Overview of the RCAP Presented at the ISRU Thermal Integration Meeting

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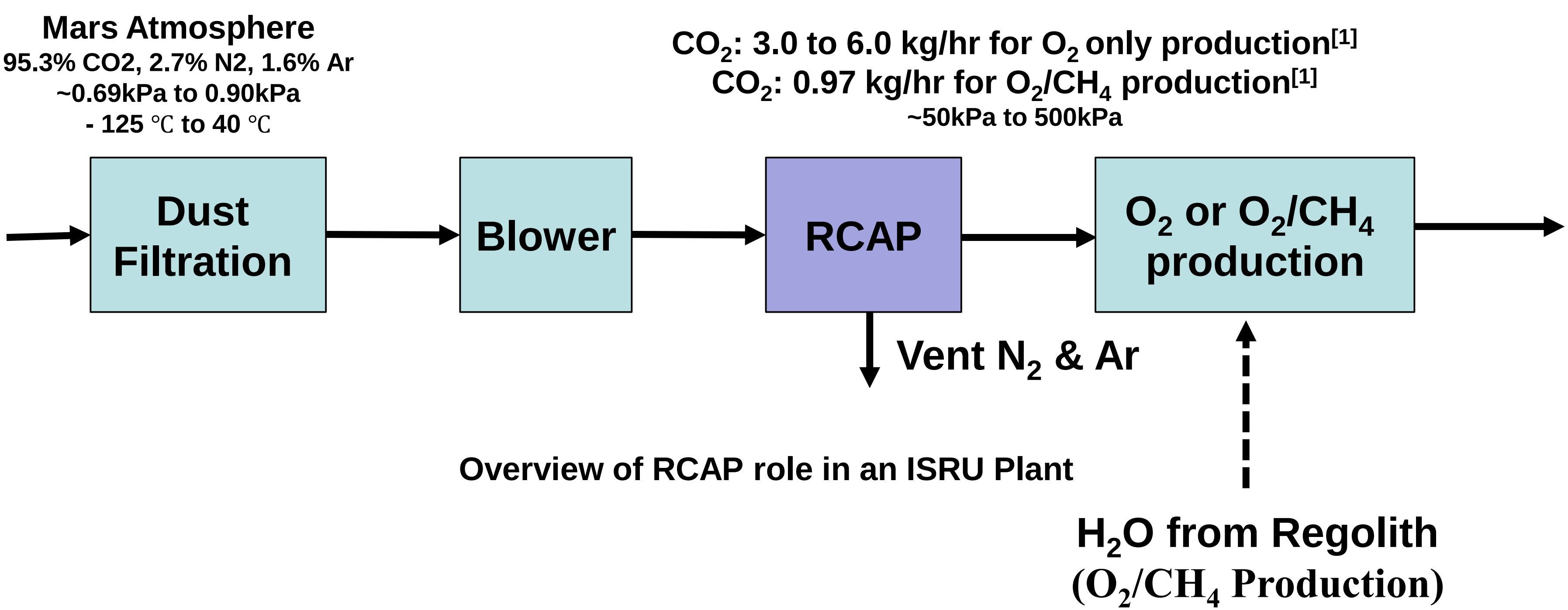
Adsorption Pump Concept

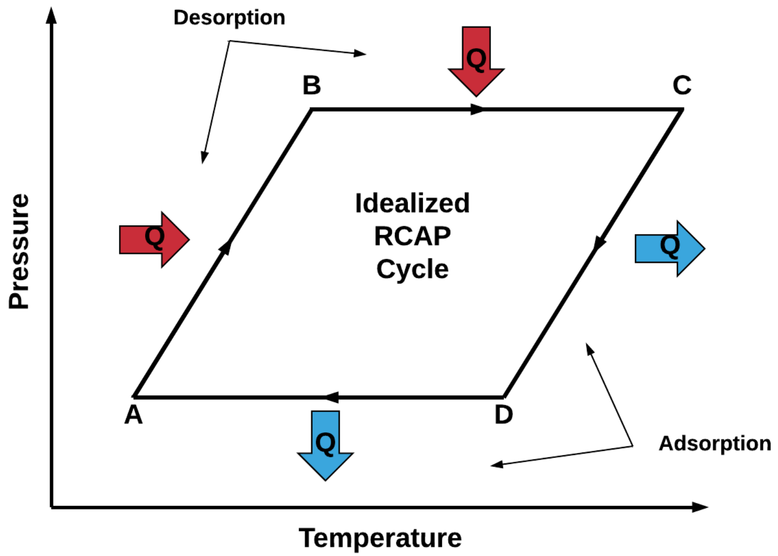
- Rapid Cycle Adsorption Pump (RCAP) Purpose:
  1. Separate carbon dioxide (95% CO_2) from the Mars atmosphere ($\sim 5\%\ N_2,\ Ar_2$)
  2. Send pressurized CO_2 to downstream processes in a Martian In-Situ Resource Utilization Plant.



Overview of RCAP role in an ISRU Plant

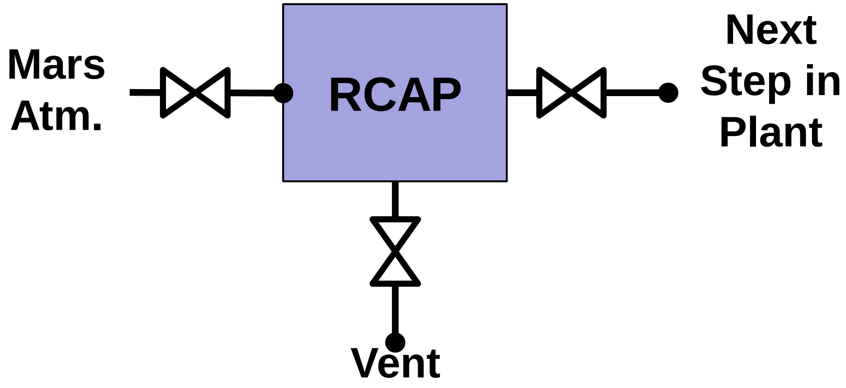
Thermodynamic Model: Adsorption Pump

- RCAP fundamentals:
  - **<u>Adsorption:</u>** Cool to adhere CO_2 particles to a material called an adsorbent. More CO_2 adsorbed with *increasing pressure* and *colder temperatures*
  - **<u>Desorption:</u>** Heat the adsorbent to release the adhered particles.
  - <u>Desorption in a closed volume will generate a pressurized product</u>



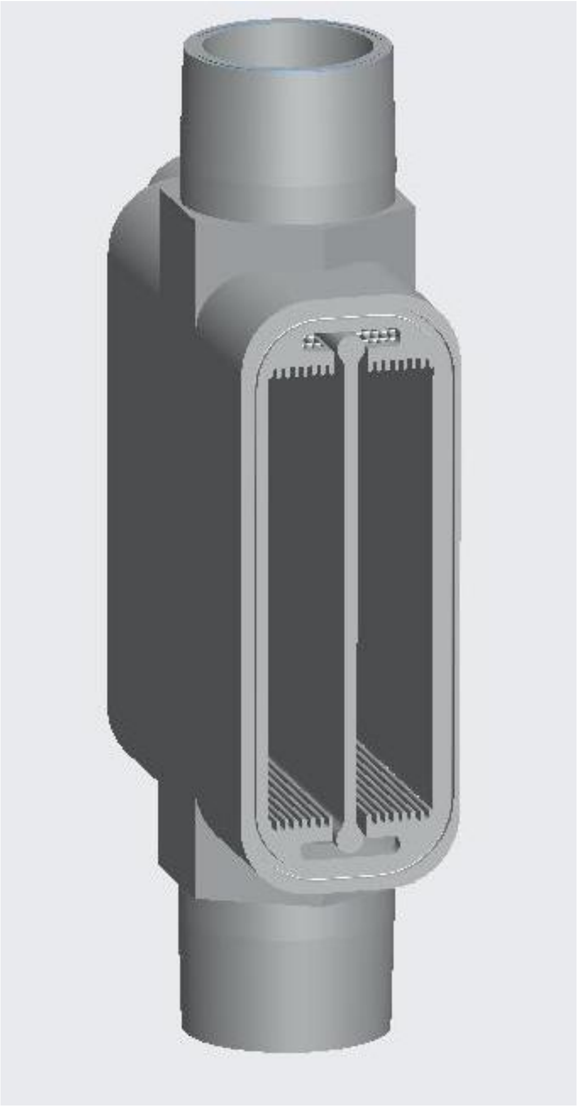
Idealized RCAP pump processes operated via temperature swing represented on a Pressure-Temperature diagram.[3]

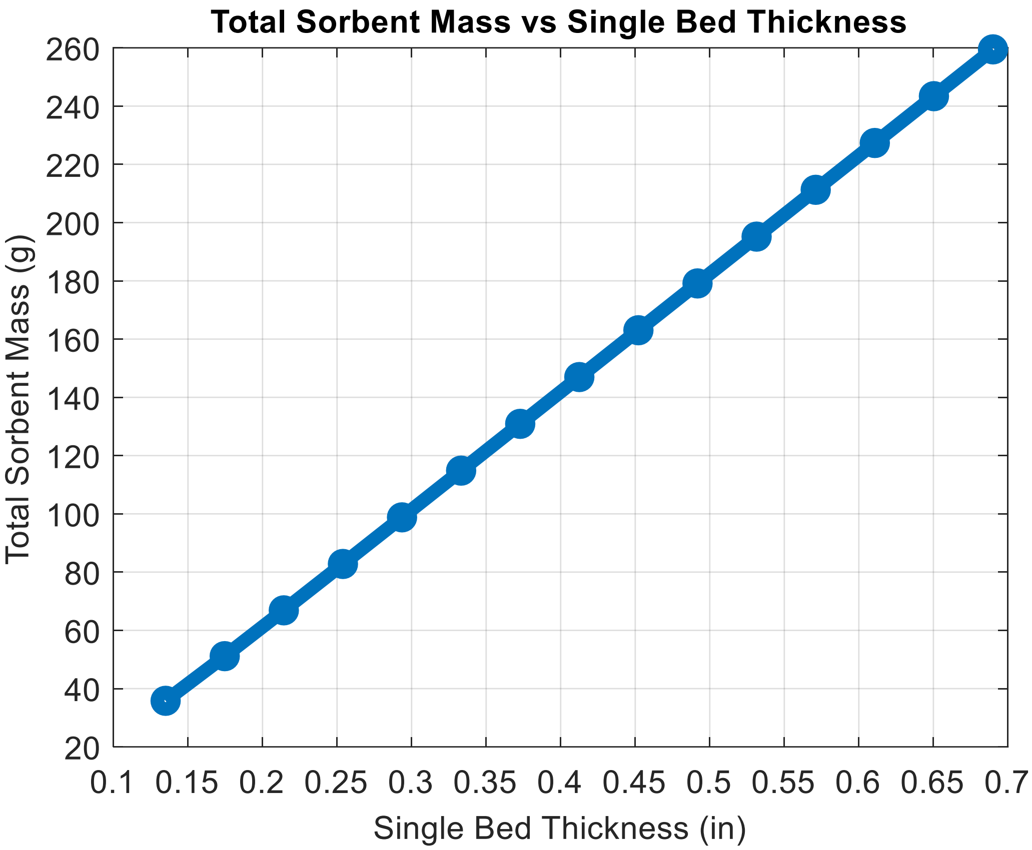
- Idealized 4 step cyclic process:
  - $A \rightarrow B$: Isovolume Heating of a saturated bed
  - $B \rightarrow C$: Isobaric Heating
  - $C \rightarrow D$: Isovolume Cooling
  - $D \rightarrow A$: Isobaric Cooling



