85 F8:86 F8:87 F8:88 F8:89 F8:88 F8:89 F8:89 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:82 F8:83 F8:84 F8:88 F8:89 F8:88 F8:89 F8:88 F8:89 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:81 F8:83 F8:81 F8:83 F8:81 F8:83 F8:83 F8:83 F8:83 F8:84 F8:88 F8:89 F8:88 F8:89 F8:81 F8:81 F8:81 F8:81 F8:83	PH1_DP_SP PH1_TM_SP PH2_P_SP PH3_DP_SP PH3_TM_SP PH4_P_SP PH4_T_SP PH5_TM_SP	Global Global Global Global Global Global	Adsorp blower speed dP SP Adsorp time SP Air evac P SP Vap strip dP SP Vap strip time SP Fin desorp P SP Fin desorp temp SP Pressurize time SP Adsorp blower speed pressure drop SP Adsorp time SP Adsorp time SP Air evac pressure SP Vap strip vac pump speed dP SP Vap strip pressure SP Fin desorp pressure SP Fin desorp Temperature SP Fin desorp Temperature SP PT1 out PT2 out PT3 out TC1 out TC2 out TC3 out TC4 out Weight scale out Pressure Transducer 1 Pressure transducer 1 Pressure transducer 2 Pressure Transducer 3 Thermocouple 1 Thermocouple 2 Thermocouple 3 Thermocouple 4 Weight scale Vac pump output Air blower output Heater output		
N7:10 N7:10/0 N7:40 N7:41 N7:42 N7:50 N7:90 N7:100 N7:101 O:2/0 O:2/1 O:2/2 O:2/4 O:2/5 O:2/5 O:2/7 O:2/9	PHS_IDX MAN_PHS_INDX CYCLE_SP HOA_MODE	Global	Phase Index Manual phase index Cycle count SP Phase index out HOA mode HOA mode in Manual phase selection command in Cycle count HMI in		

Address	Symbol	Scope	Description	Sym Group	Dev. Code	ABV
0:2/10						
0:4.0						
0:4.1 0:4.2						
5:0			Arithmetic Flags			
5:0/0			Processor Arithmetic Carry Flag			
3:0/1			Processor Arithmetic Underflow/ Overflow Flag			
3:0/2			Processor Arithmetic Zero Flag			
S:0/3 S:1			Processor Arithmetic Sign Flag Processor Mode Status/ Control			
:1/0			Processor Mode Bit 0			
3:1/1			Processor Mode Bit 1			
5:1/2			Processor Mode Bit 2			
5:1/3			Processor Mode Bit 3			
S:1/4			Processor Mode Bit 4			
S:1/5 S:1/6			Forces Enabled Forces Present			
S:1/7			Comms Active			
S:1/8			Fault Override at Powerup			
S:1/9			Startup Protection Fault			
S:1/10			Load Memory Module on Memory Error			
S:1/11 S:1/12			Load Memory Module Always Load Memory Module and RUN			
S:1/13			Major Error Halted			
S:1/14			Access Denied			
S:1/15			First Pass			
S:2/0			STI Pending			
S:2/1 S:2/2			STI Enabled STI Executing			
S:2/2			Index Addressing File Range			
S:2/4			Saved with Debug Single Step			
S:2/5			DH-485 Incoming Command Pending			
S:2/6			DH-485 Message Reply Pending			
S:2/7 S:2/15			DH-485 Outgoing Message Command Pending			
S:3			Comms Servicing Selection Current Scan Time/ Watchdog Scan Time			
S:4			Time Base			
S:5/0			Overflow Trap			
S:5/2			Control Register Error			
S:5/3			Major Err Detected Executing UserFault Routine			
S:5/4 S:5/8			M0-M1 Referenced on Disabled Slot Memory Module Boot			
S:5/9			Memory Module Password Mismatch			
S:5/10			STI Overflow			
S:5/11			Battery Low			
S:6			Major Error Fault Code			
S:7 S:8			Suspend Code Suspend File			
S:9			Active Nodes			
S:10			Active Nodes			
S:11			I/O Slot Enables			
S:12 S:13			I/O Slot Enables			
S:13			Math Register Math Register			
S:15			Node Address/ Baud Rate			
S:16			Debug Single Step Rung			
S:17			Debug Single Step File			
S:18			Debug Single Step Breakpoint Rung			
S:19 S:20			Debug Single Step Breakpoint File Debug Fault/ Powerdown Rung			
S:21			Debug Fault/ Powerdown File			
S:22			Maximum Observed Scan Time			
S:23			Average Scan Time			
S:24			Index Register			
S:25 S:26			I/O Interrupt Pending I/O Interrupt Pending			
S:27			I/O Interrupt Enabled			
S:28			I/O Interrupt Enabled			
S:29			User Fault Routine File Number			
S:30			STI Setpoint			
S:31 S:32			STI File Number I/O Interrupt Executing			
S:33			Extended Proc Status Control Word			
S:33/0			Incoming Command Pending			
S:33/1			Message Reply Pending			
S:33/2			Outgoing Message Command Pending			
S:33/3			Selection Status User/DF1			
S:33/4 S:33/5			Communicat Active Communicat Servicing Selection			
S:33/6			Message Servicing Selection Channel 0			
S:33/7			Message Servicing Selection Channel 1			
S:33/8			Interrupt Latency Control Flag			
S:33/9			Scan Toggle Flag			
S:33/10			Discrete Input Interrupt Reconfigur Flag			

