Adsorption-based DAC

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**Adsorbent Selection: MOF Examples**

<table>
<thead>
<tr>
<th></th>
<th>MIL-101 (Cr)-PEI-800</th>
<th>mmen-Mg$_2$(dobpdc)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability under humid conditions</td>
<td>Stable</td>
<td>Stable</td>
</tr>
<tr>
<td>Equilibrium capacity at 400 ppm CO$_2$ concentration</td>
<td>1 mmol/g</td>
<td>3 mmol/g</td>
</tr>
<tr>
<td>Water capacity at 35% RH</td>
<td>8 mmol/g</td>
<td>6 mmol/g</td>
</tr>
<tr>
<td>DH$_{ads}$ (kJ/mol CO$_2$)</td>
<td>55 kJ/mol</td>
<td>70 kJ/mol</td>
</tr>
<tr>
<td>DH$_{ads}$ (kJ/mol H$_2$O)</td>
<td>[25-50] kJ/mol</td>
<td>[25-50] kJ/mol</td>
</tr>
</tbody>
</table>

N,N’-dimethyl ethylene diamine (mmen)
Support Structures

Monolithic contactors

- Lower pressure drop for high gas flow compared to packed bed
- High geometric surface area to create a MOF film on the surface
- Optimization of structural parameters required to maximize mass transfer rates at minimum pressure drop and parasitic thermal mass.
- Manufactured at scale for other applications

Fiber contactors

- Higher pressure drop than monoliths
- Greater adsorbent density per unit volume
- Thermal management with bore fluid
- Based on hollow fiber membrane technology

Monolith structural parameters

<table>
<thead>
<tr>
<th>Name</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monolith length</td>
<td>cm</td>
<td>30</td>
</tr>
<tr>
<td>Monolith cell density</td>
<td>cpsi</td>
<td>400</td>
</tr>
<tr>
<td>Channel outer radius ($R_3$)</td>
<td>μm</td>
<td>635</td>
</tr>
<tr>
<td>Monolith wall thickness ($R_3-R_2$)</td>
<td>μm</td>
<td>50</td>
</tr>
<tr>
<td>Adsorbent film thickness ($R_2-R_1$)</td>
<td>μm</td>
<td>60</td>
</tr>
</tbody>
</table>
Operational Scheme: Example VTSA

Step 1: Air
Step 2: Vacuum
Step 3: Closed end
Step 4: Steam
Step 5: Vacuum

Temperature Swing
Adsorption

O₂ sensitivity of adsorbent at high T
Concentration Profile Analysis

Adsorption step

Tradeoffs

Mass Transfer vs Pressure Drop
Sorbent Utilization vs Recovery

Balancing Mass Transfer Resistances

Reducing thermal parasitic
Concentration profile analysis

Desorption step

Heat quality

CO₂ adsorbed (mmol/g)

T_{ads}

T_{des}

p_{CO₂} (mbar)

Severity of vacuum

Alternatively External Heat Supply

Steam

Gaseous CO₂ concentration

Tradeoffs

- Rate of heating vs water management
- Swing capacity vs energy consumption
- Productivity vs energy consumption

Interaction of condensing water/adsorbent/CO₂

Reducing thermal parasitic
Cost and Energy Components

Capital Cost
- Adsorbent
- Blowers
- Vacuum pumps
- Monolith

Operating Cost
- Blowers
- Steam
- Vacuum Pump

Energy
- Enthalpy losses
- CO₂ desorption
- Vacuum pumps
- Uncondensed steam
Assumptions

- Adsorbent purchase cost is determined based on lab scale prices and then scaled up for bulk production cost.
- Lifetime of the adsorbent is assumed to be 1-3 years.
- Electrical and thermal energy are converted to primary energy for fair comparison. Steam energy is calculated based on equivalent work.

<table>
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<tr>
<th>Scale up factors (for primary energy conversion)</th>
<th></th>
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<tbody>
<tr>
<td>Electricity</td>
<td>3.14</td>
</tr>
<tr>
<td>Steam</td>
<td>1.20</td>
</tr>
</tbody>
</table>

\[ W_1 = W_2 \text{ Pay for the additional HP Steam} \]


Cost Analysis

MIL-101(Cr)-PEI-800: $95-160/t-CO₂
mmen-Mg₂(dobpdc): $75-200/t-CO₂

Clear drivers for non-toxic, low cost, high capacity, stable adsorbents with low water co-adsorption
Clear need for better methods to estimate adsorbent costs at scale.
Energy Analysis

- Energy generated on burning 1 mole of CH₂ to CO₂: 0.45 MJ/mol
- Theoretical minimum energy of unmixing: 0.02 MJ/mol
Back of the envelope energy analysis

If using NG: 254 kg CO$_2$/tonne CO$_2$ captured

- CHP
  - 100 kJe/mol CO$_2$
  - 100 kJth/mol CO$_2$

Energy mix is both electrical and thermal. Renewable electricity not necessarily most efficiently used.

- U.S. Electrical Generation
  - NG 2400 kWhe/Tonne emitted
  - Coal 1020 kWhe/Tonne emitted

- 21,000 TWh Global Electricity Consumption
  - (Datacenters 416 TWh in 2016)

- 631 kWhe/Tonne captured
- 631 TWhe/GT captured

Feed Concentration of CO$_2$

- Air Capture (400ppm)
  - $\sim 20$ kJ/mol CO$_2$

- Flue Gas Capture (10%)
  - $\sim 10$ kJ/mol CO$_2$

$\eta=10\%$

$200$ kJ/mol CO$_2$

Tonnes Captured /t released

Kwhe exported/t released

NG

Coal

1

1.6

1020

2400

631 kWhe/Tonne captured
Learning Curve acceleration

How do we drive down the cost at a given installed capacity?

Modular process designs with upgrade pathways (e.g. sorbent materials)

Rate of deployment

How do we identify and promote applications at different points on the adoption curve?

Early applications utilizing CO$_2$ maybe with small fractions or zero sequestration.

Co-location with power plant CC and EOR applications
Summary of broader solid adsorbent DAC study

• Broad analysis of solid adsorption for DAC – details not presented here
  • mid-range costs $[85 215]/tonne
  • mid-range energy requirements per tonne
    • $[500 1000]$ kWh$_e$
    • $[1000 1500]$ kWh$_{th}$
• Cost analysis very sensitive to cost of adsorbent
  • Manufacturing costs at scale are highly uncertain
  • Sorbent lifetime and degradation dynamics are not well understood in real operating conditions
• Energy analysis sensitive to sorbent properties and process design
  • Operational swing capacity
  • Balance between thermal and vacuum conditions
  • Parasitic load of contactor
Overall Summary

Market & technology analysis and development

- Understanding what niche applications and locations that can support early technology development is key.

Process design & integration

- Processes that balance complex tradeoffs between capital and energy efficiency
- Processes that can be operated flexibly to mitigate performance flaws
- Modular process designs that allow technology learning to be accelerated