RCAP Flow Configuration

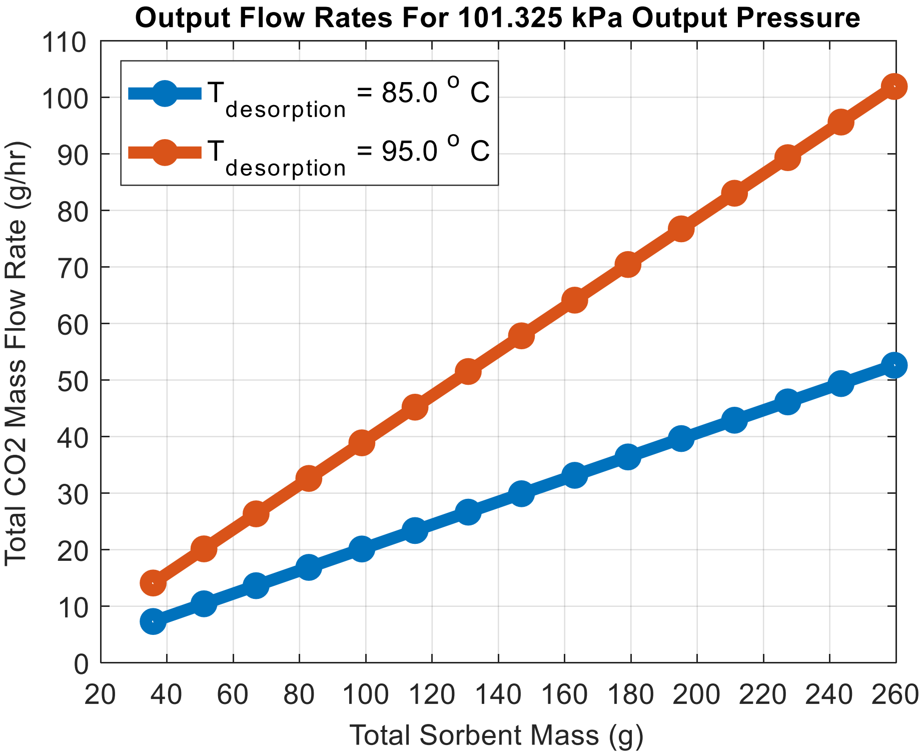
RCAP Thermo Model - Test Article

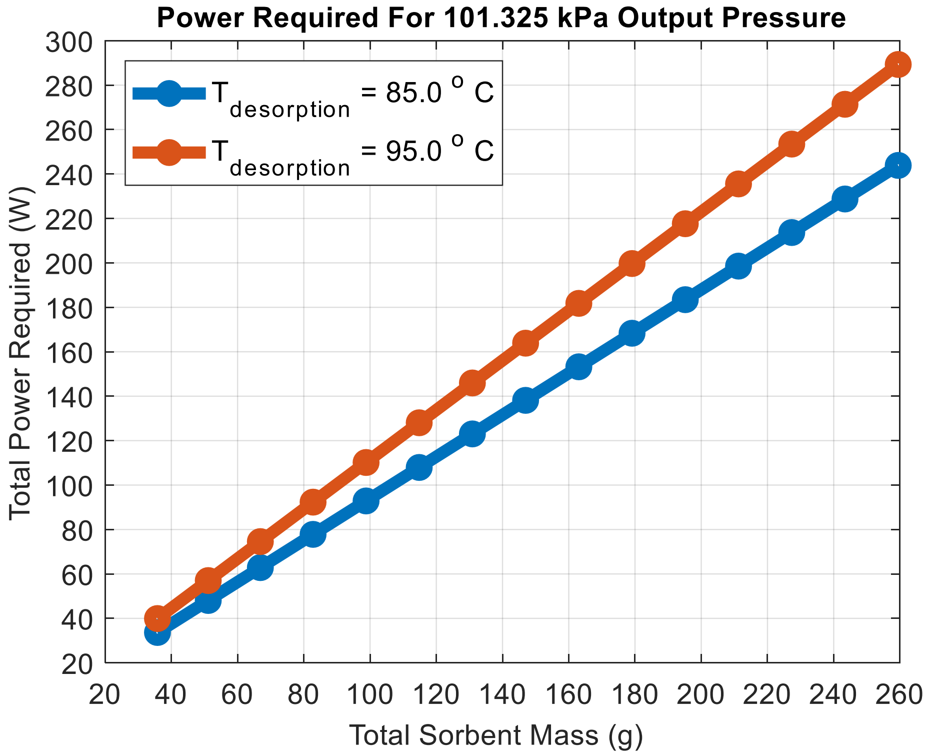




Single-Stage RCAP Test Hardware

RCAP Thermo: Idealized Cycle Analysis



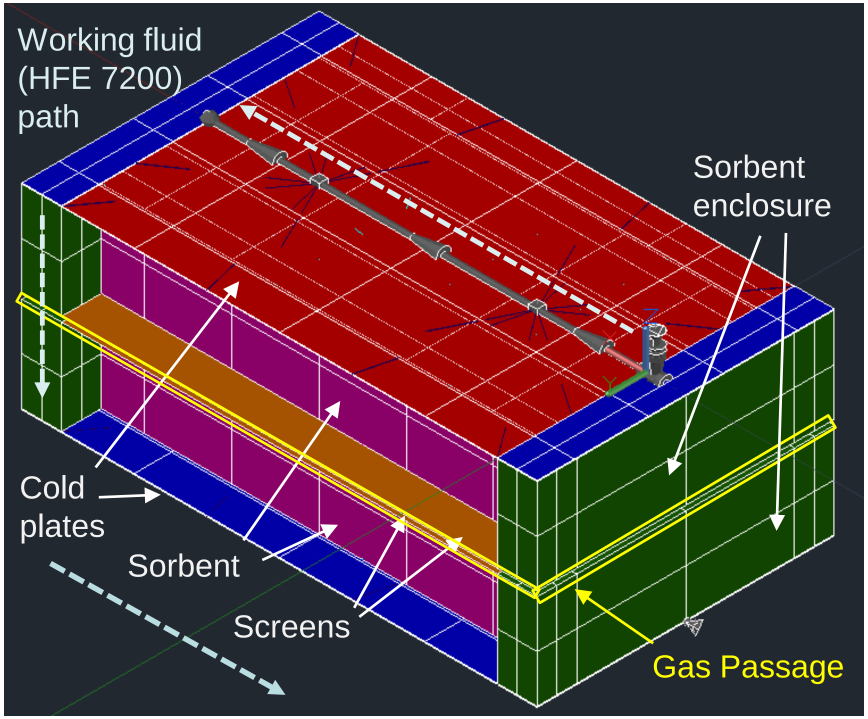


Single-Stage RCAP Test Analysis parameters:

- Adsorption Temperature = $-20\ ℃$
- Inlet Pressure = $0.933\ kPa$
- Sorbent Heat Capacity **[Ref 1]:** $0.96 \frac{kJ}{kg - K}$

RCAP Modeling – Plate Based Design

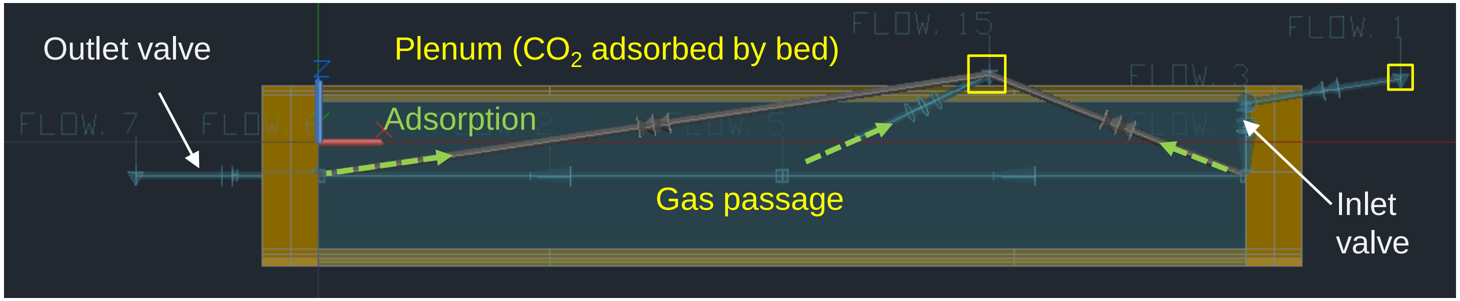
- Purpose
  - Help size and choose a material for the RCAP test article (e.g. bed height).
- Overview:
  - 1 pump stage = 1 stack
    - 2 Cold plates
    - 2 Sorbent beds (Grace 544 13X)
    - 2 Metal screens
    - 1 Gas passage
  - Increasing the width of thermal model is used to estimate real world configuration multiple plates stacked.



Thermal Desktop model layout. Finite difference objects represent solid parts. FloCAD objects (e.g. paths, junctions) represent the process gas to be pressurized and the working fluid.

RCAP Modeling – Plate Based Design

- Overview (cont.):
  - Implement adsorption/desorption via set mas flow rates of CO_2 to/from a plenum (infinite source/sink).
  - At each time step set:
    - plenum's temperature = sorbent's mass average temperature.
    - plenum's pressure = gas passage's average pressure.
  - Toth Isotherm fit predicts: 1) heat of adsorption, & 2) bed loading at equilibrium.
  - Linear driving force approximation predicts 1) sorbent heating/cooling rates, & 2) CO_2 flowing into and out of the gas passage.



