Vacuum Moisture Swing

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Project Description

- The purpose of our project is to create a **Direct Air Capture (DAC) Reactor** that uses **Vacuum Moisture Swing** as it's CO_2 collection process. This will allow us to pull air (~420 ppm CO_2) through our reactor, react it with the **sorbents to separate CO_2**, and store that CO_2 product in a large canister. **Point Source Carbon Capture** technology is already in use that collects emissions coming **directly from factories** and will likely be scaled much further with the addition of DAC Reactors. The sorbents we will be using are the same ones used for testing in Professor Wade's Climate Solution's lab.
- This process could be an important technology for **lowering global emissions to reverse climate change.** CO2 emission is the largest contributor to global warming, in addition to causing ocean acidification.

Stakeholders

Industry Sponsor: Salt River Project (SRP)

Advisor: Professor Jennifer Wade

Mentor: PhD Candidate Stephano Sinyangwe

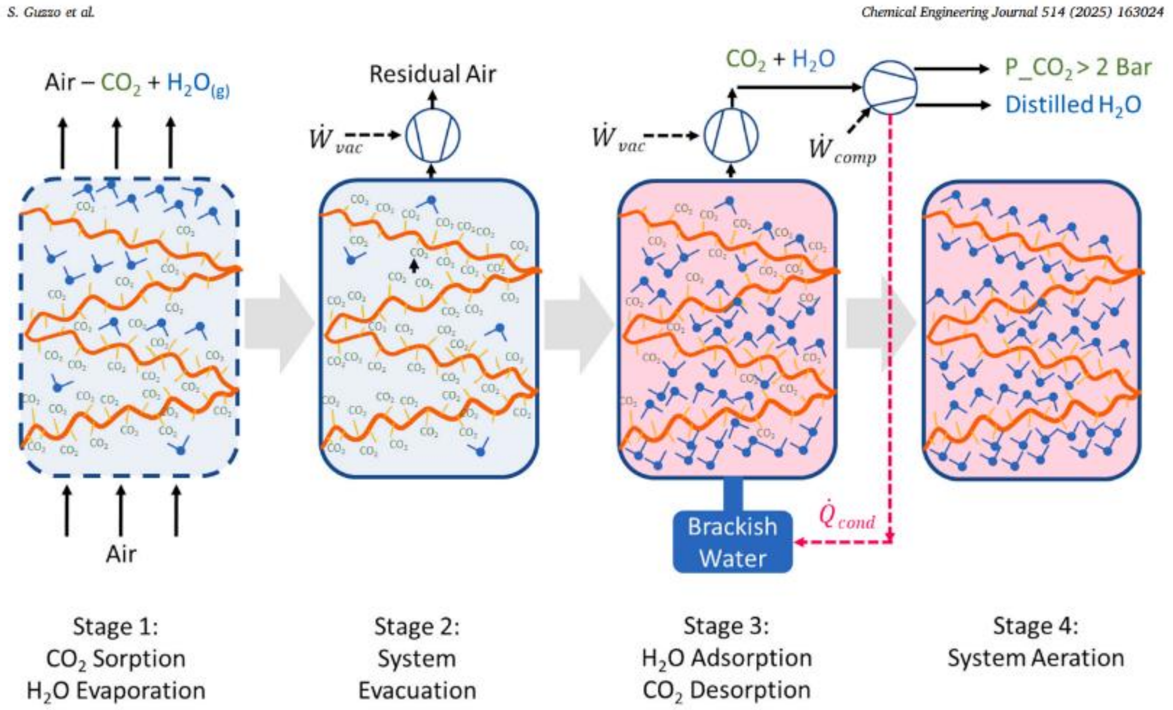
Other Stakeholders: NAU Climate Lab

Reaction Diagram

$$\mathbf{CO_3^{2-}} \cdot m_1\mathrm{H_2O} \leftrightarrow \mathbf{HCO_3^-} \cdot m_2\mathrm{H_2O} + \boldsymbol{OH^-} \cdot m_3\mathrm{H_2O} + (m_1 - m_2 - m_3 - 1)\mathrm{H_2O} \quad (1)$$

$$\mathbf{CO_2} + \boldsymbol{OH^-} \cdot m_3\mathrm{H_2O} \leftrightarrow \mathbf{HCO_3^-} \cdot m_2\mathrm{H_2O} \quad (2)$$

$$\boldsymbol{2HCO_3^-} \cdot m_2\mathrm{H_2O} + (m_1 - m_2 - m_3 - 1)\mathrm{H_2O} \leftrightarrow \mathbf{CO_3^{2-}} \cdot m_1\mathrm{H_2O} + \boldsymbol{CO_2} \quad (3)$$



A **vacuum pump** will be used to pull air through and will **boil the water at room temperature** due to the very low pressure.

