Simulation Of Unique Pressure Changing Steps And Situations In PSA Processes

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A more rigorous cyclic adsorption process simulator is being developed for use in the development and understanding of new and existing PSA processes. Unique features of this new version of the simulator that Ritter and co-workers have been developing for the past decade or so include: multiple absorbent layers in each bed, pressure drop in the column, valves for entering and exiting flows and predicting real-time pressurization and depressurization rates, ability to account for choked flow conditions, ability to pressurize and depressurize simultaneously from both ends of the columns, ability to equalize between multiple pairs of columns, ability to equalize simultaneously from both ends of pairs of columns, and ability to handle very large pressure ratios and hence velocities associated with deep vacuum systems. These changes to the simulator now provide for unique opportunities to study the effects of novel pressure changing steps and extreme process conditions on the performance of virtually any commercial or developmental PSA process.

This presentation will provide an overview of the cyclic adsorption process simulator equations and algorithms used in the new adaptation. It will focus primarily on the novel pressure changing steps and their effects on the performance of a PSA system that epitomizes the extremes of PSA process design and operation. This PSA process is a sorbent-based atmosphere revitalization (SBAR) system that NASA is developing for new manned exploration vehicles.

This SBAR system consists of a 2-bed 3-step 3-layer system that operates between atmospheric pressure and the vacuum of space, evacuates from both ends of the column simultaneously, experiences choked flow conditions during pressure changing steps, and experiences a continuously changing feed composition, as it removes metabolic CO₂ and H₂O from a closed and fixed volume, i.e., the spacecraft cabin. Important process performance indicators of this SBAR system are size, and the corresponding CO₂ and H₂O removal efficiencies, and N₂ and O₂ loss rates. Results of the fundamental behavior of this PSA process during extreme operating conditions will be presented and discussed.
Simulation of Unique Pressure Changing Steps and Situations in PSA Processes

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Introduction

1. Rigorous cyclic adsorption process simulator (Ddaspk-Fortran) being developed to assist in the design, development and understanding of new and existing PSA processes.

2. Unique features of this simulator include:
   - Multiple absorbent layers and columns
   - Pressure drop in the column
   - Entering and exiting flows defined by constant flow, valve equations, or choke flow approaches (Isentropic, Fanno, etc.)
   - Interaction with other processes: cabin, distillation units, etc.
   - Simultaneous feed, exit, pressure varying steps through multiple ports
   - Ability to handle large P ratios and v’s associated with deep vacuum systems.
   - Equalization between pairs of columns (single and dual ended) in progress.

These features provide for unique opportunities to study the performance of virtually any commercial or developmental PSA process under extreme process conditions.
Objectives

- Focus primarily on a particular PSA system that NASA is developing: referred to as the sorbent-based atmosphere revitalization (SBAR) system

  - **this PSA system is unique because it uses deep space vacuum for regeneration in lieu of processed air as purge**

- Describe NASA’s PSA System, with emphasis on the alternative regenerative steps that NASA has developed to further improve performance: single, dual, and triple ended blowdown
- Show validation of the PSA process simulator against NASA’s experimental data of an 8.8 L dual blowdown system
- Use the simulator to discuss the role of these regenerative steps on PSA performance in terms of $\text{H}_2\text{O}$ and $\text{CO}_2$ removal efficiencies

This SBAR system might be used in a new Crew Exploration Vehicle (CEV) to remove metabolic $\text{H}_2\text{O}$ and $\text{CO}_2$ from cabin air.
Schematic of Base Case Column Simulated for Water and Carbon Dioxide Removal from Cabin Air

MSFC SBAR Experimental System

- \( V_b = 8.88 \text{ L} \)
- \( L_b = 0.2654 \text{ m} \)
- \( r_b = 0.1032 \text{ m} \)
- \( \text{HCT} = 450 \text{ s} \)

- Zeolite 13X
- Zeolite 5A

\[ F (10-14.5 \text{ SCFM}) \]

\[ LP \]

\[ 2.357 \text{ kg} \]  
\[ 34\% \]

\[ 4.062 \text{ kg} \]  
\[ 66\% \]
Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization

