MODELING THE EFFECTS OF ADDING GRAPHITE FLAKES TO FAM-Z02 IN AN ADSORBER BED

Mahdi Nemati Mehr
Amir Sharafian
Khorshid Fayazmanesh
Wendell Huttema
Majid Bahrami

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Objectives

• Developing a CFD model to predict system performance under different operational conditions

• Understanding heat and mass transfer inside the adsorber bed

• Performing a comprehensive parametric study to see the effects of different parameters on the performance of the adsorption cooling system

• Studying the effects of graphite flakes additive to the adsorbent on the ACS performance

• Investigating the impact of using graphite-based heat exchangers as the adsorber bed
The U.S. consumed about 140.43 billion liters of fuel a year for AC systems of light duty vehicles in 2015\textsuperscript{[1]}. During the SFTP-SC03 driving cycle, a vapor compression refrigeration cycle of light-duty vehicle results in increasing\textsuperscript{[2]}:

- CO emissions by 71%
- NOx emissions by 81%
- Non-methane hydrocarbons by 30%

\textsuperscript{[1]} Independent Statistics and Analysis, How much gasoline does the United States consume?, US Energy Information Administration (EIA), March 2016
### Schematic of Experimental Test Setup

**Parameter** | **Value**  
--- | ---  
Working pairs | FAM Z02 – water  
Heating fluid inlet temperature | 90°C  
Cooling fluid inlet temperature | 30°C  
Coolant fluid inlet temperature | 20°C  
Chilled water inlet temperature | 20°C  
Heat transfer fluid mass flow rate to adsorber bed | Not measured  
Heat transfer fluid | Silicone oil
Literature Review

<table>
<thead>
<tr>
<th>Working pairs</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zeolite - Water</td>
<td>[1][2][3][4][5][6][7][8][9]</td>
</tr>
<tr>
<td>Silica gel – Water</td>
<td>[9][10][11][12][13]</td>
</tr>
<tr>
<td>Ammonia - Activated Carbon</td>
<td>[2]</td>
</tr>
<tr>
<td>Ethanol – Activated Carbon</td>
<td>[13]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Geometry</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D</td>
<td>[1][2][3][4][5][11]</td>
</tr>
<tr>
<td>2D</td>
<td>[6][7][8][9][10][12]</td>
</tr>
<tr>
<td>3D</td>
<td>[13][14]</td>
</tr>
</tbody>
</table>

Gaps in literature:

- FAM-Z02 as working pair
- Few 3D models
- No models with effects of thermal contact resistance (TCR)

Assumptions:

- Ideal gas behavior for adsorbate gas [1-14]
- Uniformly sized spherical particles [1-14]
- Constant thermo-physical properties for materials (except density of adsorbate) [1-14]
- Thermal equilibrium between particles and adsorbate [1-14]
- Thermal contact resistance

Numerical Tool:

- ANSYS Fluent was used to solve the Navier-Stokes, energy, and uptake equations
- User defined scalar (UDS) module was used in order to simulate uptake rate ($\omega$)
- Mass generation, heat generation, and scalar generation were simulated using user defined functions (UDF)
Governing Equations

- **Continuity**

\[
\frac{\partial (\varepsilon \rho_{\text{refrigerant}})}{\partial t} + \nabla \cdot (\rho_{\text{refrigerant}} \vec{v}) + (1 - \varepsilon) \rho_{\text{adsorbent}} \frac{d\omega}{dt} = 0
\]

- **Momentum**

\[
\frac{\partial (\rho \vec{v})}{\partial t} + \nabla \cdot \left( \frac{\rho \vec{v} \vec{v}}{\varepsilon} \right) = -\varepsilon \nabla p + \nabla \cdot (\vec{\tau}) - \left( \frac{\varepsilon \mu}{K} \vec{v} + \frac{\varepsilon C_v}{2} \rho |\vec{v}| \vec{v} \right)
\]

\[
\vec{\tau} = \mu \left[ (\nabla \vec{v} + \nabla \vec{v}^T) - \frac{2}{3} \nabla |\vec{v}| \right]
\]

- **Energy**

\[
\left[ \rho_{\text{adsorbent}} \left( (1 - \varepsilon) C_{p,\text{adsorbent}} + \omega \varepsilon C_{p,\text{refrigerant}} \right) \right] \frac{\partial T}{\partial t} + \vec{V} \left( \rho_{\text{refrigerant}} \vec{v} C_{p,\text{refrigerant}} T \right) = (1 - \varepsilon) \rho_{\text{adsorbent}} \Delta h_{\text{adsorption}} \frac{d\omega}{dt} + \vec{V} \left( k \nabla T \right)
\]
Governing Equations