A **condenser** will be used at the end of stage 3 to **condense the water vapor back into water**. This will ensure the CO_2 that is extracted is of **high purity**.

The chemical equation will **shift right if water content is high** (>90% humidity) and **shift left if water content is low** (<30% humidity)

Customer and Engineering Requirements

Customer Requirements

1. Capture as much CO_2 as possible

Engineering Requirements

1a. Maximize sorbent productivity [(mmol CO_2/g sorbent)/hour]

1b. Maximize packing density (cm^3/cm^3)

1c. Find ideal void fraction (cm^3/c^3)

Customer and Engineering Requirements

Customer Requirements

2. Minimize power requirement

Engineering Requirements

2a. Minimize pressure drop (ΔkPa/cm)

2b. Keep air velocity within practical range, <1m/s

Customer and Engineering Requirements

Customer Requirements

3. Utilize moisture swing

Engineering Requirements

3a. Vacuum pressure below water vaporization pressure at ambient temperature, <~3kPa

Customer and Engineering Requirements

Customer Requirements

4. Minimize water loss

Engineering Requirements

4a. Reuse water by condensing water vapor (°C)

4b. Heat water reservoir to offset evaporative cooling to maintain ambient temperature (~15 °C)

Customer and Engineering Requirements

Customer Requirements

5. Track the metrics of the apparatus as it runs

Engineering Requirements

5a. Incorporate pressure transducers before and after reactor chamber (kPa)

5b. Incorporate thermocouples before and after reactor chamber (°C)

Customer and Engineering Requirements

Customer Requirements

6. Be able to control flow rate and pressure

Engineering Requirements

6a. Incorporate a VFD (matched to vacuum pump, rated by kW)

6b. Incorporate control logic (most likely a PLC, possibly analogue feedback from 4-20mA sensors)

Customer and Engineering Requirements

Further Customer Requirements

7. Maintain clean lab environment by using an oil-free vacuum pump

8. Keep design compact

9. Utilize existing common vacuum parts

QFD

0
0 0
0 0 +
0 0 0 +
+ 0 0 0 +
0 - 0 0 0 +
- - - 0 0 + +
+ - - + - + + +

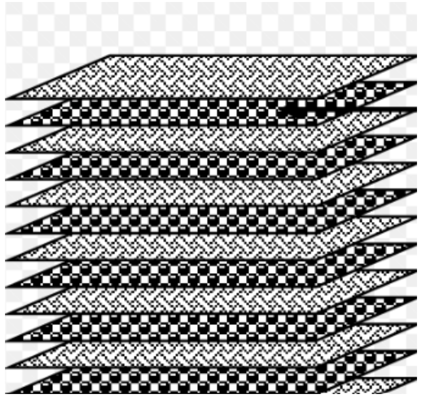
weight	Customer Requirements / Engineering Requirements	Sorbent Efficiency	Packing Density	Pressure Drop	Practical Velocity Range	Vacuum Pressures	Condensor	Sensor Integration	PLC	VFD	Packed Bed	Monolithic	Laminate
25	C02 Capture Effeciency	5	3.5	2	2.5	3	2	3	3	2	5	2	3
22.5	Minimal Power Input	1.5	2.5	4.5	3	3.5	2	2.5	3	4	1	5	4
7.5	Vaporization Without Heating	1	1.5	2	2	4.5	1.5	1.5	1.5	2	2	5	3
32.5	Measurable Results	1.5	1.5	1	2	1.5	1.5	5	2.5	1.5	2	5	4
12.5	Controllable Flow Rate	1	1.5	2	2.5	2	1.5	5	5	4.5	2	5	4
	Units	mmol/g	m^3/m^	kPa	m/s	kPa	QTY	QTY	QTY	QTY			
	Target Score	>1.5	>0.6	<0.5	<1	<3	1	6	1	1			
	Relative Importance Weight	2.275	2.225	2.2375	2.4125	2.6125	1.7375	3.675	2.975	2.6			
	Packed Bed	2	4	2	3	3	3	4	4	4			
	Monolithic	3	3	3	3	3	3	3	3	3			
	Laminate	4	4	4	3	3	3	3	3	3			