**SBAR Cycle Step Times**
- $t_F = 420$ s
- $t_{SEB} = 30$ s
- $t_{SEB} = 420$ s
- $t_{FP} = 30$ s

SEB: single ended blowdown
Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization

FP | SEB
---|---

To Cabin

FP | DEB
---|---

To Space

SBAR Cycle Step Times

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>FP</td>
<td>F</td>
</tr>
<tr>
<td>SEB</td>
<td>DEB</td>
</tr>
<tr>
<td>FP</td>
<td>F</td>
</tr>
</tbody>
</table>

Time

**SBAR Cycle Step Times**

- \( t_F = 420 \text{ s} \)
- \( t_{SEB} = 30 \text{ s} \)
- \( t_{DEB} = 420 \text{ s} \)
- \( t_{FP} = 30 \text{ s} \)

SEB: single ended blowdown
DEB: dual ended blowdown
Schematic Diagram and Cycle Sequencing of VSA Cycle Used for Air Revitalization

**FP** SEB

<table>
<thead>
<tr>
<th><strong>SEB</strong></th>
<th><strong>FP</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>PL</strong></td>
<td><strong>PH</strong></td>
</tr>
<tr>
<td><strong>PH</strong></td>
<td><strong>PL</strong></td>
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</table>

**TEB**

<table>
<thead>
<tr>
<th><strong>TEB</strong></th>
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</thead>
<tbody>
<tr>
<td><strong>PH</strong></td>
</tr>
<tr>
<td><strong>PH</strong></td>
</tr>
<tr>
<td><strong>PL</strong></td>
</tr>
</tbody>
</table>

Bed 1

1: FP F SEB TEB
2: SEB TEB FP F

**SBAR Cycle Step Times**

- $t_F = 420$ s
- $t_{SEB} = 30$ s
- $t_{TEB} = 420$ s
- $t_{FP} = 30$ s

**SEB**: single ended blowdown

**TEB**: triple ended blowdown
## Simulator Input

### Bed Characteristics and Transport Properties

**MSFC SBAR Experimental System**

<table>
<thead>
<tr>
<th></th>
<th>13X</th>
<th>5A</th>
</tr>
</thead>
<tbody>
<tr>
<td>bed layer fraction (%)</td>
<td>66%</td>
<td>34%</td>
</tr>
<tr>
<td>porosity</td>
<td>0.26</td>
<td>0.35</td>
</tr>
<tr>
<td>pellet density (kg m(^{-3}))</td>
<td>1100</td>
<td>1201</td>
</tr>
<tr>
<td>heat capacity (kJ kg(^{-1}) K(^{-1}))</td>
<td>1.10</td>
<td>0.84</td>
</tr>
<tr>
<td>heat transfer coefficient (kW m(^{-2}) K(^{-1}))(^{a})</td>
<td>0.0017</td>
<td>0.0017</td>
</tr>
<tr>
<td>mass transfer coefficients (s(^{-1}))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>H(_{2})O</td>
<td>0.00550</td>
<td>0.00310</td>
</tr>
<tr>
<td>CO(_{2})</td>
<td>0.00150</td>
<td>0.00067</td>
</tr>
<tr>
<td>O(_{2})</td>
<td>0.001</td>
<td>0.001</td>
</tr>
<tr>
<td>N(_{2})</td>
<td>0.001</td>
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</tr>
<tr>
<td>(r_{p,eff} b) (mm)</td>
<td>3.3</td>
<td>2.1</td>
</tr>
</tbody>
</table>
Motivation: Single vs Dual Ended Blowdown

Pressure profiles @ End of Blowdown Step

Single

Dual

15 SCFM
Motivation: Single vs Dual Ended Blowdown
Cycle Performance Parameters Zeolite System

15 SCFM

Single

- H2O, Blowdown Heavy End
- CO2, Blowdown, Heavy End
- CO2, Light Product
- H2O, Bed Accumulation

Dual

- H2O, Blowdown Heavy End
- H2O, Blowdown, Light End
- CO2, Blowdown, Heavy End
- CO2, Blowdown, Light End
- CO2, Light Product
- H2O, Bed Accumulation
- CO2, Bed Accumulation