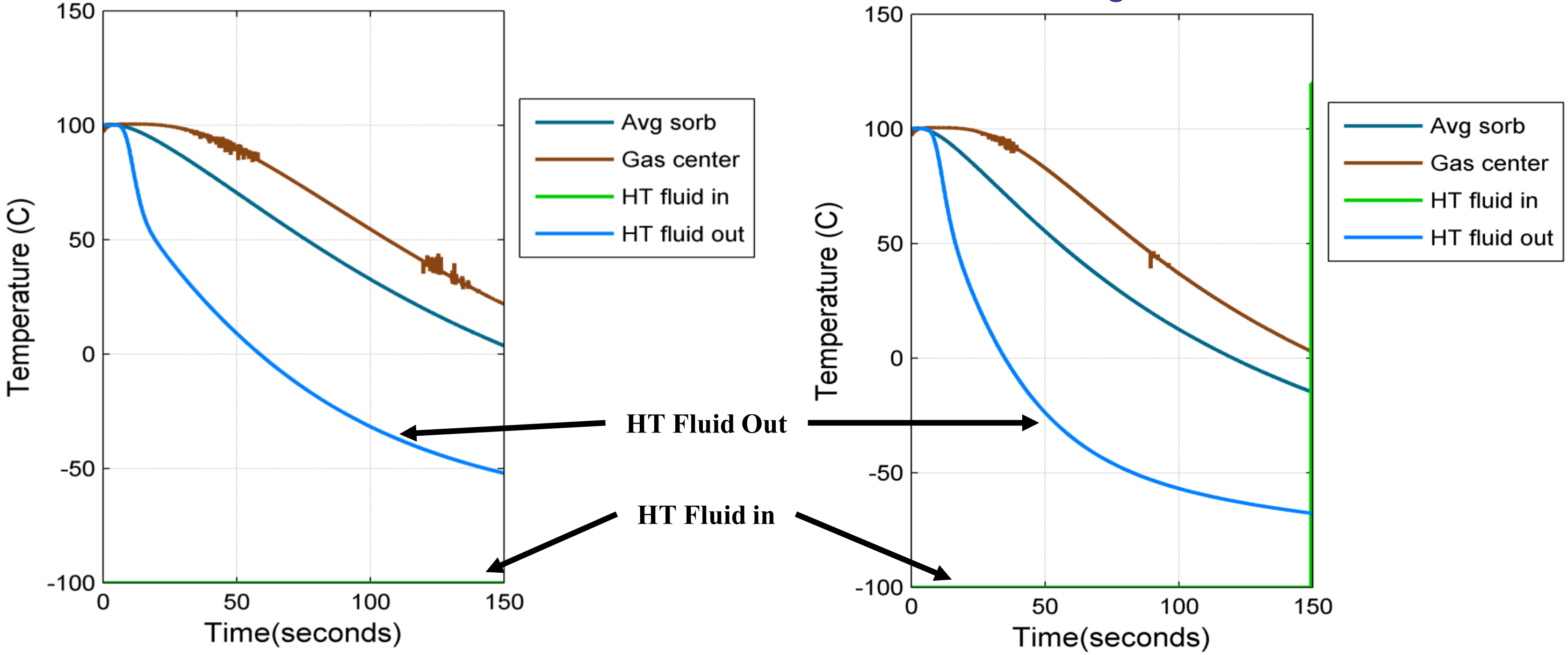
Gas passage. Set flows are used to implement 1) inlet flow rate from Mars atmosphere, and 2) flow rates from of CO2 adsorbing into or desorbing from the sorbent bed.

RCAP Modeling – Materials Trade

- Comparison Case:
  - Cooled 1.72kg sorbent from 100C in a sealed bed. (Thermal Effects Only)
  - While GRCop-84 has a much higher thermal conductivity, the AlSi10mg version had a much lower thermal mass and cooled faster.
  - Use of AlSi10mg instead of GRCop-84 resulted in $30,000 decrease in 3D printing manufacturing costs

GRCop-84 results:

AlSi10mg results:

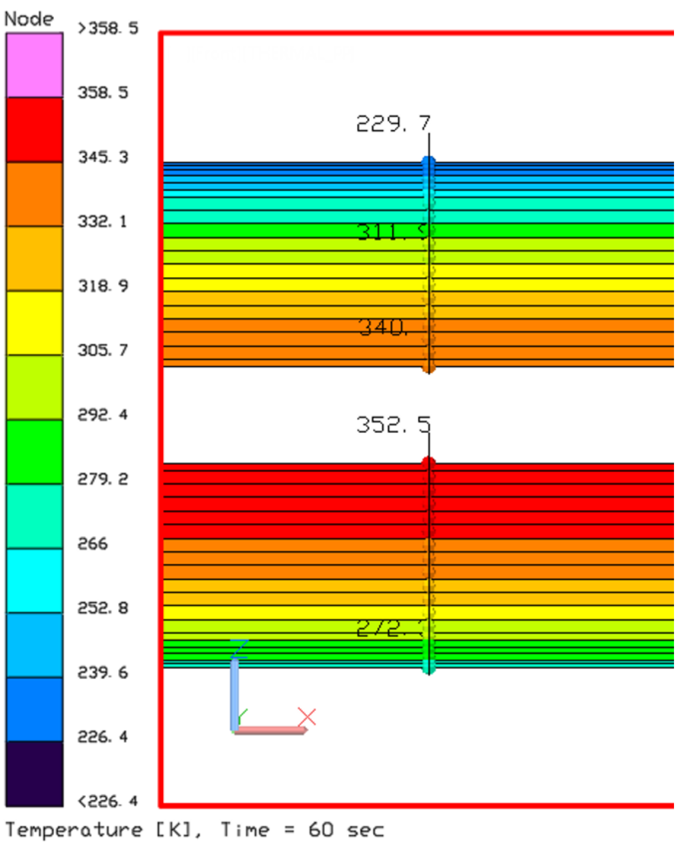


Cooling time with enclosure and cold plate set to GRCop-84. Cold plate wall could be 0.75mm thin.

Cooling time with enclosure and cold plate set to AlSi10mg. Cold plate wall could be 0.55mm thin.

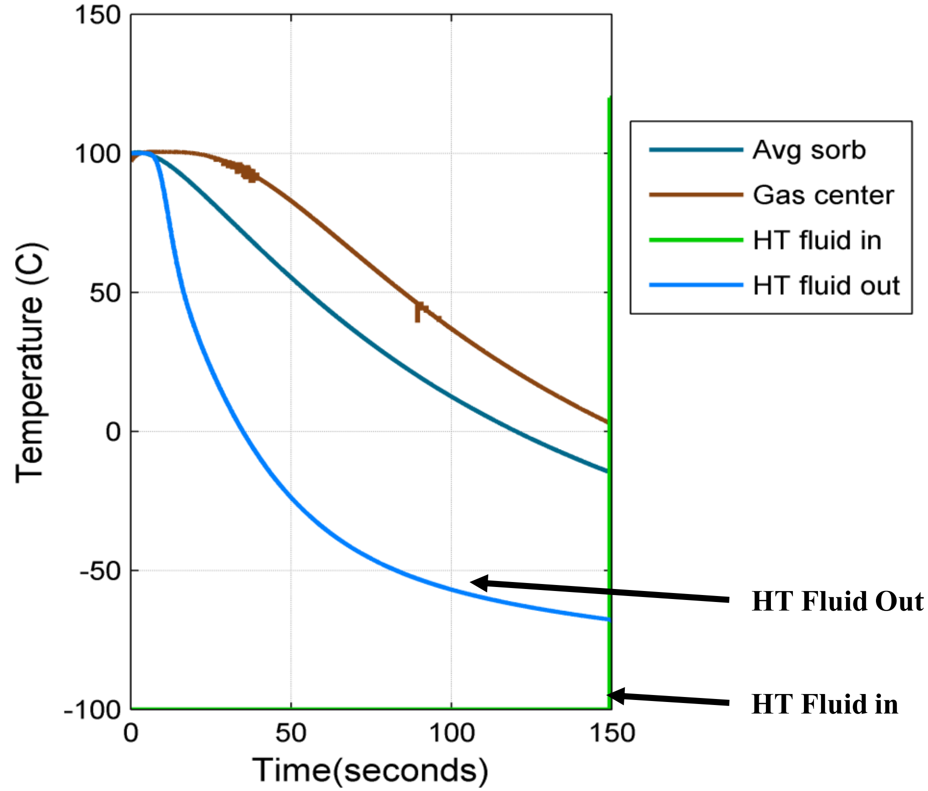
RCAP Modeling – Materials Trade

- Comparison Case:
  - Cooled 1.72kg sorbent from 100C in a sealed bed.
  - Observed large temperature gradients in the 5.23mm thick sorbent beds.



Temperature gradient in sorbent at 60s into cycle. At this point the gas passage center was at 74 C (347 K). The heat transfer fluid warmed from -100 C (173 K) to -34 C (239 K).

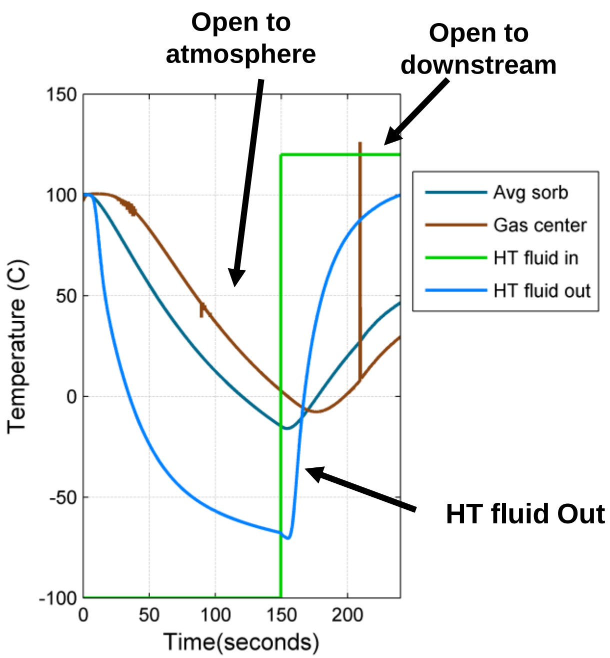
AlSi10mg results:



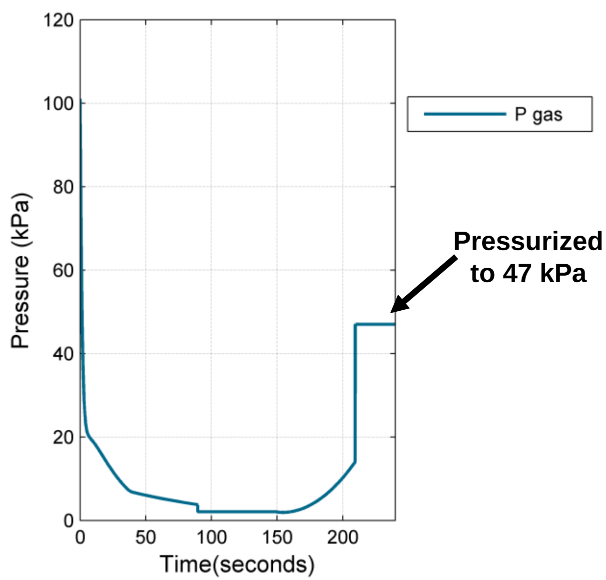
Cooling time with enclosure and cold plate set to AlSi10mg. Cold plate wall could be 0.55mm thin.