dress	Symbol	Scope	Description	Sym Group	Dev. Code	ABV
33/11			Online Edit Status			
33/12			Online Edit Status			
33/13			Scan Time Timebase Selection			
33/14 33/15			DTR Control Bit DTR Force Bit			
33/15 34			Pass-thru Disabled			
34/0			Pass-Thru Disabled Flag			
34/1			DH+ Active Node Table Enable Flag			
34/2			Floating Point Math Flag Disable, Fl			
35			Last 1 ms Scan Time			
36			Extended Minor Error Bits			
36/8			DII Lost			
36/9			STI Lost			
36/10			Memory Module Data File Overwrite Protection			
37			Clock Calendar Year			
38			Clock Calendar Month			
9			Clock Calendar Day			
10			Clock Calendar Hours			
11			Clock Calendar Minutes			
12 13			Clock Calendar Seconds			
: 4			STI Interrupt Time I/O Event Interrupt Time			
15			DII Interrupt Time			
16			Discrete Input Interrupt- File Number			
17			Discrete Input Interrupt- Slot Number			
18			Discrete Input Interrupt- Bit Mask			
19			Discrete Input Interrupt- Compare Value			
0			Processor Catalog Number			
1			Discrete Input Interrupt- Return Number			
2			Discrete Input Interrupt- Accumulat			
3			Reserved/ Clock Calendar Day of the Week			
5			Last DII Scan Time			
6			Maximum Observed DII Scan Time			
57			Operating System Catalog Number			
8			Operating System Series Operating System FRN			
51			Processor Series			
52			Processor Revision			
53			User Program Type			
54			User Program Functional Index			
55			User RAM Size			
56			Flash EEPROM Size			
57			Channel O Active Nodes			
58			Channel O Active Nodes			
59			Channel O Active Nodes			
70			Channel O Active Nodes			
71			Channel O Active Nodes Channel O Active Nodes			
72 73			Channel O Active Nodes Channel O Active Nodes			
74			Channel O Active Nodes			
75			Channel O Active Nodes			
76			Channel O Active Nodes			
77			Channel O Active Nodes			
78			Channel O Active Nodes			
79			Channel O Active Nodes			
30			Channel O Active Nodes			
31			Channel O Active Nodes			
32			Channel O Active Nodes			
33 34			DH+ Active Nodes DH+ Active Nodes			
35			DH+ Active Nodes DH+ Active Nodes			
6			DH+ Active Nodes			
0			Adsorp timer			
0.PRE			-			
0/DN						
1			Vap strip timer			
1.PRE						
1/DN						
2			Pressuize timer			
2.PRE						
2/DN 3	LS1 HIGH	Global	Water reservoir high level			
3/DN	701-111GU	GIUDAI	Macci reservoit midu reser			
4	LS2_LOW	Global	Water reservoir low level			
4/DN		0.0001				
5 5/DN			Air evac timer			
6 6/DN			Fin desorp timer			
3 1 5 5 7			HMI I/O DIGI IN DIGI OUT ANLG IN ANLG OUT			

