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 (~5% N$_2$, Ar$_2$)
  2. Send pressurized CO$_2$ to downstream processes in a Martian In-Situ Resource Utilization Plant.

Mars Atmosphere
95.3% CO$_2$, 2.7% N$_2$, 1.6% Ar
~0.69kPa to 0.90kPa
- 125 °C to 40 °C

CO$_2$: 3.0 to 6.0 kg/hr for O$_2$ only production\(^1\)
CO$_2$: 0.97 kg/hr for O$_2$/CH$_4$ production\(^1\)
~50kPa to 500kPa

Dust Filtration → Blower → RCAP → O$_2$ or O$_2$/CH$_4$ production

Vent N$_2$ & Ar

Overview of RCAP role in an ISRU Plant

H$_2$O from Regolith
(O$_2$/CH$_4$ Production)
Thermodynamic Model: Adsorption Pump

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

- **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

Idealized RCAP pump processes operated via temperature swing represented on a Pressure-Temperature diagram.\(^3\)
Single-Stage RCAP Test Hardware
Single-Stage RCAP Test Analysis parameters:

- Adsorption Temperature = −20 °C
- Inlet Pressure = 0.933 kPa
- Sorbent Heat Capacity [Ref 1]: $0.96 \frac{kJ}{kg \cdot K}$
• **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.
• Overview (cont.):
  – Implement adsorption/desorption via set mass flow rates of CO₂ 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) CO₂ flowing into and out of the gas passage.
• 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:

HT Fluid in

HT Fluid Out

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

AlSi10mg results:

HT Fluid in

HT Fluid Out

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).

Cooling time with enclosure and cold plate set to AISi10mg. 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 1/10\(^{th}\) CO\(_2\) production for full scale ISRU system.
RCAP Testing – Test Hardware

Porous Bed

Cold Plate, Heat transfer Fluid

Martian Atmosphere
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
    • N₂ (Barrier)
    • Ar (Barrier)

• Find Bed Regeneration Operational Procedure when N₂ and Ar builds up on Zeolite Adsorbent
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.
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 through them.
RCAP Revised Manufacture

RCAP Mechanical Design

Mars Gas Flow

SLS Rapid Prototyped Pump Housing (AlSi10Mg) [section view]

Silicone O-ring Seal

Al Baseplate Thermocouple Rake

Swagelok Fittings

Diffusion Bonded Cu Cold Plate [section view]

FDM Rapid Prototyped Covers (Onyx plastic)

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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

![Diagram of RCAP Vent and Compressor System]
RCAP - Closing Remarks

- Need To Improve Heat Transfer In The RCAP Porous Bed
  - Most Promising Idea Is To Add Al Shot As Conductive Paths
- 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


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-CO₂ gasses vent.
    - Adsorption occurs (CO₂ molecules bond to sorbent, e.g. zeolite) releasing heat.[²]
    - Sorbent bed is externally cooled to maintain a constant pressure.
    - State A’s temperature is called the adsorption temperature.
4 step cyclic process:
\[ A \rightarrow B: \text{Const. Volume Compression} \]
- 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.

Idealized TSA pump processes represented on a Pressure-Temperature diagram.\(^3\)
4 step cyclic process:

B → C: Isobaric Desorption

- Downstream valves 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.
• 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 CO₂ 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]
**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:
  - $\varphi = \frac{\text{total volume of voids in bed}}{\text{total bed volume}}$
  - $\varphi_{\infty} = \text{far field bulk void fraction}$
  - $y = \text{distance from wall}$
  - $d_p = \text{pellet diameter}$
  - $C = (1 - \varphi_{\infty}) / \varphi_{\infty}$
  - $N = \text{emperical constant} \sim 5^{[5]}$
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.$^5$
    • $k_{\text{slic}} = \varphi_{\text{slic}} k_{\text{CO}_2} + (1 - \varphi_{\text{slic}}) k_{\text{sorb}}$
    • $k_{\text{bulk}} = \frac{\sum_{i=0}^{n_{\text{slic}}/2} k_{\text{slic}}}{(n_{\text{slic}}/2)}$
  – Density (volume averaged):
    • $\rho_{\text{slic}} = \varphi_{\text{slic}} \rho_{\text{CO}_2} + (1 - \varphi_{\text{slic}}) \rho_{\text{sorb}}$
    • $\rho_{\text{bulk}} = \frac{\sum_{i=0}^{n_{\text{slic}}/2} \rho_{\text{slic}}}{(n_{\text{slic}}/2)}$