RCAP Modeling – Preliminary Results

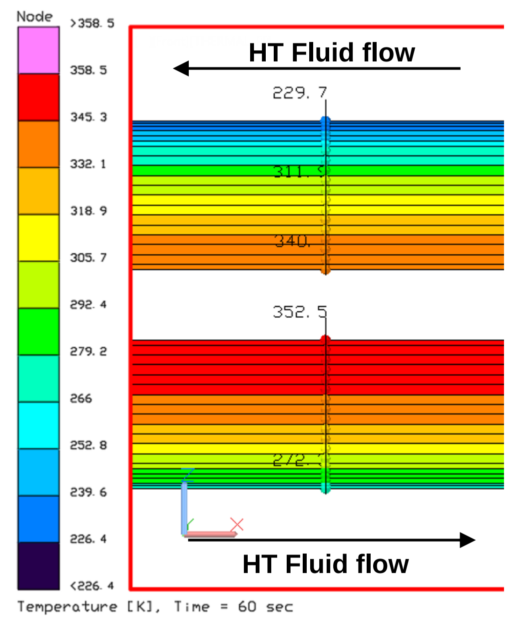
- Case:
  - 1.72kg sorbent heated/cooled with forced liquid HFE 7200 at 0.063kg/s
    - 1st stage of a 5.16kg pump.[3]
    - HFE 7200 mass flow rate loosely based on Linne (2013) experiment.[6]



Temperatures throughout one RCAP cycle



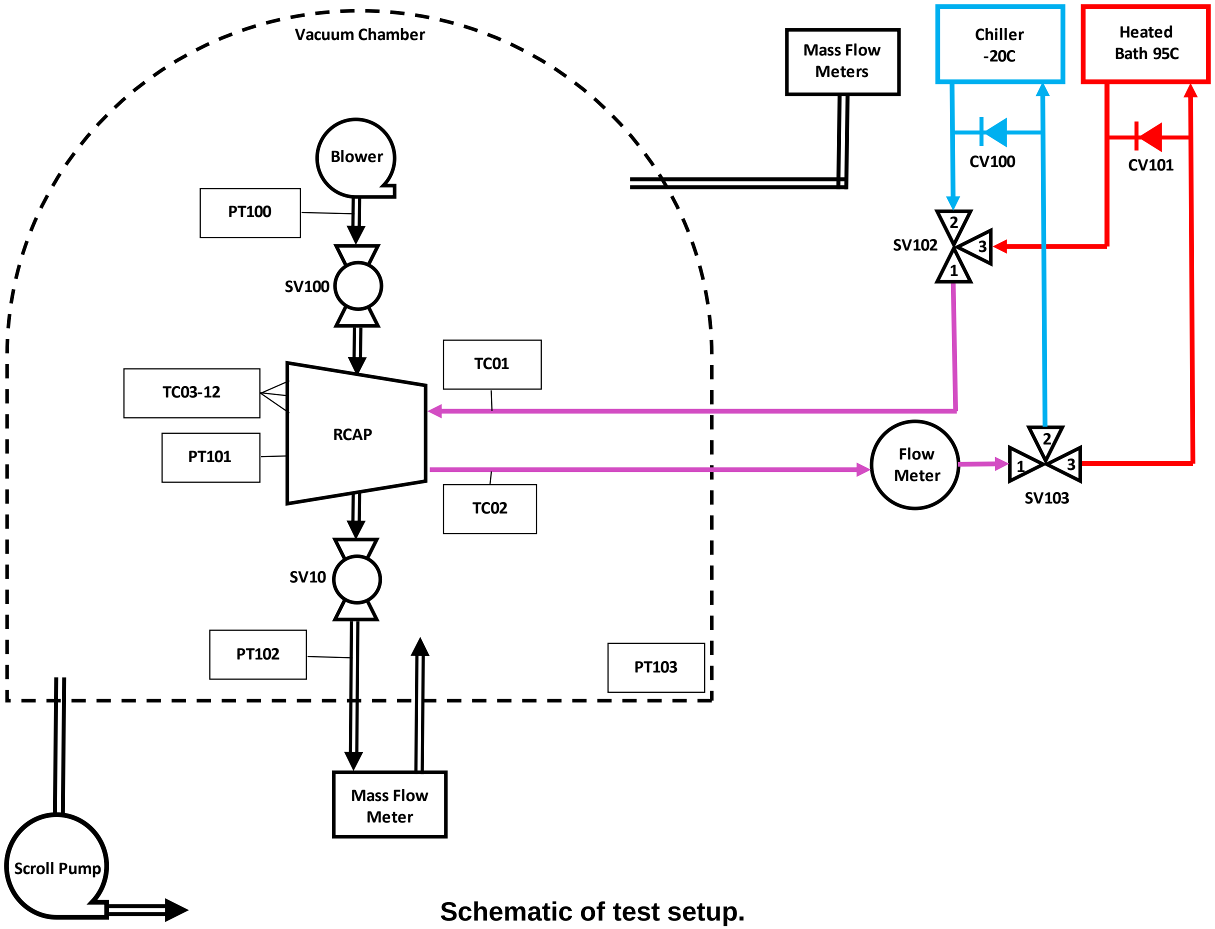
Average gas passage pressure throughout one RCAP cycle



Temperature gradient in sorbent at 60 s into cycle. At this point the gas passage center was at 74 C (347 K). The heat transfer fluid warmed from -100 C (173 K) to -34C (239 K).

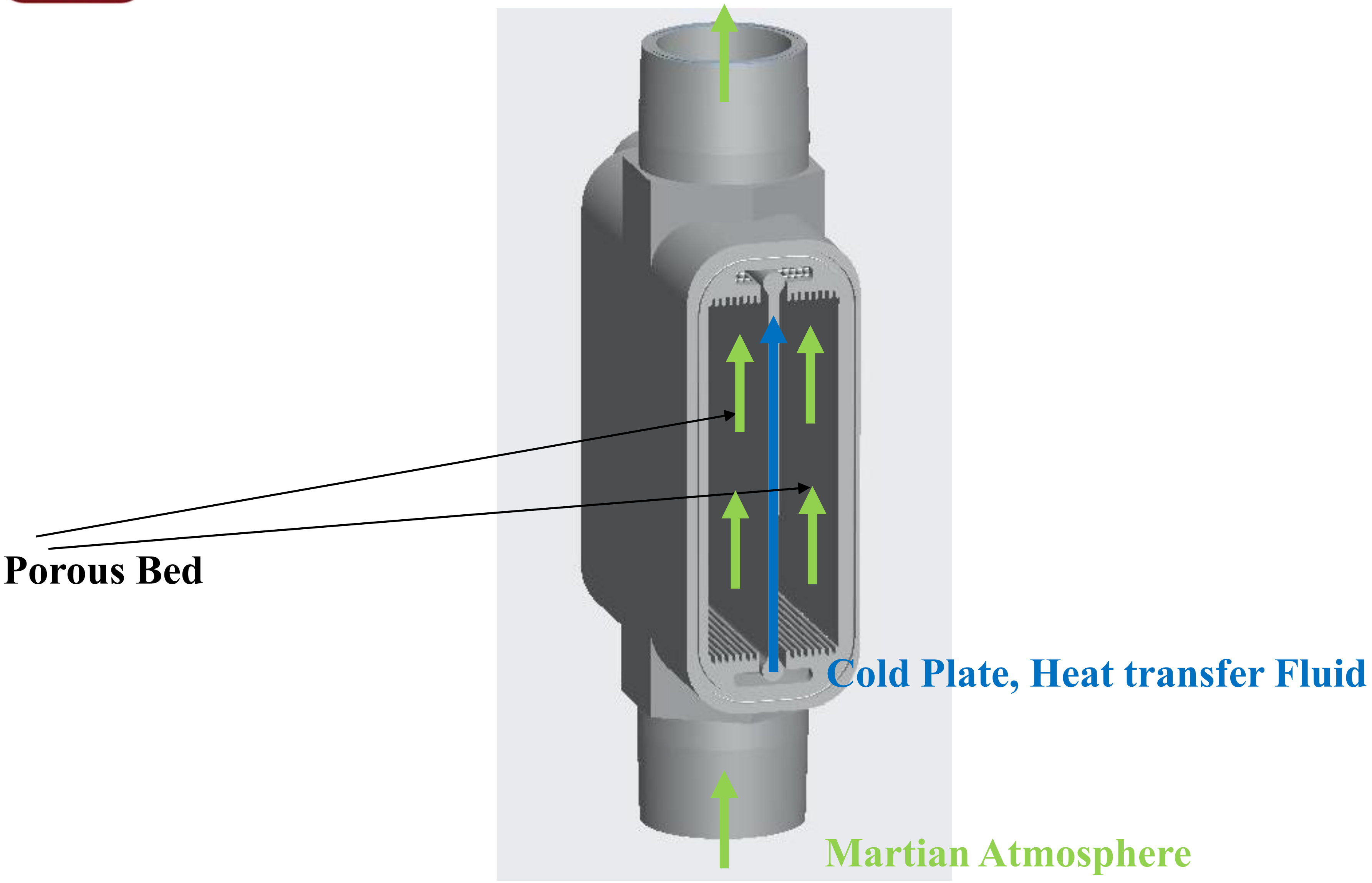
RCAP Testing – Single Plate Test

- Purpose
  - Single-Plate, Single-Stage RCAP test article – scaled down RCAP.
    - Targeting 1/10th CO_2 production for full scale ISRU system.



Schematic of test setup.

