A ONE-DIMENSIONAL HEAT AND MASS TRANSFER MODEL OF SORPTION CELLS

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ABSTRACT
In the current paper, we introduce a one-dimensional dynamic heat and mass transfer model for closed system sorption cells. The model objective is to allow the design of sorption systems for a wide range of processes such as heat storage, fluid storage, and pressure control systems. The model is based on implicit finite differences method which is implemented by Matlab™ code and governed by energy and mass equations. The current research focuses on sorption cells which are under thermal cycles which consist of heating and cooling phases. Several insulation methods are examined, and the thermal efficiency and the temperature distribution in the cell are investigated. The results show the differences between designs for maximum thermal efficiency and designs for obtaining maximum pressures. In addition, an active cooling method, which consist of a liquid coolant, is examined with five different coolants. The results show that turbulent flow in the heat exchanger is desired, whereas, the pressure drop in the heat exchanger must be considered.

INTRODUCTION
Sorption systems are used to store heat, store fluids, and for pressure management, for example, in gas storage, thermal energy storage, separation and purification systems, pressure swing adsorption (PSA), adsorption chillers, and sorption compressors. Sorption applications often operate in closed systems, where mass doesn’t enter or leave the system. In this paper, we present an investigation on heat and mass transfer in a closed sorption system, in the frame of our ongoing research on sorption compressors aiming for driving Joule-Thomson cryocoolers in space applications. An adequate heat and mass transfer model is essential for investigating the performance of sorption systems. Bahrehmand et al. [1] developed an energy and mass transfer model for a thermochemical reactor appointed for thermal energy storage. Luo et al. [4] developed a non-lumped dynamic simulation method of sorption compressors, by using computational fluid dynamic (CFD) technique. In the current research, we develop an enhanced one-dimensional heat and mass transfer model of cylindrical sorption cell, which its thermal part has already validated against reported results [5]. The model incorporates the thermal resistances at the contact areas between different materials in the cell, and it enables the investigation of using different materials, geometries, dimensions, insulation techniques, and heating and cooling methods. The main strengths of the new model are in allowing the investigation of different heaters and coolers, incorporating the heat of adsorption/desorption, and enabling the research on different insulation techniques.

NOMENCLATURE

\( a \) [MPa
\(^{-1}\)] Adsorption affinity
\( C \) [J/K] Heat capacity
\( c \) [J/kg-K] Specific heat capacity
\( C_i \) [mg/g] Adsorption concentration
\( C_{s,0} \) [mg/g] Saturated adsorption concentration
\( h \) [W/m
\(^2\)K] Convective heat transfer coefficient
\( i \) [-] Index of an element
\( k \) [W/m
\( \cdot \)K] Conductive heat transfer coefficient
\( L \) [m] Vessel length
\( n \) [-] Number of time step
\( \eta_{\text{mix}} \) [-] Heterogeneity of the adsorbate-adsorbent system
\( N_i \) [-] Number of adsorbent elements
\( P \) [MPa] Pressure
\( q_{\text{heating}} \) [W/m
\(^2\)] Heat flux
\( Q \) [W] Power
\( R \) [K/W] Thermal resistance
\( r \) [m] Radius
\( r_s \) [m] Distance from central axis
\( t \) [sec] Time
\( T \) [K] Temperature
\( V \) [m
\(^3\)] Volume
\( W \) [m] Layer thickness

Special characters
\( \theta \) [rad] Angular direction
\( \rho \) [kg/m
\(^3\)] Density
\( \sigma_y \) [MPa] Yield stress
Subscripts
0  [-]  Initial state
n  [-]  Time step index
s  [-]  Adsorbent

Abbreviations and Acronyms
ATS  [K]  Average temperature of sorbent
HC  –  Heater/Cooler device
RATS  –  Relative average temperature of sorbent
TESC  –  Thermal efficiency of sorption cell

METHOD
System Description

In the current research we examine several configurations of closed system cylindrical sorption cells, which consist of an activated carbon adsorbent, nitrogen as a working fluid, and an inner heater/cooler (HC) device. Heating and cooling in a closed sorption system increase and decrease the temperature of the cell, respectively. Consequently, the adsorption concentration and the pressure are changed. In the current research we assume a uniform pressure in the cells, due to slow thermal cycles.