Time (hr)
Modeling the SBAR DEB Experimental System
Temperature History Profiles at Three Bed Locations

120 h
F = 13.5 SCFM
V_b = 8.88 L
HCT = 450 s
t_F = 420 s
t_SEB = 30 s
t_DEB = 420 s
t_FP = 30 s

time (min)

Cycles 481-482
Modeling the SBAR DEB Experimental System
Pressure History Profiles at Three Bed Locations

120 h
F = 13.5 SCFM
V_b = 8.88 L
HCT = 450 s
t_F = 420 s
t_SEB = 30 s
t_DEB = 420 s
t_FP = 30 s

Cycles 481-482
Modeling the SBAR DEB Experimental System

$P_{CO_2}$ History Profiles at Two Bed Locations

120 h

$F = 13.5 \text{ SCFM}$

$V_b = 8.88 \text{ L}$

HCT = 450 s

$t_F = 420 \text{ s}$

$t_{SEB} = 30 \text{ s}$

$t_{DEB} = 420 \text{ s}$

$t_{FP} = 30 \text{ s}$

---

Cycles 481-482

\[ z = 0.00 \quad \text{exp, } z = 0.00 \]

\[ z = 1.00 \quad \text{exp, } z = 1.00 \]
Modeling the SBAR DEB Experimental System
Bed Profiles at End of Steps for P, T, P_{H2O} and P_{CO2}

120 h

F = 13.5 SCFM
V_b = 8.88 L
HCT = 450 s
\(t_F\) = 420 s
\(t_{SEB}\) = 30 s
\(t_{DEB}\) = 420 s
\(t_{FP}\) = 30 s
### Modeling the SBAR DEB Experimental System

#### Summary of Modeling vs Experimental Results of Eight Different Test Runs

<table>
<thead>
<tr>
<th>Test Point</th>
<th>Experimental Conditions</th>
<th>Experimental Results</th>
<th>Modeling Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Bed Size, L</td>
<td>Half Cycle Time, min</td>
<td>DED Time, min</td>
</tr>
<tr>
<td>12</td>
<td>8.88</td>
<td>7.5</td>
<td>7.0</td>
</tr>
<tr>
<td>18</td>
<td>8.88</td>
<td>7.5</td>
<td>7.0</td>
</tr>
<tr>
<td>20</td>
<td>8.88</td>
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<td>23</td>
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<tr>
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<tr>
<td>43</td>
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<td>6.0</td>
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<tr>
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<td>8.88</td>
<td>7.5</td>
<td>6.0</td>
</tr>
<tr>
<td>54</td>
<td>8.88</td>
<td>7.5</td>
<td>6.0</td>
</tr>
</tbody>
</table>
### Modeling the SBAR DEB Experimental System

**Summary of Modeling vs Experimental Results of Eight Different Test Runs: \( \text{H}_2\text{O} \) Removal**

<table>
<thead>
<tr>
<th>Test Point</th>
<th>Experimental Conditions</th>
<th>Experimental Results</th>
<th>Modeling Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Bed Size L</td>
<td>Half cycle Time min</td>
<td>DED Time min</td>
</tr>
<tr>
<td>12</td>
<td>8.88</td>
<td>7.5</td>
<td>7.0</td>
</tr>
<tr>
<td>18</td>
<td>8.88</td>
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<tr>
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<td>7.5</td>
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</tr>
<tr>
<td>42</td>
<td>8.88</td>
<td>7.5</td>
<td>6.0</td>
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<tr>
<td>43</td>
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<td>7.5</td>
<td>6.0</td>
</tr>
<tr>
<td>52</td>
<td>8.88</td>
<td>7.5</td>
<td>6.0</td>
</tr>
<tr>
<td>54</td>
<td>8.88</td>
<td>7.5</td>
<td>6.0</td>
</tr>
</tbody>
</table>
Modeling the SBAR DEB Experimental System
Summary of Modeling vs Experimental Results of Eight Different Test Runs