• Conductance at bed/wall interface
  – Use conductance, $G$, across slice nearest the wall.$^4$
    • $G_{\text{bed to flat surface}} = \frac{k_{\text{bed 1st slice}}}{L_{\text{slic}}} \left[ \frac{W}{m^2 K} \right]$
Model 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.\[^5\]
    - $k_{\text{slice}} = \phi_{\text{slice}} k_{CO_2} + (1 - \phi_{\text{slice}}) k_{\text{sorbent}}$
    - $k_{\text{bulk}} = \frac{\sum_{i=0}^{n_{\text{slices}}/2} k_{\text{slice}}}{\binom{n_{\text{slices}}}{2}}$
  - Density (volume averaged):
    - $\rho_{\text{slice}} = \phi_{\text{slice}} \rho_{CO_2} + (1 - \phi_{\text{slice}}) \rho_{\text{sorbent}}$
    - $\rho_{\text{bulk}} = \frac{\sum_{i=0}^{n_{\text{slices}}/2} \rho_{\text{slice}}}{\binom{n_{\text{slices}}}{2}}$

• **Conductance at bed/wall interface**
  - Use conductance, $G$, across slice nearest the wall. \[^4\]
    - $G_{\text{bed to flat surface}} = \frac{k_{\text{bed 1st slice}} L_{\text{slice}}}{W \left[ m^2 K \right]}$

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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]
    - $k_{\text{bed}} = 0.5k_{\text{al shot}} + (1 - 0.5)k_{\text{sorbent}}$
    - $k_{\text{slic}} = \varphi_{\text{slic}} k_{\text{CO}_2} + (1 - \varphi_{\text{slic}})k_{\text{bed}}$
    - $k_{\text{bulk}} = \frac{\sum_{i=0}^{\frac{n_{\text{slic}}}{2}} k_{\text{slic}}}{\frac{n_{\text{slic}}}{2}}$
  - Density (volume averaged):
    - $\rho_{\text{bed}} = 0.5\rho_{\text{al shot}} + (1 - 0.5)\rho_{\text{sorbent}}$
    - $\rho_{\text{slic}} = \varphi_{\text{slic}}\rho_{\text{CO}_2} + (1 - \varphi_{\text{slic}})\rho_{\text{bed}}$
    - $\rho_{\text{bulk}} = \frac{\sum_{i=0}^{\frac{n_{\text{slic}}}{2}} \rho_{\text{slic}}}{\frac{n_{\text{slic}}}{2}}$

- Conductance at bed/wall interface
  - Use conductance, $G$, across slice nearest the wall. [4]
    - $G_{\text{bed to flat surface}} = \frac{k_{\text{bed 1st slice}}}{L_{\text{slic}}} \left[ \frac{W}{m^2K} \right]$

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

$\text{mass}_{\text{sorbent}} = \frac{(1 - 0.5\rho_{\text{al shot}})}{\rho_{\text{bed}}} \text{mass}_{\text{bed}}$
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.

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

\[
m_{c_p,res} \frac{dT}{dt} = Q + \dot{m}_{c_p,avg}(T_{in} - T_{out})
\]

\[
m_{c_p,res} \frac{\Delta T}{\Delta t} = Q + \dot{m}_{c_p,avg}(T_{in,t-1} - T_{out,t-1})
\]

\[
\Delta T = \left( \frac{Q + \dot{m}_{c_p,avg}(T_{in,t-1} - T_{out,t-1})}{m_{c_p,res}} \right) \Delta t
\]

\[
T_{res} = T_{res,t-1} + \Delta T
\]
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<tr>
<th>Test Matrix #</th>
<th>Purpose</th>
<th>MACS Press (torr)</th>
<th>MACS gas</th>
<th>Cold Bath Temp (°C)</th>
<th>Hot Bath Temp (°C)</th>
<th>HX flow rate (ml/min)</th>
<th>HX cycle time (min)</th>
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<td>Checkout 1</td>
<td>Verify scroll pump operating procedures, determine bleed settings for Mars pressure, pump down</td>
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<td>Checkout 2</td>
<td>Verify chiller / heater operation, valve operation, plumbing, flow meter, temperature change in RCAP</td>
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<td>-20</td>
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<td>Checkout 3</td>
<td>Verify isolation valve operation, pressure transducer, flow through mass flow meter, purging</td>
<td>760,7</td>
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<td>Checkout 4</td>
<td>Run full adsorp / desorb, verify time to steady state, verify labview operation for cycle (Max bed size, 1/8&quot; pellet)</td>
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