A sorption cell description

The cylindrical sorption cell consists of six axisymmetric sections (S1 – S6), as described in Fig.1, where each section can be defined as a different material. In this paper, S1 and S3 present the adsorbent, S4 and S6 are an inner and an outer insulation, respectively, S2 is a HC device and S5 is a stainless-steel vessel. Every section can be eliminated by applying zero thickness.

Numerical model

A dynamic heat transfer model is developed, based on a finite differences method, implemented in Matlab™ software. The sorption cell is modelled as one-dimensional, in the radial direction only, due to the assumption that its length is at least ten times larger than its outer diameter [6]. The model consists of six sections, S1 – S6, where each section is divided into elements with a central node. Each element is defined as a lumped capacity and all its thermal properties are temperature dependent. The model is based on energy equations and allows the investigation of different insulation methods, active heating and cooling, natural and forced convection to the surrounding, and contact heat resistances between different materials. The heat transfer method has been already validated, as presented in previous work [5].

Figure 2 shows a schematic view of the elements and the nodes. Every element is defined by the distance from the central axis, $r_m$, and its width, $\Delta r$, which is a function of the radial thickness of a section and the number of elements in the section.

Adsorbent elements, section S1 and S3, consist of three phases: solid adsorbent, adsorbed fluid, and gaseous fluid, see Fig. 3. Effective thermal properties of the adsorbent elements are determined, and the elements can generate and absorb heat, according to the heat of adsorption which is determined by the adsorption isotherms [7].

Figure 1 A schematic view of the sorption cell

Figure 2 A schematic view of the elements

Figure 3 A schematic view of an adsorbent element
The HC elements, section S2, can function as a heater or a cooler, meaning, they generate or absorb heat, respectively. Assuming constant heating and cooling powers per surface area, the total heating and cooling power of a HC device is a function of its dimensions.

Elements of the inner insulation section, S4, can depict porous insulation materials, therefore, they allow mass transfer of a gaseous fluid between elements.

System thermal performance

Two non-dimensional thermal parameters are defined and discussed: thermal efficiency of sorption cell (TESC) and relative average temperature of sorbent (RATS). TESC, is the ratio between the energy transferred to or from the adsorbent and the total energy invested or rejected in the cell, at a time step:

\[
TESC_n = \frac{\sum_i^{N_i} (C_{\text{in}}^{n+1} - C_{\text{in}}^{n})/C_{\text{in}}}{Q_{\text{in}}/\Delta t}
\]

where \(Q_{\text{in}}\) is the power invested or rejected (W), \(n\) indicates the time step, \(i\) is an element index, \(T\) is the temperature (K), \(C\) is the heat capacity of an element \((\Delta C)\), \(\Delta t\) is the time step (sec), and \(N_i\) is the number of adsorbent elements. In order to calculate the thermal efficiency during a process, TESC is calculated as follows:

\[
TESC = \frac{\sum_{n=0}^{N_i} TESC_n}{(t-t_0)/\Delta t}
\]

where \(t_0\) is the initial time, \(t\) is the end time of the process and \(t_0\) is the initial time step, assuming a constant time step during the process.

An average temperature of sorbent (ATS) is also defined. In every time step, ATS, is calculated as follows:

\[
ATS_n = \left(\frac{\sum_{i=1}^{N_i} \Delta T_{\text{ads}}^{n+1} V_i^{n+1}}{V_S^{n+1}}\right)_{n}
\]

where \(V_s\) is the total adsorbent volume in the cell and \(V_i\) is a volume of an element \(i\). RATS is then determined as the ratio between ATS and the maximum temperature in the cycle.

\[
RATS = \frac{ATS_n}{T_{\text{max}}}
\]

Mass transfer

In closed system sorption cells, mass transfer occurs when an adsorbed fluid becomes a gaseous fluid, or vice versa, or when gas fluid transfer between absorbent elements and void volumes. Changes in adsorption concentration, which are characterized by the adsorption isotherms, drive the mass transfer in the cell. In previous work [8] several models were examined for describing the adsorption of nitrogen on activated carbon, and the Sips model is found as the most appropriate one:

\[
\frac{C_s}{C_{s,0}} = \frac{(a \cdot p)^{-n_{\text{ads}}}}{1 + (a \cdot p)^{-n_{\text{ads}}}}
\]

where \(C_s\) is the adsorption concentration, \(C_{s,0}\) is the saturated adsorption concentration, \(p\) is the pressure, (MPa), \(a\) is the adsorption affinity (MPa\(^{-1}\)), and \(n_{\text{ads}}\) is a dimensionless parameter that qualitatively characterizes the heterogeneity of the adsorbate-adsorbent system.