Address	Symbol	Scope	Description	Sym Group	Dev. Code	ABV
U:8 U:9 U:10			STATE CTRL CTRL LOGIC			
U:20 U:21 U:22 U:23			IDLE ADSORP AIR EVAC VAPOR STRIP			
U:24 U:25			FIN DESORP PRESSURIZE			

9.2 Appendix B: condenserCalcs.m

```
clear
Gsorbent=200; % grams of sorbent
Volume=1/8; %m^3
utarget=1; %m/s
n=.002*Gsorbent; %moles of co2
massCO2 = n * 44.01; % grams of CO2
Pressure=(linspace(1,31,(31-1)*4+1));
Tempsat=[];
hwsat=[];
hvexes=[];
Wdensity=[];
for I=Pressure./100
Tempsat(1,end+1)=XSteam('tsat_p',I); %temp of sat water
hwsat(1,end+1) = XSteam('hL_p', I); % enthalpy of sat water
hvexes(1,end+1) = XSteam('h_pt', I,Tempsat(end)+5); % enthalpy steam slightly above
saturation
Wdensity(1,end+1) = XSteam('rhoL p',I);
Tempsat=Tempsat+274.15; %convert to kelvin
Mdot=utarget*.0027229.*(Pressure./Tempsat);
Qcooler=Mdot.*(hvexes-hwsat); %cooling power to condense
Qfreezer=Mdot.*(hvexes-333.55); %cooling power to freeze
figure(1)
plot(Pressure, [Qcooler; Qfreezer])
legend('Q freezer (kW)','Q condenser (kW)','Location','northwest')
xlabel('Pressure (Kpa)');
vlabel('Cooling Power (kW)');
title('Cooling Power vs Pressure');
grid on;
% Given a constant pressure and concentration of steam find the pressure
% drop caused by condensation
Ppc=(n*.008314*(Tempsat+5))/Volume; %partial pressure due to a fixed quantity of co2
Ppw=(Pressure-Ppc).*(Pressure>Ppc);
Xw= Ppw./(Pressure); %percent pressure water
MdotW=utarget*.0027229.*(Ppw./Tempsat);
Pafter=(Pressure-Ppw).*(Tempsat./(Tempsat+5)).*(Volume./(Volume-MdotW./Wdensity));
Pdrop=Pressure-Pafter;
figure(2)
plot(Pressure,Pdrop)
xlabel('Pressure (Kpa)');
ylabel('Pressure Drop (Kpa)');
title('Pressure Drop vs Pressure');
grid on;
figure(3)
area(Pressure,[Ppc;Ppw]')
legend('P_ CO2', 'P_ Steam', 'Location', 'northwest')
title('Partial pressures')
xlabel('Pressure (Kpa)');
ylabel('Pressure (Kpa)');
```