Background & Benchmarking

- Loose Sorbents
  - Packed Bed
- 3D Printed Sorbents
  - Monolithic
  - Laminate

- Packed Bed Metrics:
  - Highest adsorbent loading capacity (+)
  - Lowest flow uniformity (-)
  - Highest pressure drop (-)
- Monolithic Metrics:
  - Lowest adsorbent loading capacity (-)
  - Hihgest flow uniformity (+)
  - Lowest pressure drop (+)
- Laminate Metrics:
  - Middle adsorbent capacity (~)
  - Middle flow uniformity (~)
  - Middle pressure drop (~)

Monolithic structure example



Laminate structure example

Lit review 1: Sorbent properties/3D printed sorbents

1. AmberLite™ IRA900 Cl Ion Exchange Resin (https://www.lenntech.com/Data-sheets/DuPont-AmberLite-IRA900-Cl-Ion-Exchange-Resin-L.pdf)
   - This source includes all sorbent properties for our IRA900 sorbent that were used in many of our calculations.
2. Moisture-driven CO2 pump for direct air capture (file:///C:/Users/jpatt_dmk2jue/Downloads/MembranePump_JMS_WadeLopezMarquesWangFloryFreeman2023.pdf)
   - This source is Wade's paper that gives us the basic chemical formulas for moisture swing
3. CO_2 Capture From Air in a Radial Flow Contactor: Batch or Continuous Operation? (https://www.frontiersin.org/journals/chemical-engineering/articles/10.3389/fceng.2020.596555/full)
4. Analysis of direct capture of from ambient air via steam-assisted temperature–vacuum swing adsorption (https://link.springer.com/article/10.1007/s10450-020-00249-w)
   - Both of these sources are great baseline standards for our prcoess that use very similar sorbents and operating conditions that we can use to predict output data and compare based on their outputs. We will mainly use these sources after we are able to test our reactor.
5. Scaling up 3D printed hybrid sorbents towards (cost) effective post-combustion CO2 capture: A multiscale study (file:///C:/Users/jpatt_dmk2jue/Downloads/1-s2.0-S1750583624000124-main.pdf)
6. Investigating The Performance Of 3-D Printed Sorbents For Direct Air Capture Of CO2 by Terry Obeng-Ampomah (file:///C:/Users/jpatt_dmk2jue/Downloads/ObengAmpomah_asu_0010N_20002.pdf)
7. 3D-Printing of Adsorbents for Increased Productivity in Carbon Capture Applications (3D-CAPS) (file:///C:/Users/jpatt_dmk2jue/Downloads/ssrn-3811591%20(1).pdf)
   - These 3 sources are focused on 3D printing of sorbent structures. They primarily focus on optimizing cost vs surface area in addition to some different ideas for structure shapes for stability/air flow.

Lit review 2: Vacuum equipment

8. Flanges and Fittings, Leybold Vacuum (CP_080_EN_T_809-882_Flange_and_Fittings.pdf)
   - This source provides a standard in the form of specs for all standard vacuum part fittings
9. Fundamentals of Vacuum Technology, Oerlikon Leybold Vacuum (Grundlagen E)
   - 200pg document from a manufacturer, covering basic physics to how to quantify all aspects of vacuum
10. Introduction to Vacuum Technology, Hata; Brewer; Louwagie (Introduction to Vacuum Technology – Simple Book Publishing)
    - A guide intended for technicians maintaining vacuum systems
11. A Guide to Vacuum Pump Sizing, Blower and Vacuum Best Practices (A Guide to Vacuum Pump Sizing | Blower & Vacuum Best Practices)
    - A distributor website discussing the more qualitative aspects and overview
12. Sizing Vacuum Pumps, VTech Cool Industries (Sizing Vacuum Pumps)
    - A manufacturer of refrigeration systems, has basic calculations for flow speeds and conductance
13. Handbook of Mechanical Engineering Equations, Hicks (VACUUM-PUMP SELECTION FOR HIGH-VACUUM SYSTEMS | McGraw-Hill Education – Access Engineering)
    - Broad scope, has a chapter on vacuum systems
14. Conductance & Throughput in Vacuum Pipelines, Vac Aero (Conductance & Throughput in Vacuum Pipelines)
    - From a manufacturer of vacuum furnaces, covers resistance to gas flow in vacuum pipelines