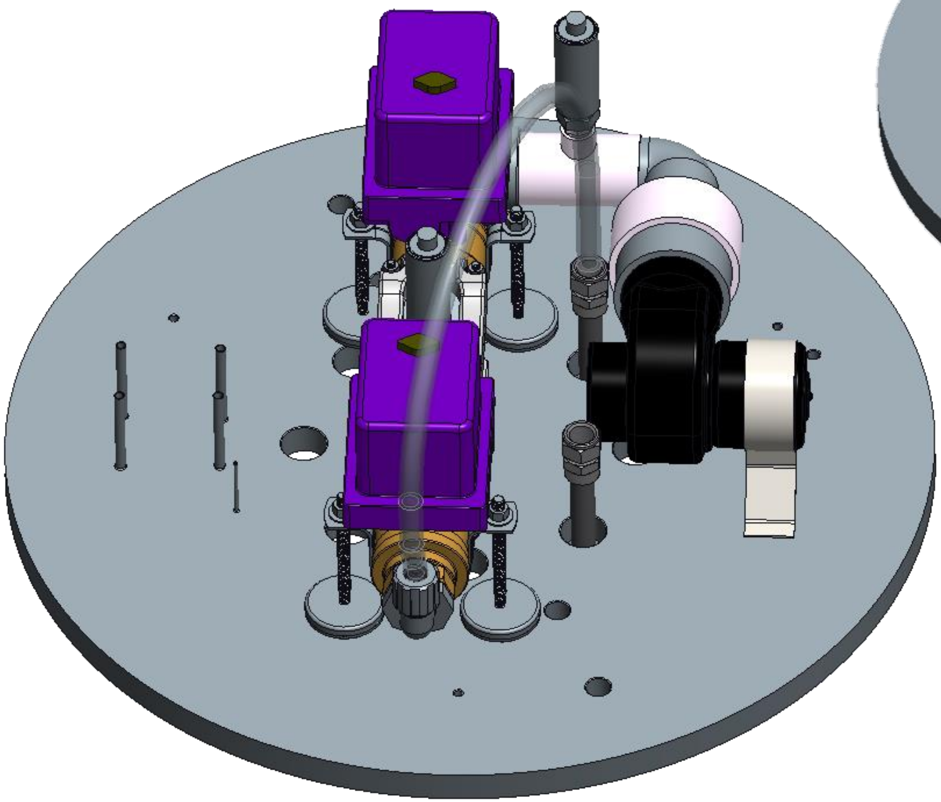
RCAP Testing – Test Hardware

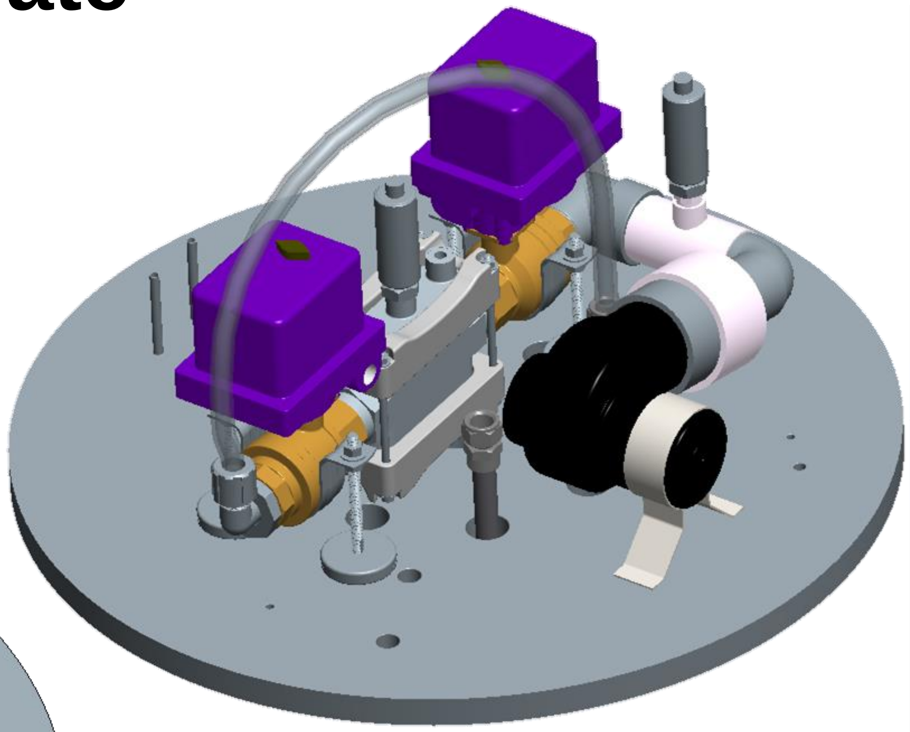


RCAP Testing

RCAP in the Mars Air Chamber Simulator

Complete Assembly on Base Plate



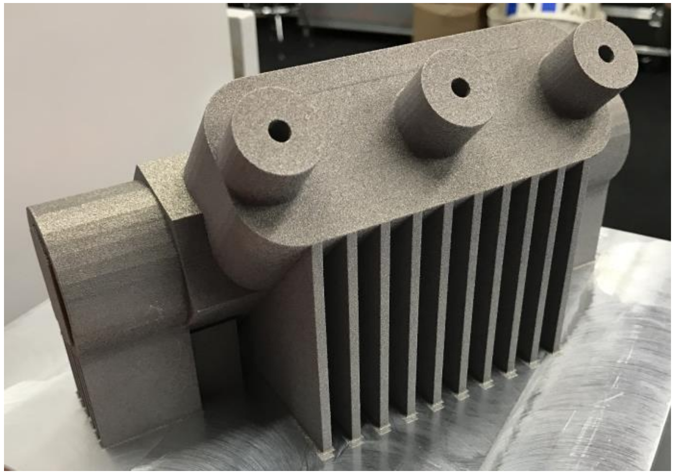


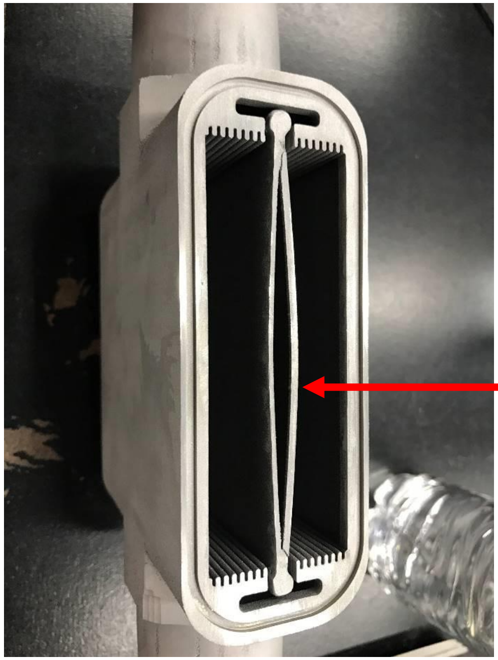
RCAP Testing

- Validate Thermal Desktop Single-Stage Model Against Experimental Results
  - Measure Temperature Distribution in the Porous Bed
  - Confirm pressurization of CO2
  - Measure mass flow rate of the CO2
- Possibly look at improving Heat Transfer in the Bed
  - Conductive Paths
    - Metal Foam (Cu, Al)
    - Al Shot
- Degradation issues
  - Adsorbent Poisoning
    - Water
    - N_2 (Barrier)
    - Ar (Barrier)
- Find Bed Regeneration Operational Proceedure when N_2 and Ar builds up on Zeolite Adsorbent

RCAP Manufacturing

- The RCAP container was created using a Selective Laser Sintering (SLS) additive manufacturing process out of aluminum alloy (AlSi10Mg).
- It underwent post machining which included:
  - The removal of support material.
  - The creation of an o-ring groove to create a face seal.
  - The re-surfacing of certain regions to create an o-ring seal for Swagelok fittings.
  - The creation of NPT and SAE threads to allow valves and tube fittings to attach on to the RCAP.



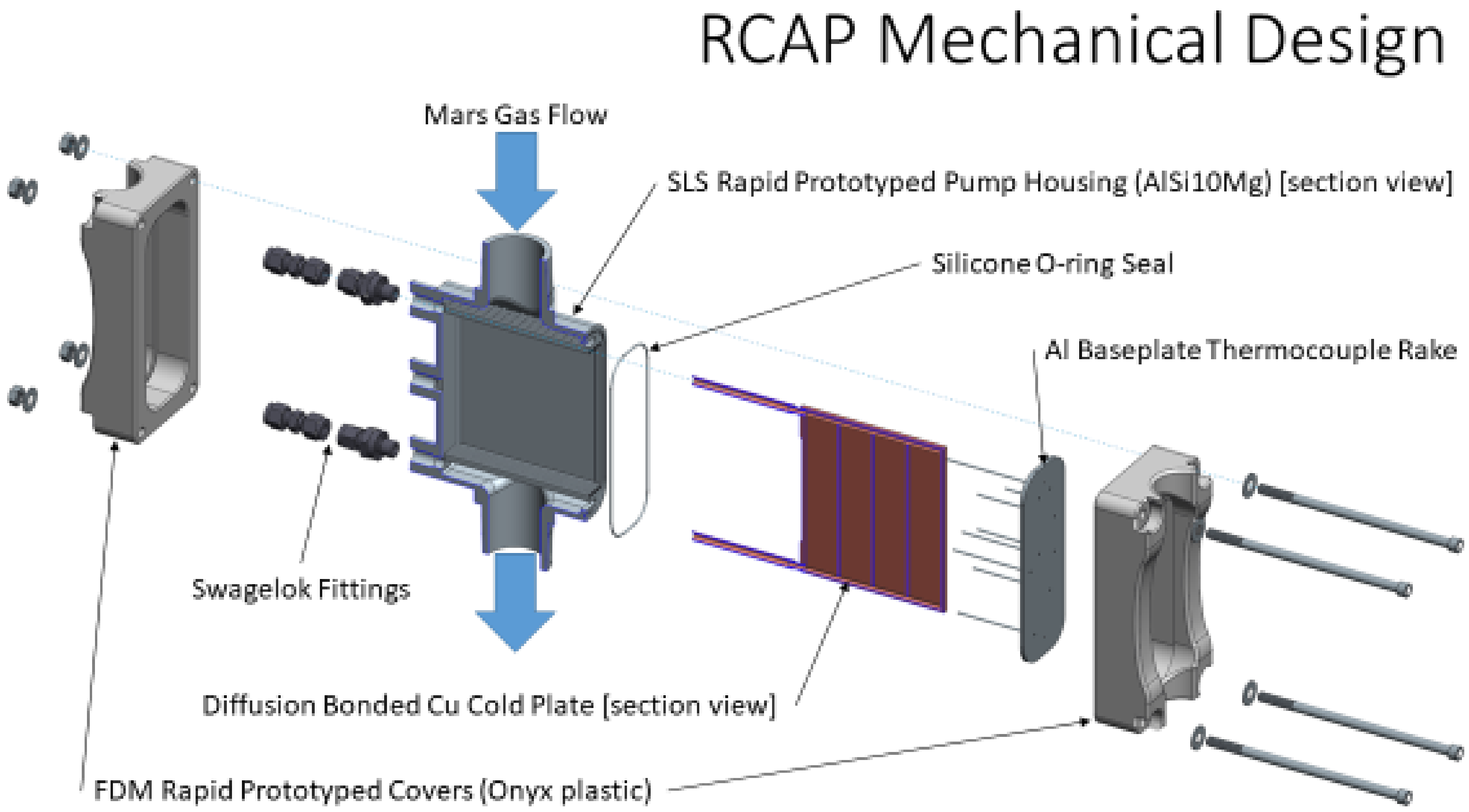


Failed Cold Plate

RCAP Manufacturing

- The RCAP covers were created using an additive manufacturing process called Fused Deposition Modeling (FDM) out of a material called Onyx.
  - Onyx is proprietary plastic compound produced by Markforged that performs well throughout our temperature range.
- The RCAP instrumentation plates were cut using a water knife out of 0.125 inch steel.
- Holes for thermocouple tubes were drilled out at pre-specified locations to allow for steel hypo-tubes to be epoxied in to rigidize thermocouple wires passing though them.