9.3 Appendix C: BOM

М			
el Designation		Manufacturer	Link
Boiler	Water reservoir with top and bottom KF40 ports, two threaded ports.		
	•	Ideal vaccum	https://www.idealvac.com/en-us/Mini-Degassing-Vacuum-Chamber-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Band-Clamper-43-Liters-with-KF-40-Ports-Includes-Lid-Centering-Ring-Ring-Ring-Ring-Ring-Ring-Ring-R
	Open container, TBD		
	Weight scale, TBD		
Sa althrough	Thermocouple + power feedthrough (if scale is internal to		
Feedthrough	•	Ideal vaccum	https://www.idealvac.com/en-us/Electrical-Thermocouple-and-Power-Feedthrough-Type-K-5KV-30A-UHV-Rated-118-in-dia-KF16/pp/P108
HE .	blanket, 120V,	Brisk Heat	https://www.briskheat.com/economy-silicone-rubber-heating-blanket-srw.html
K/O reservoir	Water reservoir with top and bottom ports, two threaded ports, INSULATED		
	KF40 flange		
		Ideal vaccum	Ideal Vacuum Tee Adapter KF-40 to NPT 1/4 in, Female Pipe, Flange Size ISO-KF NW-40 to NPT-F, Stainless Steel
•			Ideal Vacuum Elbow 90 Degrees KF-40 Vacuum Fittings, ISO-KF Flange Size NW-40, Stainless Steel
1" Npt Ball	3 wire electrically actuated ball		
	1" NPT to KF40	U.S. 50tia	Amazon.com: U.S. Solid Motorized Ball Valve-1" Stainless Steel Electrical Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 3 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial Ball Valve with Full Port, 9-24V AC/DC and 9 Wire Setup: Industrial
		Ideal vaccum	ldeal Vacuum Adapter KF-40 to NPT1 in. Male Pipe, ISO-KF Flange Size NW-40, Stainless Steel
	KF40 4 way		https://www.idealvac.com/en-us/Cross-4-Way-KF-40-Vacuum-Fittings-ISO-KF-Flange-Size-NW-40-Stainless-Steel/pp/P101207
Manual	KF40 manual		
	Boiler reservoir Feedthrough HE K/O reservoir NPT single adaper Elbow 1" Npt Ball Valve 1" NPT adapter Cross	Water reservoir with top and bottom KF40 ports, two threaded Boiler ports, reservoir uninsulated Open container, TBD Weight scale, TBD Thermocouple + power feedthrough (if scale is internal to Feedthrough vessel) Feedthrough vessel) Silicon heating blanket, 120V, 6 "x40" Water reservoir with top and bottom ports, two threaded K/O ports, reservoir INSULATED KF40 flange NPT single with NPT 1/4", adaper single port Selbow Selbow 3 wire electrically 1" Npt Ball actuated ball valve valve 1" npt 1" NPT to KF40 1" NPT adapter for adapter ball valve KF40 4 way 1 Cross cross Manual KF40 manual	Water reservoir with top and bottom KF40 ports, two threaded Boiler ports, reservoir uninsulated Ideal vaccum Open Container, TBD Weight scale, TBD Thermocouple + power feedthrough (if scale is internal to Feedthrough vessel) Ideal vaccum Silicon heating blanket, 120V, HE 6"x40" Brisk Heat Water reservoir with top and bottom ports, two threaded K/O ports, reservoir INSULATED KF40 flange NPT single with NPT 1/4", adaper single port Ideal vaccum 3 wire electrically 1" Npt Ball Valve valve 1" npt U.S. Solid 1" NPT of KF40 1" NPT adapter for adapter ball valve Ideal vaccum KF40 4 way 1 Cross cross Ideal vaccum KF40 manual KF40 manual