Lit review 3: Reactor types

15. 50 years of Geldart classification (https://www.sciencedirect.com/science/article/pii/S0032591023006459)
    - A meta-analysis and summary of modern research and fluidization behavior.
16. Flow Through Packed Beds (https://faculty.washington.edu/finlayso/Fluidized_Bed/FBR_Fluid_Mech/packed_beds_fbr.htm#ergun)
    - Pressure drop through a packed bed
17. Fluid Mechanics for Fluidized Beds (https://faculty.washington.edu/finlayso/Fluidized_Bed/FBR_Fluid_Mech/fluid_bed_scroll.htm)
    - Pressure drop and critical velocities for fluidized beds
18. Structured adsorbents in gas separation processes (https://doi.org/10.1016/j.seppur.2009.10.004)
    - Alternatives to packed or fluidized beds and how they perform
19. Analysis of maximum pressure drop for a flat-base spouted fluid bed (https://www.osti.gov/servlets/purl/1477173)
    - Describes a 36% drop in stable pressure when a spouting state is achieved, making it worthwhile to pursue if possible
20. Properties of Water and Steam (https://www.ski-gmbh.com/swa/tools/steam)
    - Steam table and calculator
21. Aeration, Fluidization, Permeability of powders (https://powderprocess.net/Powder_Flow/Aeration_Permeability.html)
    - Fluidization volume and pressure constancy
22. Comparison of Attrition Test Methods: ASTM Standard Fluidized Bed vs Jet Cup (https://pubs.acs.org/doi/10.1021/ie990730j)
    - Two standards of catalyst testing in fluidized beds

Lit review 4: CFD Simulation and Validation

23. Simulating flow through multi-layer reactor using Ansys Fluent (Energy and productivity efficient vacuum pressure swing adsorption process to separate CO2 from CO2N2 mixture using Mg-MOF-74_ A CFD simulation)
    - Provides extensive optimization results that have been found using Ansys Fluent and validated with experimental data
24. Simulating VMS packed bed (Simulation of elevated temperature solid sorbent CO2 capture for pre-combustion applications using computational fluid dynamics)
    - Provides many user defined functions to model flow through sorbent reactor and provides validated results
25. Simulating VMS packed bed (Simulation and Airflow Experimentation of a Multi-Layer Adsorbent Chamber for Enhanced Direct Air Capture Efficiency)
    - Similar to the last article with different parameters
26. Adding sorbent expansion to CFD model (Regenerable MgO-based sorbent for high temperature CO2 removal from syngas: 2. Two-zone variable diffusivity shrinking core model with expanding product layer)
    - Provides user defined functions required to model sorbents expanding in Ansys Fluent
27. CFD, packed bed vs 3D printed structure (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)
    - Explains the CFD modeling process used to compare packed bed to 3D printed structures
28. Modeling 3D printed sorbent structure (3D-printing of adsorbents for increased productivity in carbon capture applications (3D-CAPS))
    - Overview on how 3D printed structure can reduce pressure drops using Ansys Fluent
29. CFD validation and verification (Quantitative V&V of CFD simulations and certification of CFD codes.)
    - Overview of validation and varification of CFD simulation
    - (AIAA G-077-1998) standard for validation and verification of CFD software