• Uptake

\[ \omega = \frac{\text{mass of adsorbed material (kg of adsorbate)}}{\text{mass of adsorbent (kg of adsorbent)}} \]

\[ \frac{d\omega}{dt} = \frac{15D_{s0}}{R_p^2} \exp\left( -\frac{E_a}{R_u T_{adsorbent}} \right) \left( \omega_{eq} - \omega \right) \quad \text{[1]} \]

\[ \omega_{eq} = f(T, p) \]

\[ \omega_{eq} = \frac{\sum_{j=1}^{n_j} \left( \frac{K^0 P}{P^0} \right)^j \exp\left( -\frac{\Delta h_j}{RT} \right) / (j-1)!}{1 + \sum_{j=1}^{n_j} \left( \frac{K^0 P}{P^0} \right)^j \exp\left( -\frac{\Delta h_j}{RT} \right) / (j)!} \quad \text{water-FAMZ02 [2]} \]

\[ \omega_{eq} = \frac{k_0 p \exp\left( \frac{\Delta h}{RT} \right)}{\left[ 1 + \left( \frac{k_0 p \exp\left( \frac{\Delta h}{RT} \right)}{\omega_{max}} \right)^{\frac{1}{n}} \right]^{\frac{1}{n}}} \quad \text{water-silica gel [1]} \]

Thermal Contact Resistance (TCR)

\[ \delta + 2\delta_{TCR} \]

\[ k_{yy} = k_{ads} \]
\[ k_{xx} = k_{zz} = 0 \]
\[ \rho = c_p = 0 \]

\[ k_{yy} = k_{ads} \]
\[ k_{xx} = k_{zz} = 0 \]
\[ \rho = c_p = 0 \]
HEX and Vacuum Chamber Arrangement

- Heat transfer fluid
- Vacuum chamber wall
- Gap between HEX and vacuum chamber
- Front View
- Side View
- Adsorbent
- HEX fin
- TCR
Initial and Boundary Conditions

Initial Conditions:

- The final solution does not depend on initial conditions due to cyclic operation of ACSs.
- Incorrect initial conditions can result in divergence (esp. for pressure)

Boundary Conditions:

- Pressure at outlet / inlet → Represents pressure at evaporator / condenser
- Temperature at outlet / inlet → Representative for temperature of vapor coming from (or going to) at evaporator (condenser)
- Temperature at heat exchanger walls → Represents temperature of heating/cooling fluid
Results – Equilibrium Uptake

Adsorption

Desorption

Water Uptake % (kg/kg)

Time (min)

Experimental

Numerical

Water Uptake % (kg/kg)

Time (min)

Numerical

Experimental
Δω: the difference between the maximum and the minimum values of the uptake
Graphite Doped Adsorbent

- 0% graphite
- 5% graphite
- 10% graphite
- 20% graphite

Δω (kg/kg) vs. Cycle time (s)
Conclusions and Future Works

Conclusions

• A full three-dimensional finite volume based computational fluid dynamic model was developed.

• It was shown that if thermal conductivity improvement is performed by adding some non-adsorptive material like graphite, it could decrease the adsorption performance of the adsorber bed.

Future Works

• Adding the effects of uptake value on thermo-physical properties of an adsorbent.

• Studying the effects of the ideal evaporator and condenser.
THANK YOU!

Q&A
Boundary Conditions

Rectangular Wave (Ideal Case)

Trapezoidal Wave

Fourier Series of Rectangular Wave

Actual Case
Graphite HEX vs. Aluminum HEX

- **Fin**
- **TCR**
- **Adsorbent**

Dimensions:
- 3 mm
- 10 mm
- 20 mm
- 50 mm
- 1 mm
- 0.7 mm
- 0.6 mm
Graphite HEX vs. Aluminum HEX
Boundary Conditions

- Temperature
- Pressure

Graph showing the variation of temperature and pressure over time.
Results - Graphite HEX vs. Aluminum HEX

The graph shows the uptake percentage (kg/kg) over time (s) for both Aluminum and Graphite HEX. The data indicates:

- Aluminum:
  - 1.58% at 300 s
  - 2.06% at 150 s

- Graphite:
  - 2.21% at 300 s
  - 2.39% at 600 s

The graph highlights the differences in uptake efficiency between the two materials.
## Results - Graphite HEX vs. Aluminum HEX