In order to determine the fluid mass in the gas phase the specific volume of the gas phase is calculated by the Peng-Robinson equation of state. When the temperature of an adsorbent element is changed, the adsorption concentration varies, and the pressure is iteratively determined.

Test Cases

Three cell configurations are investigated during the heating phase. Fig. 4 describes the three configurations: Cell-A is adiabatic, Cell-B has an outer insulation, and Cell-C has an inner insulation, where all three cells have equal outer radius of the adsorbent section. An inner insulation consists of porous materials which increase the void volume in the cell. Thus, a “sealed Cell-C” is investigated as well, where an inner thin metal foil prevents the incorporation of the insulation pores in the cell void volume. The Outer insulation of Cell-B is a Pryogel XTE\textsuperscript{TM} blanket, having a conductive heat coefficient which equals 0.03 \((W/(m \cdot K))\). The inner insulation in Cell-C must be rigid to comply with the inner pressure, therefore, a ceramic ZYFB-3 insulation layer is used, with a conductive heat coefficient which equals 0.08 \((W/(m \cdot K))\).

Every configuration is examined with two different vessels, which their dimensions are listed in table \(1\), and the thermal properties of the different sections are provided in table \(2\). Table \(3\) describes eight parameters that are maintained constant: the HC heat flux, the maximum allowed temperature and pressure in the sorption cell, the HC and insulation thicknesses, the yield stress of the vessel, the convective heat transfer coefficient with the surroundings, and the ambient temperature.
The HC dimensions can be changed, and therefore, the total heating and cooling power are changed. The heating phase starts with a uniform temperature distribution of 300 K and a pressure of 0.2 MPa, and it stops at a maximum allowed temperature of 750 K in the cell.

The cooling phase is investigated with the configuration of Cell-B and Vessel-1. In the current paper, we focus on cooling with a liquid coolant which flows in copper pipes in the cell. Two options are discussed: two U shape 1/4-inch pipes with a total length of 1 m each, and three U shape 3/16-inch pipes with a total length of 1 m each. Five different coolants are considered.

### Table 1. Vessel dimensions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Vessel-1</th>
<th>Vessel-2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inner vessel radius (mm)</td>
<td>25</td>
<td>30</td>
</tr>
<tr>
<td>Vessel length (mm)</td>
<td>720</td>
<td>720</td>
</tr>
<tr>
<td>Vessel volume (cc)</td>
<td>1,400</td>
<td>2,000</td>
</tr>
<tr>
<td>Vessel wall thickness (mm)</td>
<td>2.4</td>
<td>2.8</td>
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### Table 2. Constant thermal properties

<table>
<thead>
<tr>
<th>Material</th>
<th>Section: Adsorbent</th>
<th>HC</th>
<th>Vessel</th>
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<tbody>
<tr>
<td></td>
<td>Chemviron</td>
<td>CrNi Steel</td>
<td>SS 316L</td>
</tr>
<tr>
<td>k (W/m·K)</td>
<td>0.2</td>
<td>16</td>
<td>20</td>
</tr>
<tr>
<td>ρ (kg/m³)</td>
<td>400</td>
<td>8000</td>
<td>8000</td>
</tr>
<tr>
<td>c (J/kg·K)</td>
<td>1000</td>
<td>500</td>
<td>500</td>
</tr>
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</table>