Calculations 1- Sorbent Density, Volume and CO_2 capture capacity

$$\frac{\left(\rho_{particle} + \left(H_c \cdot \rho_{water}\right)\right) \cdot V_{dry\ bead}}{V_{wet\ bead}}$$

$$\frac{100g}{2.126\ \frac{g}{cm^3}} = 47.04\ cm^3$$

$$\frac{\left(1.06\ \frac{g}{cm^3} + \left(.64 \cdot 1\ \frac{g}{cm^3}\right)\right) \cdot .000524\ cm^3}{.00419\ cm^3} = 2.126\ \frac{g}{cm^3}$$

$$.8\ \frac{mmol}{g} CO_2 \cdot 100g \cdot \frac{1\ mol}{1000\ mmol} = .08\ mol\ CO_2$$

$$.08\ mol\ CO_2 \cdot 44.01\ \frac{g}{mol} = 3.521\ g\ CO_2$$

$$30\ \frac{mmol}{g} H_2O \cdot 100g \cdot \frac{1\ mol}{1000\ mmol} = 3\ mol\ H_2O$$

$$3\ mol\ H_2O \cdot 18.02\ \frac{g}{mol} = 54.06\ g\ H_2O$$

- What question does this answer?

Density in addition to Volume and CO_2/H_2O capacity per 100 grams of sorbent

- Why were these calculations needed?

These calculations were used in the Irgun equation to find pressure drop and other metrics. It will also be used to help with sizing our housing vessel for our sorbents and the water tank.

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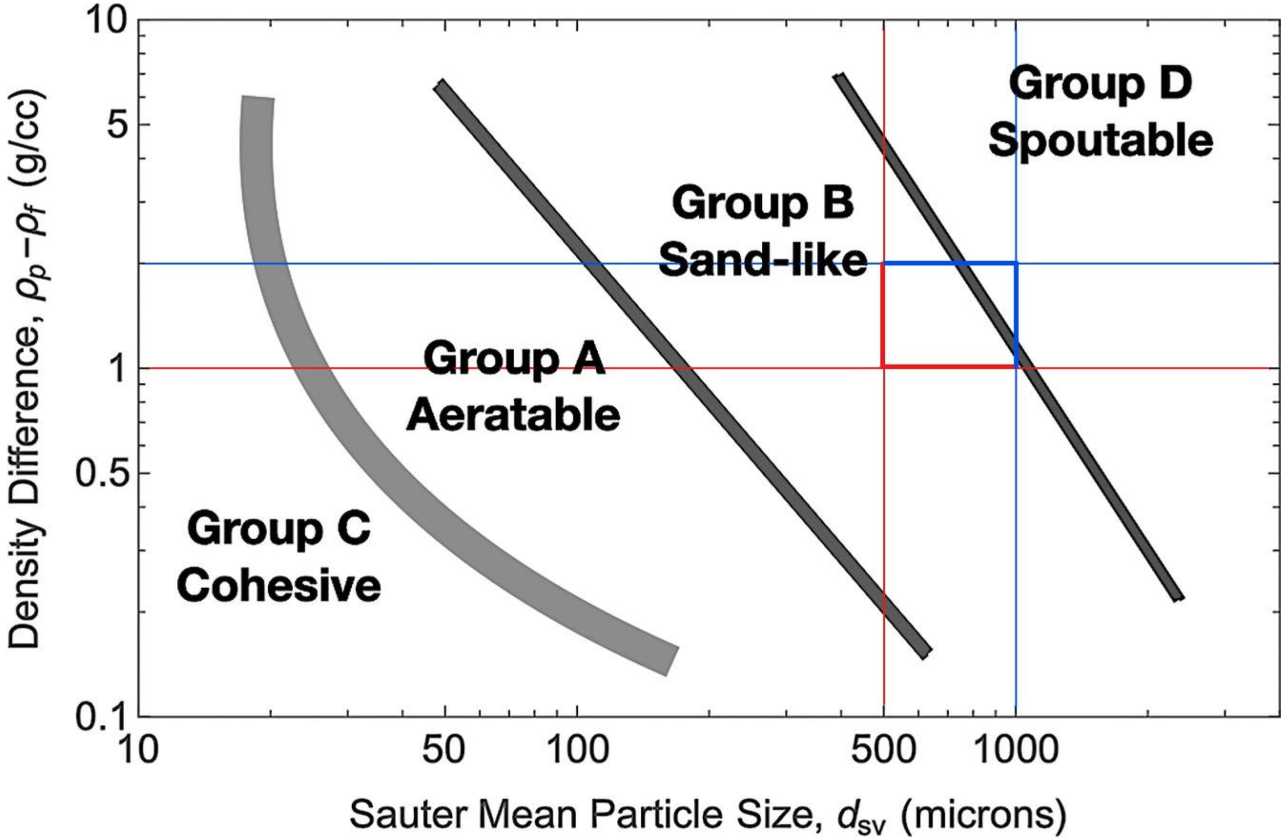
Different sources provide values closer to 2 mmol/g CO_2 which would result in 8.8 grams of CO_2 captured per 100 grams of sorbent