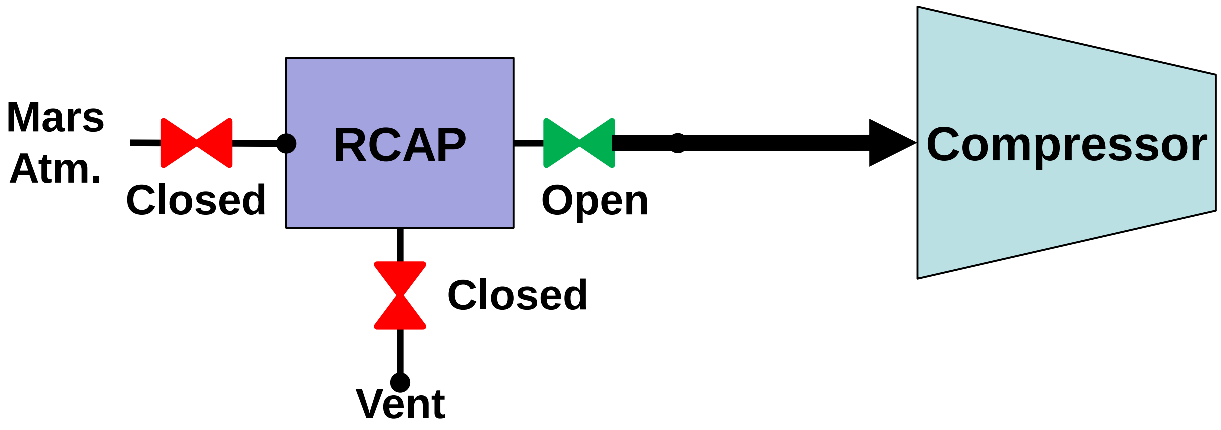
RCAP Revised Manufacture



RCAP Improvements - Hybrid System

- An RCAP designed for high pressure targets(~ 75 psi) is energy intensive may have high fractional mass for the ISRU system
  - Desorption becomes harder in higher pressure environments; thereby requiring more mass and more energy (e.g. multi-stage RCAP)
  - Can separate CO_2 from Mars atmosphere

- On Earth, small mechanical air compressors can easily hit 100 psi. However, Mars' atmospheric pressure is ~ 0.135 psi (555 : 1 CR !!)
  - High power requirement to compress to 75 psi
  - High temperature output, which may exceed material limits
    - May result in multi-stage compressors that require intercooling (i.e. increased complexity, and mass)
  - Doesn't have separation capabilities



RCAP - Closing Remarks

- Need To Improve Heat Transfer In The RCAP Porous Bed
  - Most Promising Idea Is To Add Al Shot As Conductive Paths
- Single-plate, Single-stage Tests Will Give A Better Understanding Of The Heat Transfer In The Porous Bed
- Don't Know If Adding A Compressor With Help Overall System Thermal Performance
  - Material Limits On Compressor Versus Desired Inlet Temperatures To Solid Oxide Electrolyzer (SOE) Or Sabatier Reactor
- Add Recuperation To RCAP To Improve Overall ISRU System Thermal Efficiency
- RCAP Heat Transfer Working Fluid Hot Source, A Reactor Port
  - Possibly Utilize Waste Heat From Kilopower Nuclear Reactor

References

1. National Aeronautics and Space Administration, “NextSTEP-2 BAA Appendix D: In Situ Resource Utilization (ISRU) Technology - NNH16ZCQ001K-ISRU,” *FedBizOpps*. FedBizOpps. [Accessed: 30-Jul-2018]. https://www.fbo.gov/index?s=opportunity&mode=form&tab=core&id=34eb0ba219ff3a8d97c9c4b2c9302bf1
2. R. T. Yang, Gas Separation by Adsorption Processes. Kent: Elsevier Science, 01.
3. Hasseeb, Hashmatullah and Iannetti, Anthony, “A System Level Mass and Energy Calculation for a Temperature Swing Adsorption Pump used for In-Situ Resource Utilization (ISRU) on Mars,” presented at the TFAWS, 2017.
4. R. Schunk, W. Peters, and J. Thomas, “Four Bed Molecular Sieve – Exploration (4BMS-X) Virtual Heater Design and Optimization,” Jul. 2017.
5. D. Nield and A. Bejan, *Convection in Porous Media*. New York, NY: Springer New York, 2006.
6. D. Linne *et al.*, “Demonstration of Critical Systems for Propellant Production on Mars for Science and Exploration Missions,” 2013.

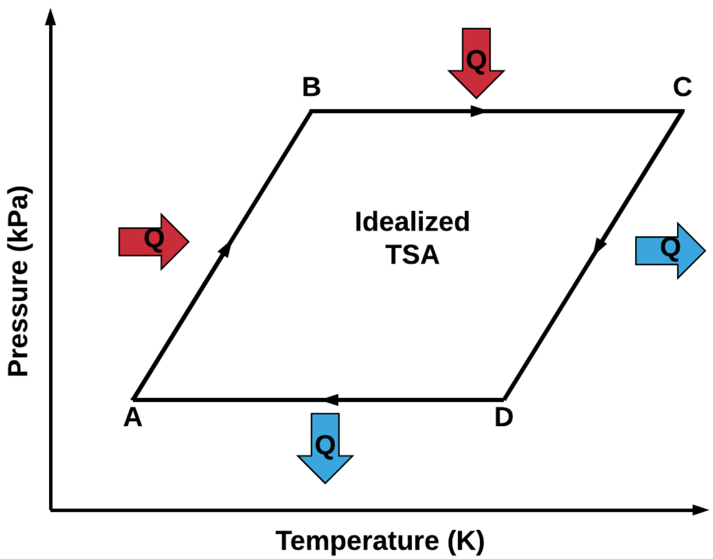
Backup

Adsorption Pump Concept

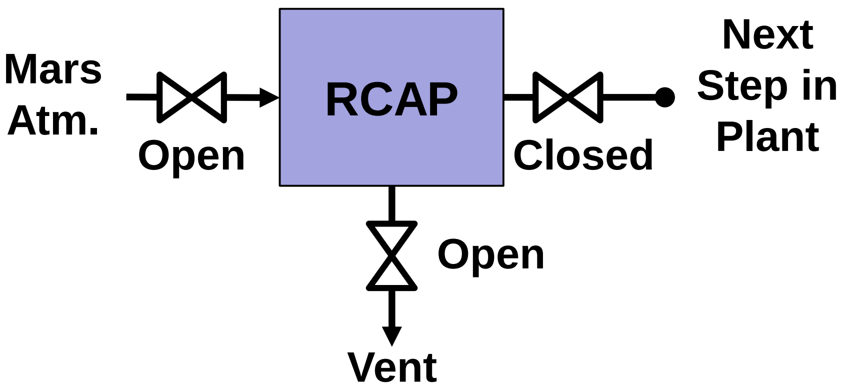
- 4 step cyclic process:

D → A: Isobaric Adsorption

- Start with cooled sorbent bed.
- Upstream valves open.
- Blower directs flow through the bed. Non-CO_2 gasses vent.
- Adsorption occurs (CO_2 molecules bond to sorbent, e.g. zeolite) releasing heat.[2]
- Sorbent bed is externally cooled to the maintain a constant pressure.
- State A's temperature is called the adsorption temperature.



Idealized TSA pump processes represented on a Pressure-Temperature diagram.[3]



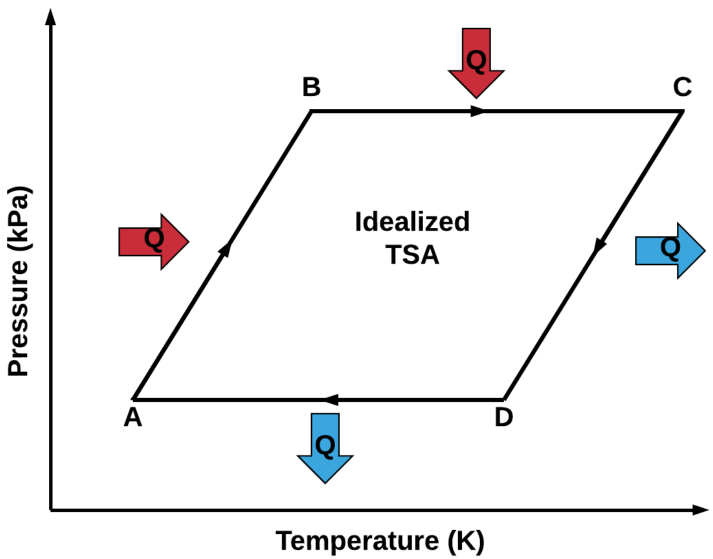
RCAP flow configuration during D to A transition.

Adsorption Pump Concept

- 4 step cyclic process:

A → B: Const. Volume Compression

- Start at adsorption temperature.
- All system valves close.
- Sorbent bed is externally heated until the target pressure is reached.
- Desorption occurs:
  - "Pulls" heat from the system
  - And pressurizing the bed's enclosure.



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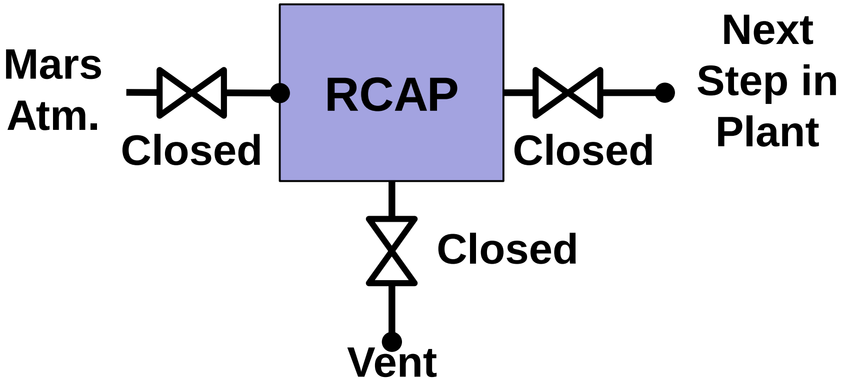


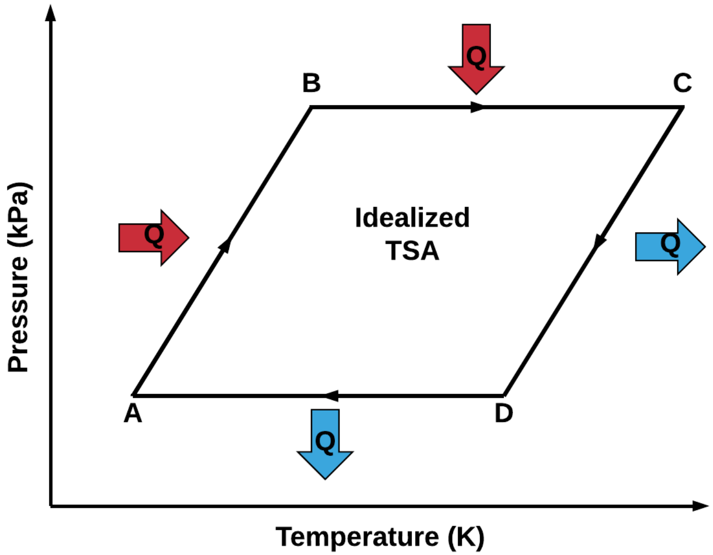
RCAP flow configuration during A to B transition.