		used while waiting on		
		peiffer		
		Adapt from		
		KF40 to		
		whatever air		
13	•		Ideal vaccum	Ideal Vacuum Reducer Conical KF-25 to KF-40 , KF25 to KF40, Vacuum Fittings, ISO-KF Flange Size NW-25 to NW-40, Stainless Steel
11		Hepa filter for	ld salvasaum	
14			Ideal vaccum	https://www.idealvac.com/en-us/Filter-Media-Activated-Alumina-for-Foreline-Trap-KF40/pp/P101869
		KF40 flange		
15	•	with NPT 1/4",	Idealyaccum	
15	•		Ideal Vaccuiii	https://www.idealvac.com/en-us/Adapter-KF-40-to-14-in-Triple-NPT-Female-Flange-Size-ISO-KF-NW-40-Stainless-Steel/pp/P106832
		Centering ring with mesh,		
16	•		Ideal vaccum	The state of the s
10		Custom	lucat vaccum	https://www.idealvac.com/en-us/Centering-Ring-Assembly-KF-40-with-Screen-ISO-KF-Flange-Size-NW-40-210-micron-Maximum-Vacuur
		sorbent bed		
		with KF40		
		flanges		
		(innitaly kf NPT		
		single port		
17	Sorbent bed	- ·	Ideal vaccum	Ideal Vacuum Tee Adapter KF-40 to NPT 1/4 in, Female Pipe, Flange Size ISO-KF NW-40 to NPT-F, Stainless Steel
		•		https://www.idealvac.com/en-us/Tee-KF-40-Vacuum-Fittings-ISO-KF-Flange-Size-NW-40-Stainless-Steel/pp/P101211
		KF40 vacuum		III,US.//WWW.IUEGIVGL.bumen-us/ ree-to
19			Ideal vaccum	Ideal Vacuum MKS Series 225 Auto-Soft Start Check Valve - Flow Actuated - Spring Loaded - Stainless Steel - Viton - NW40 KF40 Centerin
		Heat		INVICTIONAL II I I I I I I I I I I I I I I I I I
		exchanger,	Yamato	
20			Scientific	Amazon.com: Yamato Scientific cold trap
		PVC Flex Hose		
		Kit, 6 Foot		
21	Pipe	Length	Ideal vaccum	https://www.idealvac.com/en-us/PVC-Flex-Hose-Kit-6-Foot-Length-with-Clear-Reinforced-Hose-KF-16-Stainless-Steel-Flanges-and-Hose
		Electrically		
		actuated water		
		valve		
		(Probably		
		needle, needs		
22	Water valve	· · · · · · · · · · · · · · · · · · ·	U.S. Solid	https://www.dwyeromega.com/en-us/2-way-nc-direct-acting-brass-solenoid-valves/SV3100-Series/p/SV3110
	KF40-KF25	•		
23	adapter	KF40 to KF25	Ideal vaccum	https://www.idealvac.com/en-us/Reducer-Conical-KF-25-to-KF-40-Vacuum-Fittings-ISO-KF-Flange-Size-NW-25-to-NW-40-Stainless-Stee
		Pfeiffer		
		Highcroll 12+		
24	pump	controller	Pfeiffer	https://www.pfeiffer-vacuum.com/global/en/product/hiscroll-6-18.html
25	KF25 tee	KF25 tee	Ideal vaccum	Ideal Vacuum Tee KF-25 Vacuum Fittings, ISO-KF Flange Size NW-25, Stainless Steel
_	VEOF value		Pfeiffer	
26	KF25 valve	KI 25	i icilici	· ·

		electrically actuated valve (needle, gate, ball?)		
	CO2	TBD, may need		
27	collection	adapters also		
28	KF40 Clamp	KF40 clamp	Ideal vaccum	Ideal Vacuum Hinge Clamp KF-40, KF40, Vacuum Fittings, ISO-KF Flange Size NW-40, NW40, Aluminum
29	KF40 centering ring	KF40 centering ring, viton?	Ideal vaccum	Ideal Vacuum Centering Ring KF-40 Vacuum Fittings, ISO-KF Flange Size NW-40, Stainless Steel
30		KF25 clamp	Ideal vaccum	MANAGEMENT CONTROL OF THE STATE
31	KF25 centering ring	KF25 centering ring, viton?	Ideal vaccum	
32	Plug	1/4" plug for future gas detection port	Joywayus	Joywayus 4Pcs Stainless Steel Outer Hex Thread Socket Pipe Plug Fitting 1/4" NPT Male: Amazon.com: Industrial & Scientific.