<table>
<thead>
<tr>
<th>Cycle Time (s)</th>
<th>$\Delta \omega$ with Aluminum HEX (SCP)</th>
<th>$\Delta \omega$ with Graphite HEX (SCP)</th>
<th>Enhancement of $\Delta \omega$</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>1.58 % (132)</td>
<td>2.02 % (168)</td>
<td>31 %</td>
</tr>
<tr>
<td>480</td>
<td>3.11 % (161)</td>
<td>3.56 % (185)</td>
<td>15.7 %</td>
</tr>
<tr>
<td>600</td>
<td>4.12 % (171)</td>
<td>4.62 % (192)</td>
<td>12.1 %</td>
</tr>
<tr>
<td>900</td>
<td>6.57 % (154)</td>
<td>7.05 % (175)</td>
<td>7.3 %</td>
</tr>
</tbody>
</table>
Vapor Compression Refrigeration (VCR) vs. Adsorption Cooling System (ACS)

\[ \dot{Q}_{ih} + \dot{Q}_{ibd} = \dot{W}_{comp} \]

**Symbols:**
- \( \dot{Q}_{ih} \): isosteric heating
- \( \dot{Q}_{ibd} \): isobaric desorption
- \( \dot{Q}_{ic} \): isosteric cooling
- \( \dot{Q}_{iba} \): isobaric adsorption

**Components:**
- Evaporator
- Condenser
- Adsorber beds
- Expansion valve
- Compressor

**Equation:**

\[ \dot{Q}_{evap} = \dot{Q}_{cond} = \dot{Q}_{ic} + \dot{Q}_{iba} \]
ACS Working Pairs

ACS sorbent material (adsorbent):
- Activated carbon [6]
- Silica gel [7]
- Zeolite [8]

ACS refrigerant (adsorbate):
- Water
- Methanol
- Ethanol
- Ammonia

LDF model:
\[
\frac{\partial \omega}{\partial t} = K(\omega_{eq} - \omega)
\]
\[
\omega_{eq} = F(T, P)
\]

How to improve adsorption cycle

- Adsorbate/Adsorbent Pair
  - Material
  - Physical shape (consolidated, powder, pelletized particles)

- Heat Exchanger Design
  - Dimensions
  - Weight
  - Mass transfer resistance

- Thermodynamic cycle
  - Heat Recovery
  - Mass Recovery
  - Heat and Mass Recovery
  - Temperature range
    - Heat source (Exhaust gas, Coolant)
    - Refrigerant
Adsorption Concepts

Adsorption is the adhesion of atoms, ions, or molecules of gas, liquid, or dissolved solids to a solid surface.

<table>
<thead>
<tr>
<th>Adsorbents</th>
<th>Adsorbates</th>
</tr>
</thead>
<tbody>
<tr>
<td>silica gel</td>
<td>water</td>
</tr>
<tr>
<td>zeolite</td>
<td>methanol/ethanol</td>
</tr>
<tr>
<td>activated carbon</td>
<td>ammonia</td>
</tr>
<tr>
<td>FAM-Z02</td>
<td></td>
</tr>
</tbody>
</table>

Two main processes:

- **Cooling → Adsorption → Evaporation at evaporator**
- **Heating → Desorption → Condensation at condenser**

Uptake: \[ \omega = \frac{\text{mass of adsorbed material}}{\text{mass of adsorbent}} \] \( \frac{\text{kg of adsorbate}}{\text{kg of adsorbent}} \)
Advantages of ACS [1,2]:

- Utilization of waste heat
- Few moving parts (valves) ⇒ less maintenance is required
- Non toxic materials
- Environmental friendly refrigerants

Major challenges facing commercialization of ACS [2,3]:

- Low working pressure in many cases (1 kPa – 7kPa for the case of water)
- Small specific cooling power values
- Small COP values
- Bulky and heavy systems

\[
SCP = \frac{Q_{evap}}{m_{ads} \tau_{cyc}} \quad 10<\text{typ.}<270
\]

\[
COP = \frac{Q_{evap}}{Q_{ih} + Q_{ibd}} \quad 0.02<\text{typ.}<0.6
\]

Adsorber Bed Designs

- Spiral plate
- Shell and tube
- Finned tube
- Plate
- Hairpin
- Annulus tube
- Plate-tube
- Tube
- Plate fin
## Literature Review on Mass Measurement

<table>
<thead>
<tr>
<th>Mass of adsorbent</th>
<th>Reference</th>
<th>Working pair</th>
</tr>
</thead>
</table>
silica gel + CaCl₂ (SWS-1L)-water  
FAM-Z02-water  
zeolite-water  
activated carbon-methanol |
| 1 g < mass of adsorbent < 100 g | [10] [10] [11] [8] [12] [13] [9] [14] | silica gel-water  
silica gel + CaCl₂ (SWS-1L)-water  
zeolite-water  
SAPO 34-water |
| 100 g < mass of adsorbent < 1 kg | [15] [16] | zeolite 13X-water  
FAM-Z02-water |
| 1 kg < mass of adsorbent | [17] [17] [16] | silica gel-water  
zeolite-water  
FAM-Z02-water |