Adsorption Pump Concept

- 4 step cyclic process:

B → C: Isobaric Desorption

- Downstream vales are opened to allow pressurized CO_2 to exit the bed.
- Desorption continues.
- Bed is heated to maintain constant pressure.
  - Desorption is endothermic.
  - Hotter beds hold less gas.
- State C's temperature is called the desorption temperature.



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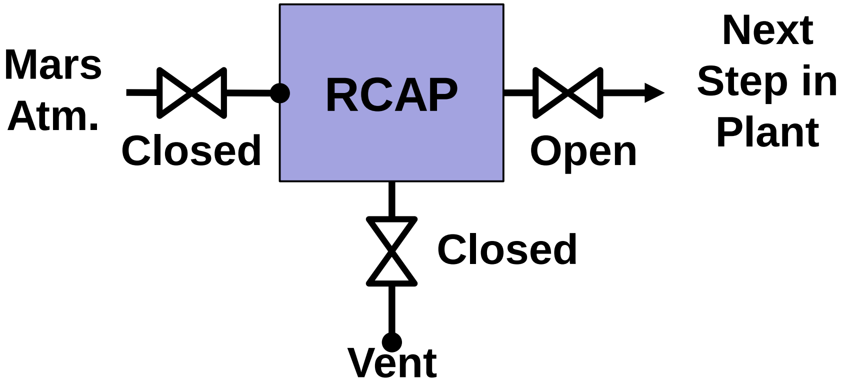


RCAP flow configuration during B to C transition.

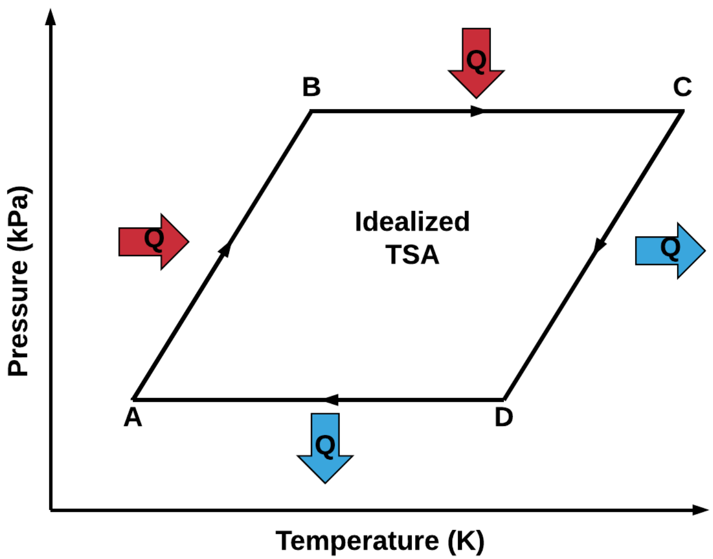
Adsorption Pump Concept

- 4 step cyclic process:

C → D: Const. Volume Cooling

  - Start at target desorption temperature.
  - Starts at max desorption temperature, and max bed pressure.
  - System valves are closed.
  - Bed is cooled in preparation for state D.
  - Remaining free CO_2 in the enclosure will start to adsorb, decreasing pressure in the enclosure.

To optimize required power & sorbent mass this cyclic process will be split into multiple stages.[3]



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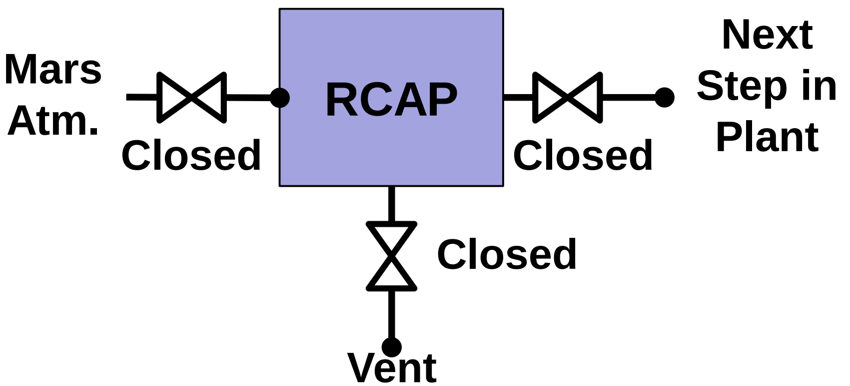
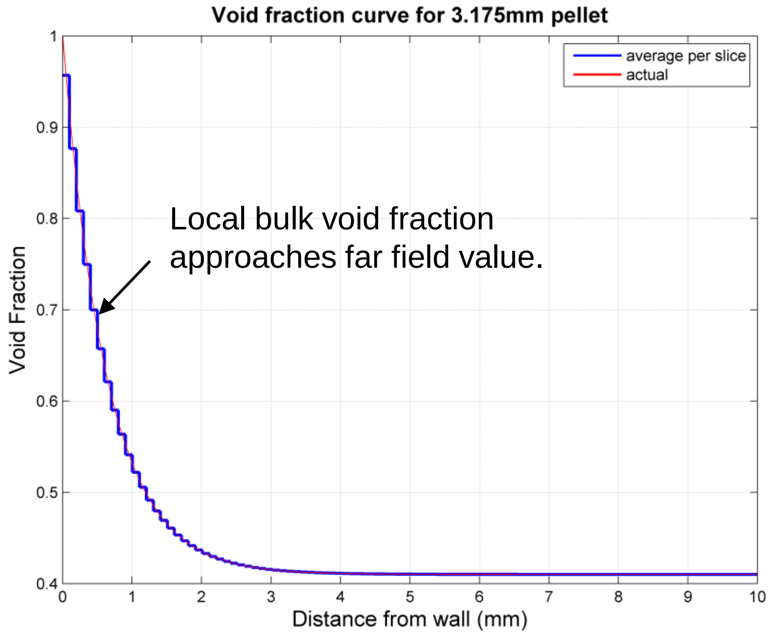


RCAP flow configuration during C to D transition.

Modeling Approach - Sorbent

- Sorbent = Finite Difference solid
  - Assumed free CO_2 in the bed to be static (e.g. no convection).
  - Follow approach in MSFC's Four Bed Molecular Sieve (4BMS-X) model to calculate 1) void fractions, and 2) conductance at bed/wall interfaces.[4]
  - Uniform bulk properties calculated with bed's bulk void fraction.
- Void fraction
  - $$\varphi_{local} = \varphi_\infty \left[1 + C \exp\left(-N \frac{y}{d_p}\right)\right]$$

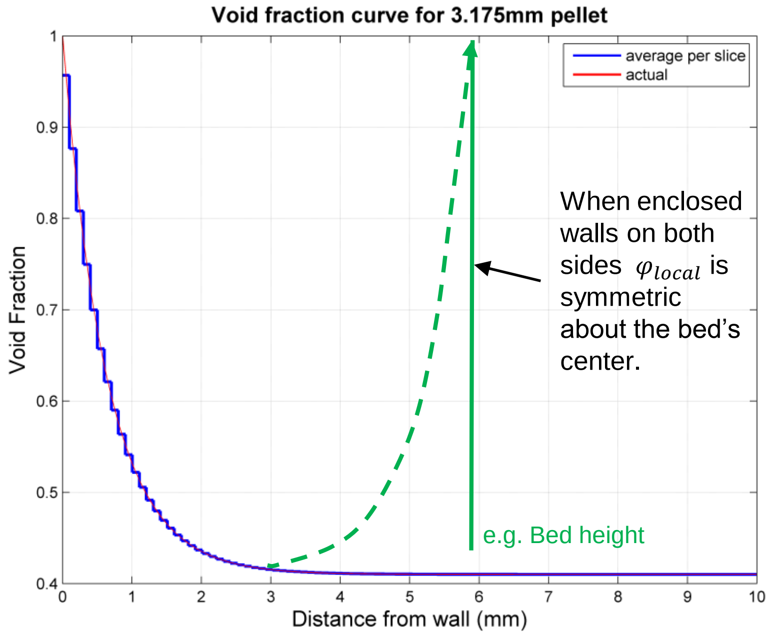
    where:
    - $\varphi = \frac{total\ volume\ of\ voids\ in\ bed}{total\ bed\ volume}$
    - $\varphi_\infty = far\ field\ bulk\ void\ fraction$
    - $y = distance\ from\ wall$
    - $d_p = pellet\ diameter$
    - $C = (1 - \varphi_\infty)/\varphi_\infty$
    - $N = emperical\ constant \sim 5$[5]



Bulk local void fraction vs. distance from a flat wall. Steps show average value at each 0.1mm slice.