Update with new sorbent measurements/calcs

Calculations 2: packed and fluidized beds



- Behavior range verified through Geldart classification
- Fluid assumptions
  - Air at standard atmospheric conditions
    - μ= .00001846 pa*s ρ=1.225 kg/m^3
  - Steam @ 5 Kpa & 33 deg C
    - μ= .000001 pa*s ρ=.035 kg/m^3
- Particle assumptions
  - d_{dry} = .5 mm = .0005 m d_{wet}=1 mm = .001 m
  - ρ_{dry}= 1.06 g/cm^3 ρ_{wet}= 2.126 g/cm^3
- Packed bed ΔP

$$\frac{\Delta P}{L} = \frac{\left(150 \cdot \mu \cdot (1-\varepsilon)^2 \cdot U_0\right)}{\varepsilon^3 \cdot d^2} + \frac{\left(1.75 \cdot (1-\varepsilon) \cdot \rho \cdot U_0^2\right)}{\varepsilon^3 \cdot d}$$

- Results
  - Air : .5332*U_0^2 + .8678*U_0 = 1.4 Kpa/cm @ 1 m/s
  - Steam: .007618*U_0^2 + .01175*U_0 = .019372 Kpa/cm @ 1 m/s

Include calcs on monolith + other one

- MATLAB plots

What: critical velocities and pressure drop for fluidization

Why: to determine applicability of fluidized beds

Is it valid: This matched what would be expected due to the steam properties and will inform our prototyping decisions

Calculations 2: packed and fluidized beds

$$g \cdot (\rho_s - \rho) = \frac{\left(150 \cdot \mu \cdot (1-\varepsilon)^2 \cdot U_0\right)}{\varepsilon^3 \cdot d^2} + \frac{\left(1.75 \cdot (1-\varepsilon) \cdot \rho \cdot U_0^2\right)}{\varepsilon^3 \cdot d}$$

- Fluidized bed critical velocities
  - U_{min}

    Fluidized pressure drop
    - Air : .5332* U_0 ^2 + .8678* U_0 = g*(ρ_p - ρ) = .1038 kpa/cm => U min = .1119 m/s
    - Steam: .007618* U_0 ^2 + .01175* U_0 = g*(ρ_p - ρ) = .2084 kpa/cm => U min = 4.515 m/s
  - U_{max} Dry

Air easily fluidizes but never reaches critical.
steam never fluidizes

$$\mathrm{Re} = \frac{\rho u d_p}{\mu} \text{ ; variables defined above except } C_D$$

$$\mathrm{Re} < 1 \quad \Rightarrow u_t = \frac{(\rho_s - \rho) g d_p^2}{18\mu}$$

$$1 < \mathrm{Re} < 500 \quad \Rightarrow u_t = \left[\frac{4(\rho_s - \rho) g d_p}{3\rho C_D}\right]^{\frac{1}{2}}$$

$$\text{where } C_D = \frac{18}{\mathrm{Re}^{\frac{3}{5}}},$$

$$500 < \mathrm{Re} < 2*10^5 \quad \Rightarrow u_t = \left[\frac{3(\rho_s - \rho) g d_p}{\rho}\right]^{\frac{1}{2}}$$