# Adsorber Bed Design – 3 fin per inch – Design I

## Design Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of supply pipes</td>
<td>1</td>
</tr>
<tr>
<td>Supply pipes size</td>
<td>1/2 in</td>
</tr>
<tr>
<td>No. of return pipes</td>
<td>6</td>
</tr>
<tr>
<td>Return pipes size</td>
<td>3/8 in</td>
</tr>
<tr>
<td>No. of fins</td>
<td>17</td>
</tr>
<tr>
<td>Fin spacing</td>
<td>9 mm</td>
</tr>
<tr>
<td>Fin diameter</td>
<td>6 in</td>
</tr>
<tr>
<td>Fin thickness</td>
<td>1/16 in</td>
</tr>
<tr>
<td>Fin material</td>
<td>Copper</td>
</tr>
</tbody>
</table>

## Working Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle time</td>
<td>60 – 90 – 120 – 180 min</td>
</tr>
<tr>
<td>Mass of adsorbent</td>
<td>0.620 kg</td>
</tr>
</tbody>
</table>
### Design Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. of passes</td>
<td>1</td>
</tr>
<tr>
<td>Branch pipes size</td>
<td>½ in</td>
</tr>
<tr>
<td>Fitting Size</td>
<td>¾ in</td>
</tr>
<tr>
<td>No. of return pipes</td>
<td>6</td>
</tr>
<tr>
<td>Fin spacing</td>
<td>10 fpi</td>
</tr>
<tr>
<td>Overall Size</td>
<td>12 ⅞ x 18 x 1 ½ in</td>
</tr>
<tr>
<td>Fin width</td>
<td>1 ½ in</td>
</tr>
<tr>
<td>Fin thickness</td>
<td>0.2 mm</td>
</tr>
<tr>
<td>Fin material</td>
<td>Aluminum</td>
</tr>
</tbody>
</table>

### Working Parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cycle time</td>
<td>8 – 10 – 20 – 30 – 60 – 90 – 120 min</td>
</tr>
<tr>
<td>Mass of adsorbent</td>
<td>1.5 kg</td>
</tr>
</tbody>
</table>
In-situ Uptake Measurement Setup – Design I

**EXPERIMENTAL SETUP**

- Pressure transducers
- Heat transfer fluid (at 30 and 90°C)
- Adsorber bed
- Evaporator/Condenser (at 20°C)
- Hosing
- Scale
- Chiller
- Aluminum lid

**Introduction**

**Numerical Modeling**

**Conclusion**
In-situ Uptake Measurement Setup – Design II

FAM Z02 in new adsorber bed

Evaporators 1 and 2

Adsorber bed
Challenges

- Low working pressure of adsorption system (1 kPa – 7 kPa)
  - Designing vacuum chamber
  - Leaking (Helium leak detector)
- Changes of the density of the heat transfer fluid (silicone oil) with temperature
- Changes of hosing stiffness with temperature
Measured Parameters

**Temperature**
- **Design II**
- Cycle time = 60 min

**Adsorption** | **Desorption**
---|---
25°C | 95°C
35°C | 85°C
45°C | 80°C
55°C | 75°C
65°C | 70°C
75°C | 65°C
85°C | 60°C
95°C | 55°C

**Mass**
- **Design II**
- Cycle time = 60 min

**P_{\text{evap/cond}}**
- **Design I**
- **Design II**

---

**Psat at 20°C**

---

**Mass change of silicone oil**
FAM Z02- Equilibrium Uptake

**Adsorption**

![Graph of Adsorption]

**Desorption**

![Graph of Desorption]

FAM Z02- Cyclic Operation

- Δω% (kg/kg adsorbent) vs. Cycle time (min)
- SCP_{ideal} (W/kg) vs. Cycle time (min)
- COP_{ideal} vs. Cycle time (min)

FAM-Z02

\( T_{\text{des}} = 90^\circ C \)
\( T_{\text{ads}} = 30^\circ C \)
\( T_{\text{evap/cond}} = 20^\circ C \)

Design I
Design II

LAEC
Laboratory for Alternative Energy Conversion
Ideal SCP vs. Actual SCP

\[ SCP_{\text{Ideal}} = \frac{\Delta \omega \times h_{fg}}{\tau_{cycle}} = \frac{\Delta m_{ref} \times h_{fg}}{m_{ads} \times \tau_{cycle}} \]