**CO₂ Removal**

**Cycle Bed Temperatures**

- Maximum
- Minimum

\( Z/L = 0.5 \)
Triple Ended Blowdown

Effect of Location of Third Exhaust Port

Test Run 18

\[
\begin{align*}
F &= 13.5 \text{ SCFM} \\
V_b &= 8.88 \text{ L} \\
HCT &= 450 \text{ s} \\
t_F &= 420 \text{ s} \\
t_{SED} &= 30 \text{ s} \\
t_{DED} &= 420 \text{ s} \\
t_{FP} &= 30 \text{ s}
\end{align*}
\]

Third Port Location

\[
z/L = 0.2, 0.3, 0.4, \text{ or } 0.5
\]
Triple vs Dual Ended Blowdown
Bed Pressure Profiles at the End of the Blowdown step

Significant Increase of Driving Force
Triple vs Dual Ended Blowdown
History of $\text{H}_2\text{O}$ and $\text{CO}_2$ Removal Per Cycle

DUAL

Triple, $z/L=0.50$

[Graph showing comparative removal of $\text{H}_2\text{O}$ and $\text{CO}_2$ for DUAL and Triple systems over time.]
Triple vs Dual Ended Blowdown
History of H$_2$O and CO$_2$ Removal Per Cycle

DUAL

Triplet, $z/L=0.40$

![Graph showing the removal of H$_2$O and CO$_2$ over time for both DUAL and Triple systems.](attachment:image.png)
Triple vs Dual Ended Blowdown
History of H$_2$O and CO$_2$ Removal Per Cycle

DUAL

Triple, z/L=0.30

Fraction of Feed (%) vs Time (hr)

H$_2$O, Blowdown Heavy End
CO$_2$, Blowdown, Heavy End
CO$_2$, Light Product
CO$_2$, Blowdown, Light End
Triple vs Dual Ended Blowdown
History of H₂O and CO₂ Removal per Cycle

DUAL

Triple, $z/L=0.20$

![Graph showing the comparison of H₂O and CO₂ removal in single and dual ended blowdown systems.](image-url)
## Triple vs Dual Ended Blowdown

### H₂O and CO₂ Removal after 120 hr

### Optimal Third Port Location

<table>
<thead>
<tr>
<th>Test Point</th>
<th>Conditions</th>
<th>Modeling Results</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Third Port Location, L</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Third Port location zL</td>
<td>CO₂ Removal, L/h</td>
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<tr>
<td>18 Triple</td>
<td></td>
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<tr>
<td>0.5</td>
<td>8.88 7.5 7.0 5.0</td>
<td>0.50</td>
</tr>
<tr>
<td>0.4</td>
<td>8.88 7.5 7.0 5.0</td>
<td>0.53</td>
</tr>
<tr>
<td>0.3</td>
<td>8.88 7.5 7.0 5.0</td>
<td>0.55</td>
</tr>
<tr>
<td>0.2</td>
<td>8.88 7.5 7.0 5.0</td>
<td>0.54</td>
</tr>
</tbody>
</table>

- Table includes columns for Bed Size, L, Half Cycle Time, min, DED Time, min, TED Time, min, Inlet pCO₂, torr, Inlet pH₂O, torr, Flow Rate, scfm, Inlet Temp, degF, CO₂ Removal, L/h, CO₂ Removal Eff, H₂O Removal Eff.
- Values for 18 Triple: 8.88 7.5 7.0 5.0.
- Values for 0.5: 8.88 7.5 7.0 5.0.
- Values for 0.4: 8.88 7.5 7.0 5.0.
- Values for 0.3: 8.88 7.5 7.0 5.0.
- Values for 0.2: 8.88 7.5 7.0 5.0.
Conclusions

- A description of the new NASA SBAR PSA system for H₂O and CO₂ removal, with particular emphasis on its purgeless deep vacuum regenerative steps has been given.

- Regeneration consisted of blowdown steps subject to deep vacuum through an increasing number of evacuation ports, i.e., single, dual and triple ended blowdown was studied.

- The USC PSA process simulator, for which adsorbent and adsorbate properties were independently obtained, successfully predicted NASA’s experimental results of a dual ended system.

- The USC PSA process simulator was also used to discern the role of the regenerative steps on the performance of NASA’s SBAR PSA system.

The USC PSA process simulator is currently being used in other projects of equal complexity.
Acknowledgements

Funding being provided by the NASA MSFC is greatly appreciated!

Thank You!