Re=33.179

0<U<.03 Ut=7.815 m/s

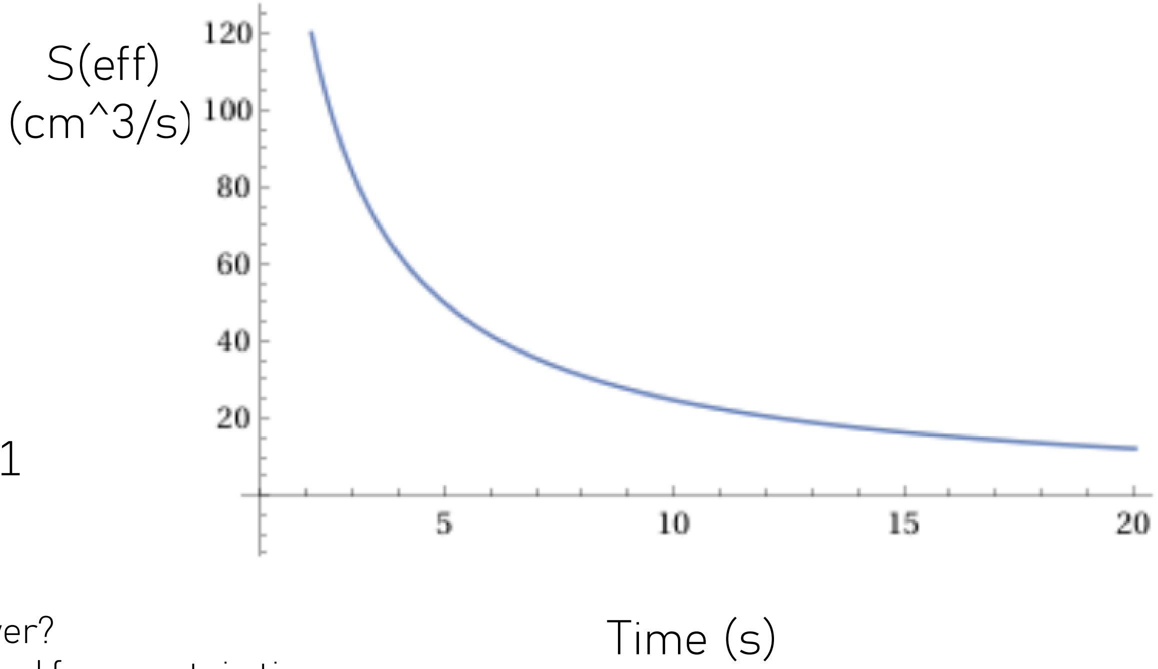
.03<U<15.07 Ut=(2.5674*U^(3/5))^(½) => Ut = U @ 1.961 m/s

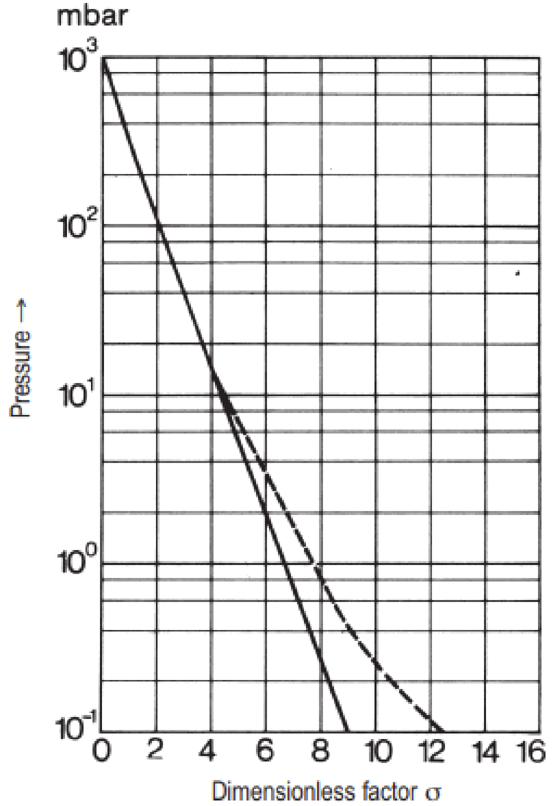
Calculations 3: Vacuum pump effective speed vs time

$$-\frac{dp}{dt} = \frac{S_{eff}}{V} \cdot p$$

$$S_{eff} = \frac{V}{t} \cdot \sigma \qquad \sigma = \ell n \frac{1013}{p}$$

0.5kpa = 5mbar
Ln(1013/5mbar)=5.311
S(eff)=47.03cm^3/t*5.311
S(eff)=249.77cm^3/t





- What question does this answer?
  Effective pump speed needed for a certain time.
- What was the answer?
  A graph to show pump performance based on time cycle.
  Will be sanity checked with pump salesperson.
- How does this answer inform the design?
  This will inform the sizing of the vacuum pump.