Sensors

вом			
Level D	Designation	Description	Manufacturer _{Link}
		1/4 in npt high	
		accuracy	
		pressure	
33 P	PΤ	transducer	https://www.dwyeromega.com/en-us/configurable-high-accuracy-pressure-transducers/PX409-Series/p/PX409-015Al-XL
34 T		1/4 in npt thermocouple	https://www.dwyeromega.com/en-us/pipe-plug-thermocouple-probes-with-npt-fitting-and-lead-wire/TC-NPT/p/TC-K-NPT-U- 72?utm_source=google&utm_medium=cpc.&utm_campaign=Omega-PLA-US-GGL-Connector-CatchAll&utm_content=undefined&utm_te 141571748582_ad-640145425429_pla-294682000766_dev-c_extprd-TC-K-NPT-U-72_mca-97897_sig_CjwKCAjwx- zHBhBhEiwA7Kjq6zateGXEyz/G4sUAGWDt3vFFdDbE/mwqMZhjw8LwYU_X0w0wo71dnhoCOT4OAvD_BwE&gad_source=1&gad_campaign zHBhBhEiwA7Kjq6zateGXEyz/G4sUAGWDt3vFFdDbE/mwqMZhjw8LwYU_X0w0wo71dnhoCOT4OAvD_BwE
35 T		thermocouple in the bed	https://www.dwyeromega.com/en-us/pipe-plug-thermocouple-probes-with-npt-fitting-and-lead-wire/TC-NPT/p/TC-K-NPT-U- 72?utm source=google&utm medium=cpc&utm campaign=Omega-PLA-US-GGL-Connector-CatchAll&utm content=undefined&utm te 141571748582 ad-640145425429 pla-294682000766 dev-c ext- prd-TC-K-NPT-U-72 mca-97897 sig-CjwKCAjwx- zHBhBhEiwA7Kjq6zateGXEyzJG4SUAGWDt3vFFdDbEfmwqMZhjw8LwYU X0w0wo71dnhoCQT4QAvD_BwE&gad source=1&gad campaign zHBhBhEiwA7Kjq6zateGXEyzJG4sUAGWDt3vFFdDbEfmwqMZhjw8LwYU_X0w0wo71dnhoCQT4QAvD_BwE
36 L	LS	level sensor	https://www.mcmaster.com/products/float-level-sensors/through-wall-horizontal-mount-float-switches-for-water/

Automation

вом			
Leve	l Designatio	n Description	Manufacturer Links
37	PLC		Rockwell
		DI, DO, AI, AO,	
		thermocouple	
38	PLC cards	card	Rockwell
	120-24V	Need to	
39	power	calculate	Rockwell

	supply	amperage	
40	PC	(Do we want dedicated PC, or just use personal laptop?)	Anything but Apple
<i>A</i> 1	Ethernet cable	~6ft length	
42	Wire	12awg and 16awg?	

Miscellaneous

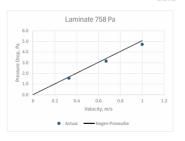
ВОМ		
	gnation Description	Manufacturer Links
	Hardware to	LINA
	hold rig	
	(saddle	
	clamps,	
	scaffolding,	
43	etc)	
	Board to	
	mount on,	
	unless	
44	scaffolding is sufficient?	
44	Electrical	
45	enclosure	
46	DIN rails	
40	Wire	
47	connectors	
7/	Terminal	
48	blocks	
	Terminal block	
49	ends	
50	Cable glands	
	Cable and	
	male plug for	
51	power source	
52	Wire ferrules	
53	Screws	
54	Washers	
1 34	vvasiicis	

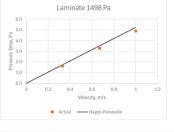
9.4 Appendix D: ANSYS Simulations

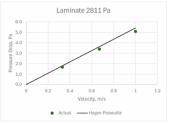
Laminate Data

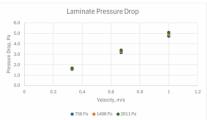
Temp (C)	Psat (Pa)	density kg/r kin visc (m² dyn visc (Pas)							
3	758	0.	.006	1.52E-03	9.03E-06				
13	1498	0.	.011	8.22E-04	9.33E-06				
23	2811	0.	.021	4.68E-04	9.64E-06				
Vi (m/s)									
0.33	0.26499								
0.67	0.53801								
1	0.803								
Tube Dia	0.032738	m							
Tube Ax	0.000842	m^2							
Dhyd	0.001882	m							
width	0.016	m							
height	0.001	m							
	0.0468								
const:	5.07	4	5.24	5.41					
V	P1	P2	P	3					
0	0.00	(0.00	0.00					
1	5.07		5.24	5.41					