Modeling Approach - Sorbent

- Bed properties
  - Bed is enclosed on both sides → bulk properties are for a specific height
  - Use upper bound thermal conductivity, k, estimate – treats heat flow as parallel through sorbent and gas.[5]
    - $k_{slice} = \varphi_{slice}\, k_{CO_2} + (1-\varphi_{slice})k_{sorbent}$
    - $k_{bulk} = \dfrac{\sum_{i=0}^{i=n_{slices}/2} k_{slice}}{\left(\frac{n_{slices}}{2}\right)}$
  - Density (volume averaged):
    - $\rho_{slice} = \varphi_{slice}\rho_{CO_2} + (1-\varphi_{slice})\rho_{sorbent}$
    - $\rho_{bulk} = \dfrac{\sum_{i=0}^{i=n_{slices}/2} \rho_{slice}}{\left(\frac{n_{slices}}{2}\right)}$
- Conductance at bed/wall interface
  - Use conductance, G, across slice nearest the wall. [4]
    - $G_{bed\ to\ flat\ surface} = \dfrac{k_{bed\ 1st\ slice}}{L_{slice}} \left[\dfrac{W}{m^2 K}\right]$



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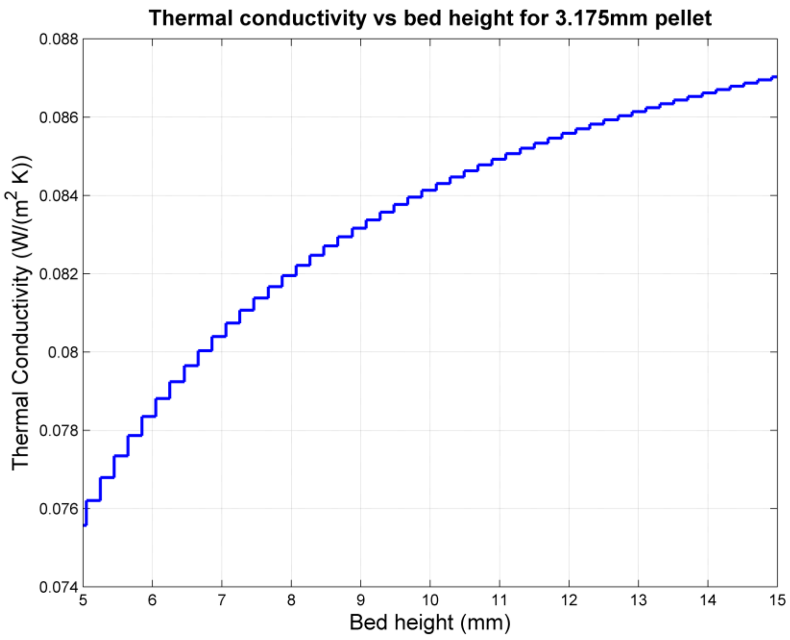

Bulk thermal conductivity vs bed height, used 0.1mm slices.

Model Approach - Sorbent

- Bed properties with Al shot
  - Bed is enclosed on both sides → bulk properties are for a specific height
  - Use upper bound thermal conductivity, k, estimate – treats heat flow as parallel through sorbent and gas.[5]
    - $k_{bed} = 0.5k_{al\ shot} + (1-0.5)k_{sorbent}$
    - $k_{slice} = \varphi_{slice}\, k_{CO_2} + (1-\varphi_{slice})k_{bed}$
    - $k_{bulk} = \dfrac{\sum_{i=0}^{i=n_{slices}/2} k_{slice}}{\left(\frac{n_{slices}}{2}\right)}$
  - Density (volume averaged):
    - $\rho_{bed} = 0.5\rho_{al\ shot} + (1-0.5)\rho_{sorbent}$
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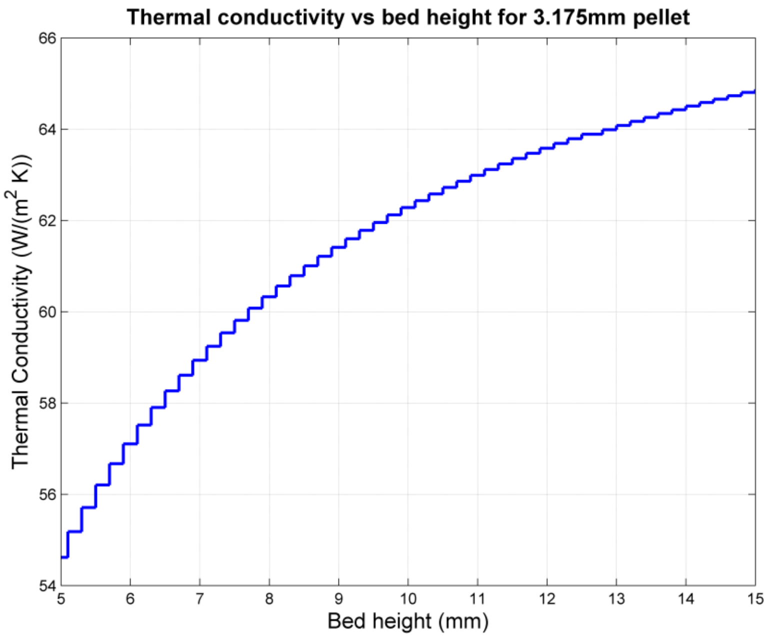


Bulk thermal conductivity vs bed height, used 0.1mm slices. The bed has 50% aluminum shot and 50% sorbent.

$$mass_{sorbent} = \frac{(1-0.5\rho_{al\ shot})}{\rho_{bed}} mass_{bed}$$

HT Fluid "Loop"

To account for chiller's cooling capacity or heater's heating capacity (fake a loop):

1) Calculate chiller and heater reservoir temperatures using max heating or cooling capacities.

2) Set inlet plenums to calculated reservoir temperature unless the chiller or heater's set point is exceeded. If a set point is surpassed, use the set point as the plenum's temperature.

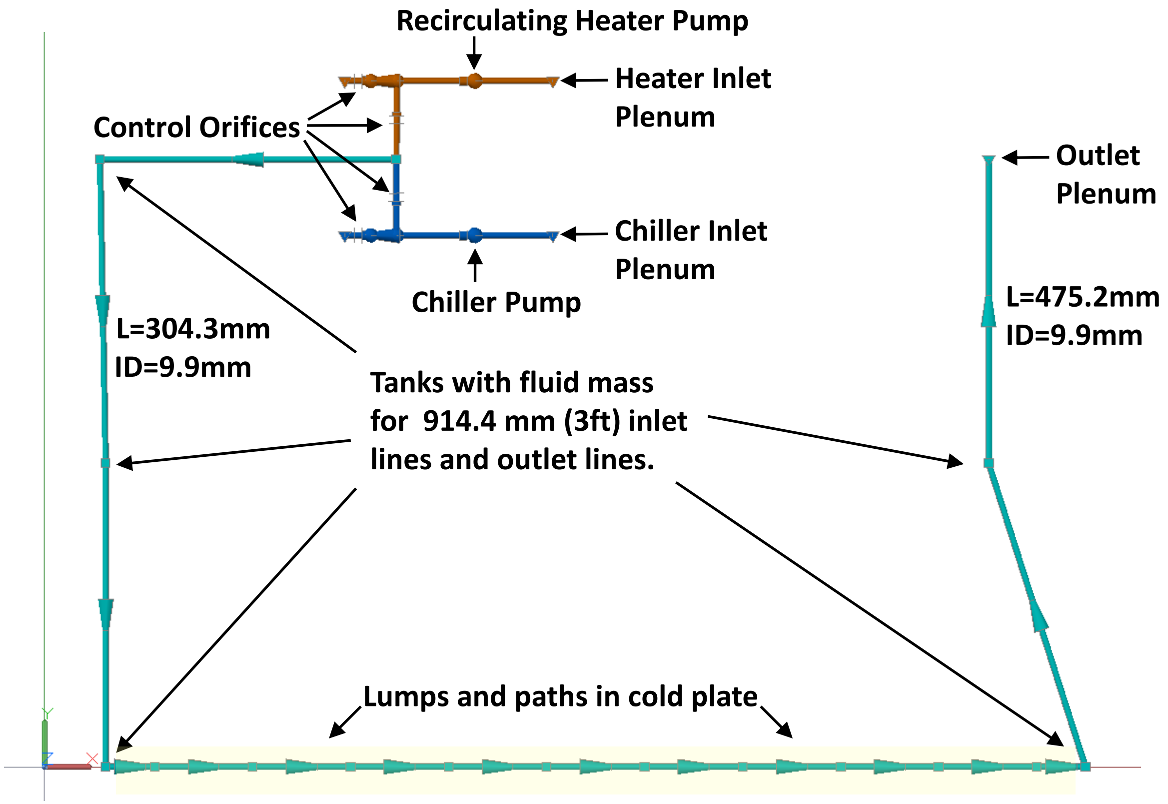
$$\frac{dU}{dt} = Q + \sum m_{in}h_{in} - \sum m_{in}h_{in}$$

$$mc_{p,res}\frac{dT}{dt} = Q + \dot{m}c_{p,avg}(T_{in} - T_{out})$$

$$mc_{p,res}\frac{\Delta T}{\Delta t} = Q + \dot{m}c_{p,avg}(T_{in,t-1} - T_{out,t-1})$$

$$\Delta T = \left(\frac{Q+\dot{m}c_{p,avg}(T_{in,t-1} - T_{out,t-1})}{mc_{p,res}}\right)\Delta t$$

$$T_{res} = T_{res,t-1} + \Delta T$$



RCAP Test Matrix

Test Matrix #	Purpose	MACS Press (torr)	MACS gas	Cold Bath Temp (°C)	Hot Bath Temp (°C)	HX flow rate (ml/min)	HX cycle time (min)
Checkout 1	Verify scroll pump operating procedures, determine bleed settings for Mars pressure, pump down	7	CO2, Mars	N/A	N/A	0	0
Checkout 2	Verify chiller / heater operation, valve operation, plumbing, flow meter, temperature change in RCAP	760	air	-20	95	?	?
Checkout 3	Verify isolation valve operation, pressure transducer, flow through mass flow meter, purging	760,7	air	N/A	N/A	0	0
Checkout 4	Run full adsorp / desorb, verify time to steady state, verify labview operation for cycle (Max bed size, 1/8" pellet)	7	CO2	-20	95	?	?
1	Max bed size, 1/8" pellet	7	CO2	-20	95	?	?
2	Mid bed size, 1/8" pellet	7	CO2	-20	95	?	?
3	Min bed size, 1/8" pellet	7	CO2	-20	95	?	?
4	Max bed size, 1/16" pellet	7	CO2	-20	95	?	?
5	Mid bed size, 1/16" pellet	7	CO2	-20	95	?	?
6	Min bed size, 1/16" pellet	7	CO2	-20	95	?	?
7	Max bed size, 600 mesh pellet	7	CO2	-20	95	?	?
8	Mid bed size, 600 meshpellet	7	CO2	-20	95	?	?
9	Min bed size, 600 mesh pellet	7	CO2	-20	95	?	?
10	Max bed size, 1/8" pellet	7	Mars	-20	95	?	?
11	Mid bed size, 1/8" pellet	7	Mars	-20	95	?	?
12	Min bed size, 1/8" pellet	7	Mars	-20	95	?	?
13	Max bed size, 1/16" pellet	7	Mars	-20	95	?	?
14	Mid bed size, 1/16" pellet	7	Mars	-20	95	?	?
15	Min bed size, 1/16" pellet	7	Mars	-20	95	?	?
16	Max bed size, 600 mesh pellet	7	Mars	-20	95	?	?
17	Mid bed size, 600 meshpellet	7	Mars	-20	95	?	?
18	Min bed size, 600 mesh pellet	7	Mars	-20	95	?	?