Maybe can update

Calculations 3: Pumping Throughput & Conductance

$$q_{pV} = C(p_1 - p_2) = \Delta p \cdot C$$

Where C is conductance

$$\frac{1}{S_{net}} = \frac{1}{S_{pump}} + \frac{1}{C_{piping}}$$

Net speed, client specified 1 m/s

$$\frac{1}{C} = \frac{1}{C_1} + \frac{1}{C_2} + \frac{1}{C_3} + \ . \ . \ . \frac{1}{C_n}$$

Conductance can be calculated as the inverse of resistors

Calculations4 – Condensation Requirement

First Law of Thermodynamics – conservation of energy

$$\frac{dE_{cv}}{dt} = \dot{Q}_{cv} - \dot{W}_{cv} + \sum_i \dot{m}_i\left(h_i + \frac{V_i^2}{2} + gz_i\right) - \sum_e \dot{m}_e\left(h_e + \frac{V_e^2}{2} + gz_e\right)$$

Assumptions: steady state, no work done to system

KE and PE negligible

$$\dot{Q}_{out} = \dot{m} * (h_{in} - h_{out})$$

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

$$\dot{Q}_{out} = 33.5\ Watts$$

What: Refrigeration power required to condense water vapor to separate from CO_2 after leaving reactor

Why: to determine what kind of apparatus is needed to condense vapor

Is it valid: This power is similar to that of many small cooling devices

Known Values [1]:

$$T_{sat} = 27.1°F \quad (1kPa)$$

$$h_{in} = h_{steam} = 2540\frac{kj}{kg} \quad (1kPa, 70°F)$$

$$h_{out} = h_{liquid} = 18.7\frac{kj}{kg} \quad (1kPa, 40°F)$$

$$\rho_{steam} = 0.007\frac{kg}{m^3} \quad (1kPa, 70°F)$$

$$v_{steam} \approx 1\frac{m}{s}$$

$$A_{reactor} \approx 19.1cm^2$$

Budget

Due to a capstone requirement of 10% of total budget must be fundraised, we are attempting to apply for a Green Fund Grant from NAU. Professor Wade had the idea to put the money towards an experimental 3D printer that can be used as an extension of this project to test solid sorbent structures that can be made into all shapes.

On the very small chance that all our parts are on there higher estimate of cost and we run out of funds; we will likely use the grant money from Green Fund or complete additional fundraising.

	Low Estimate	High Estimate
INCOME		
Budget Grant from SRP	+$50,000	+$50,000
Possible Green Fund Grant	+$5,000	+$8,000
EXPENSES		
Oil Free Vacuum Pump (1mBar, 10 LPM)	-$6,000	-$15,000
Variable Frequency Drive	-$500	-$1,000
Cold Trap & Chiller	-$2,500	-$5,000
Water Vessel w/ Thermal Jacket & Temp Control	-$3,000	-$5,000
KF40 Vessel	-$100	-$200
KF25/40 Adapters & Sorbent Bed Supports	-$5,000	-$10,000
Instrumentation (pressure transducers, thermocouples)	-$4,000	-$12,000
Welding 316 stainless steel	-$1,500	-$3,000
Experimental 3D Printer (Green Fund)	-$5,000	-$8,000
TOTALS		
Total Income	+$55,000	+$58,000
Total Expenses	-$27,600	-$59,200
Net Balance	+$27,400	-$1,200

Schedule

• HW 3,	Oct 4,	All
• Presentation 2,	Oct 9,	All
• Website Check 1,	Oct 24,	All
• Presentation 3,	Nov 6,	All
• Prototype 1,	Nov 13,	All
• HW 4,	Nov 24,	All
• Report 2,	Nov 26,	All
• Prototype 2, CAD	Dec4,	All

• Green fund application,	Oct 1,	Justin
• Initial Cad,	Oct 1,	Eli
• Initial Ansys Simulations,	Oct 6,	Branden
• Vacuum Pump Sizing,	Nov 1,	Randy

Thank You

Questions?

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