Trial	Psat		dyn visc	Vi		m flow	Inter Re	super Re	Pin (Pa)	Pout (Pa)	dP (Pa)	hagen dP		
	1	758	9.03E-06	6	0.33	1.33837E-06	0.41	5.58	757.994	756.44	1.55	1.67	0.928381	
	2	758	9.03E-06	6	0.67	2.71729E-06	0.83	11.33	757.996	754.84	3.16	3.40	0.928648	
	3	758	9.03E-06	6	1	4.05565E-06	1.24	16.91	757.992	753.27	4.72	5.07	0.930926	0.932651
	4	1498	9.33E-06	3	0.33	2.45367E-06	0.76	10.31	1497.999	1496.39	1.61	1.73	0.930636	
	5	1498	9.33E-06	i	0.67	4.9817E-06	1.53	20.94	1497.998	1494.725	3.27	3.51	0.932414	
	6	1498	9.33E-06	3	1	7.43537E-06	2.29	31.26	1497.996	1493.099	4.90	5.24	0.934691	
	7	2811	9.64E-06	i	0.33	4.68428E-06	1.33	18.12	2810.999	2809.334	1.67	1.79	0.932263	
	8	2811	9.64E-06	6	0.67	9.51051E-06	2.69	36.78	2810.997	2807.602	3.39	3.63	0.936162	
	9	2811	9.64E-06	6	1	1.41948E-05	4.02	54.90	2810.993	2805.907	5.09	5.41	0.939734	
							channel	entrance						









Monolith Data

Temp (C) Psat (Pa) density kg/ kin visc (m' dyn visc (Pr Trial 3 756.00 0.01 0.00 9.05E-06 13 1498.00 0.01 0.00 9.05E-06 23 2811.00 0.02 0.00 9.64E-06 Vi (m/s) Vs (m/s) 0.33 0.21 0.67 0.43 1 0.64 Tube Dia 0.03 m	Psat dyn visc V m flow 1/4 m flow int Re Sup Re Pin (Pa) Pout (Pa) dP (Pa) hagen dP	1.011881
Tube Ax 0.00 m^2	Monolith at 758 Pa Monolith at 1498 Pa	
side length 0.00 m length 0.05 m^2	3.5	
const: 3.01 3.11 3.21 Vi (m/s) P1 dP P2 dP P3 dP 0 0.00 0.00 0.00 0.05 0.15 0.16 0.16 0.1 0.30 0.31 0.32	3	
0.15 0.45 0.47 0.48	0 02 0.4 0.6 0.8 1 1.2 0 0.2 0.4 0.6 0.8 1 1.2	
0.2 0.60 0.62 0.64 0.25 0.75 0.78 0.80	Velocity, m/s Velocity, m/s	
0.3 0.90 0.93 0.96	Actual — Darcy-Weisbach Actual — Hagen-Poiseuille	
0.35 1.05 1.09 1.12 0.4 1.20 1.24 1.28		
0.45 1.35 1.40 1.44	Monolith at 2811 Pa Monolith Pressure Drop	
0.5 1.50 1.55 1.60	3.5	
0.55 1.65 1.71 1.76 0.6 1.80 1.86 1.92	8 25	
0.65 1.95 2.02 2.09	d d d d d d d d d d d d d d d d d d d	
0.7 2.10 2.17 2.25 0.75 2.25 2.33 2.41	2 1.5	
0.8 2.41 2.48 2.57	3 1 S 1	
0.85 2.56 2.64 2.73 0.9 2.71 2.79 2.89	0.5	
0.9 2.71 2.79 2.89 0.95 2.86 2.95 3.05	0 0.2 0.4 0.6 0.8 1 1.2 0 0.2 0.4 0.6 0.8 1 1.2	
1 3.01 3.11 3.21	Velocity, m/s Velocity, m/s	
	● Actual — Hagen-Poiseuille ●758 Pa ●1498 Pa ●2811 Pa	
0 2811.00 0.01016 2810.39 0.02032 2809.69 0.030345 2806.99 0.04064 2806.30 0.0508 2807.72	Pressure Across Monolith (2811 Pa, 1 m/s) 2811.00 2810.00 2810.00 2800.00 2800.00 2800.00 2800.00 2800.00 2800.00 Position in Monolith, m	