\{ Numerical Modeling \}

\{ Mass Measurement \}

\[ SCP_{\text{Actual}} = \frac{Q_{evap}}{m_{ads} \times \tau_{cycle}} \]

\{ Cooling Effect at Evaporator \}
1. Spiral plate
2. Shell and tube
3. Hairpin
4. Annulus tube
5. Plate fin
6. Finned tube
7. Plate-tube
8. Simple tube
9. Plate

Single-Bed ACS Equipped with Capillary-Assisted Evaporator

Adsorber bed

Condenser

Evaporator

FAM Z02 in new adsorber bed
Two-Adsorber Bed FAM-Z02-Water ACS

- Adsorber bed 1
- Condenser
- Evaporator
- Adsorber bed 2
Modified Test Setup

- Heat transfer fluid flow rate $\approx 4$ lit/min
- Evaporator flow rate $\approx 3$ lit/min
## Adsorber Bed Designs

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Design I</th>
<th>Design II</th>
</tr>
</thead>
<tbody>
<tr>
<td>Working pairs</td>
<td>AQSOA FAM-Z02/water</td>
<td></td>
</tr>
<tr>
<td>Adsorbent particles diameter (m)</td>
<td></td>
<td>0.002</td>
</tr>
<tr>
<td>Mass of adsorbent (kg)</td>
<td>0.62</td>
<td>1.50</td>
</tr>
<tr>
<td>Metal mass of adsorber bed (kg)</td>
<td>2.80</td>
<td>2.87</td>
</tr>
<tr>
<td>Adsorber bed heat transfer surface area, $A_{bed}$ (m²)</td>
<td>0.235</td>
<td>2.80</td>
</tr>
<tr>
<td>Fin spacing (mm)</td>
<td>6.47 (3.5 fins per inch)</td>
<td>2.34 (10 fins per inch)</td>
</tr>
<tr>
<td>Fin dimensions</td>
<td>12.7 cm (5”) diameter</td>
<td>43.18×30.48 cm (17”×12”)</td>
</tr>
<tr>
<td>Heating fluid mass flow rate to adsorber bed (kg/s)</td>
<td>0.058 (4.1 L/min of silicone oil)</td>
<td></td>
</tr>
<tr>
<td>Cooling fluid mass flow rate to adsorber bed (kg/s)</td>
<td>0.062 (4.1 L/min of silicone oil)</td>
<td></td>
</tr>
<tr>
<td>Heat capacity of silicone oil (kJ/kgK)</td>
<td>1.8</td>
<td></td>
</tr>
<tr>
<td>Heating fluid inlet temperature (°C)</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>Cooling fluid inlet temperature (°C)</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>Evaporation/condensation temperature (°C)</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>
Pressure – 10 fpi, 1500gr

Graph showing pressure versus time for Evaporator and Bed, with pressure in kPa and time in minutes.
Pressure - 3 fpi, 620 gr – Cycle time 60 min

![Graph showing pressure over time for Bed and Evaporator/Condenser with cycle time 60 min.](image-url)
Pressure within Bed and Evaporator – Design II Modified

Graph showing the pressure within the Bed (P Bed) and Evaporator (P Evap) over time. The pressure is measured in kPa and time is measured in minutes.
SCP – Two different Design Comparison

![Graph showing SCP (W/kg) vs Cycle Time (min) for 3 fpi and 10 fpi.]
Results – effects of silicon oil density change

![Graph showing the results](chart)

- **Total Mass Reading**
- **Oil Mass Reading**

<table>
<thead>
<tr>
<th>Mass (gr)</th>
<th>Time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>20</td>
<td>60</td>
</tr>
<tr>
<td>40</td>
<td>120</td>
</tr>
<tr>
<td>60</td>
<td>180</td>
</tr>
<tr>
<td>80</td>
<td>240</td>
</tr>
<tr>
<td>100</td>
<td>300</td>
</tr>
</tbody>
</table>

**Notes:**
- The graph illustrates the changes in mass over time for total and oil mass readings.
- The density changes are evident through the peaks and troughs in the graph.
Low Pressure Evaporator

- Using the new evaporator (capillary assisted)
- Decreasing cycle time to reach the maximum SCP
The First Generation

HTF\textsubscript{in} \hspace{1cm} HTF\textsubscript{out}

TC0 \hspace{1cm} TC8

TC1 \hspace{1cm} TC2

TC3 \hspace{1cm} TC4

TC5 \hspace{1cm} TC6

11.4 cm

9.5 mm (3/8”) fin spacing

50 Bodies
511,000 Cell
Geometries

Flow in

Flow in