### Table 3. Input parameters.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>Value</th>
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<tbody>
<tr>
<td>$q_{heating}$</td>
<td>kW/m²</td>
<td>13.53</td>
</tr>
<tr>
<td>$T_{max, HC}$</td>
<td>(K)</td>
<td>750</td>
</tr>
<tr>
<td>$P_{max}$</td>
<td>(MPa)</td>
<td>4</td>
</tr>
<tr>
<td>$P_{min}$</td>
<td>(MPa)</td>
<td>0.2</td>
</tr>
<tr>
<td>Heater thickness</td>
<td>(mm)</td>
<td>2</td>
</tr>
<tr>
<td>Insulation thickness</td>
<td>(mm)</td>
<td>5</td>
</tr>
<tr>
<td>σ$_r$, vessel</td>
<td>(MPa)</td>
<td>170</td>
</tr>
<tr>
<td>h (natural convection)</td>
<td>W/m²K</td>
<td>5</td>
</tr>
<tr>
<td>$T_{ambient}$</td>
<td>(K)</td>
<td>300</td>
</tr>
</tbody>
</table>

**RESULTS AND DISCUSSION**

Figure 5 shows $TESC$ during heating phase for the different cell configurations, as a function of the HC radius. For all configurations, an increase in the HC radius decreases $TESC$. Cell-C provides the highest $TESC$ for all HC dimensions, due to its lowest thermal mass of the non-adsorbent sections. Cell-B has the lowest $TESC$ due to the largest heat losses to the surroundings. For the optimal HC dimensions Cell-C and Cell-A obtain the highest $TESC$, in comparison to Sealed Cell-C and Cell-B which provide 94% and 89% of the highest TESC, respectively.

Figure 6 presents the pressure and $RATS$ obtained at the end of the heating phase as a function of the HC location in the cell. A relation between $RATS$ and the pressure is obtained, having the same locations for the minimum and maximum values. For all cases, higher values of both $RATS$ and pressure are achieved for cylindrical HCs located close to the outer radius of the adsorbent section. Figure 6 shows that each insulation method has a different maximum pressure at a different HC dimensions. In respect to Cell-B, which reaches the highest pressure, both Cell-A and Sealed Cell-C obtain 95%, and Cell-C obtains 69%. Figure 7 shows the temperature distribution in the radial direction at the end of the heating phase for the four cell configurations. The results in figure 7 are for the optimal HC dimension to obtain the maximum pressure. Cell-B reaches the highest pressure (see Fig 6(a)) due to its highest temperature uniformity (Fig 7). On the other hand, Cell-B requires the longest heating duration due to its highest heat losses to the surroundings. Sealed Cell-C and Cell-A achieve the same maximum pressure with the same HC dimensions, and they both have similar heating time.
Five coolants are examined at the cooling phase. The cooling phase is investigated by Cell-B and Vessel-1 configuration with HC radius which equals 21 mm, for obtaining a maximum pressure. Figure 8 presents the average cooling power of the five coolants, during a cooling phase, as a function of the mass flow. At low flow rates, laminar flows provide low cooling power, where Duratherm G provides the highest cooling power which equals 350 Watt. The transition to turbulent flow allows significantly higher cooling power. Dowtherm A transfers to turbulent flow at the lowest mass flow rate, relative to the other coolants. In addition to the cooling power of a coolant, its pressure drops, and maximum operating temperature are also of great concern in designing a cooling system. Table 4 shows these parameters for four of the examined coolants while providing an average cooling power of 1600 Watt. Duratherm G is not able to provide an average cooling power of 1600 Watts; therefore, it is not presented in Table 4.

<table>
<thead>
<tr>
<th>Coolant</th>
<th>Avg Cooling Power (W)</th>
<th>$T_{\text{max,coolant}}$ (K)</th>
<th>$\Delta P_{\text{coolant}}$ (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Duratherm 450™</td>
<td>1340</td>
<td>425</td>
<td>0.128</td>
</tr>
<tr>
<td>Duratherm G™</td>
<td>1400</td>
<td>375</td>
<td>0.28</td>
</tr>
<tr>
<td>Therminol 62™</td>
<td>1400</td>
<td>375</td>
<td>0.73</td>
</tr>
<tr>
<td>Dowtherm A™</td>
<td>1340</td>
<td>425</td>
<td>0.108</td>
</tr>
<tr>
<td>Dynalene MT™</td>
<td>1340</td>
<td>425</td>
<td>0.6</td>
</tr>
</tbody>
</table>

The results in Table 4 show that Dowtherm A has the lowest pressure drop in the heat exchanger while achieving a maximum temperature of 447 K, which is lower than its maximum allowed operating temperature of 530K at 0.101 MPa.
Figure 9 shows the cooling power as a function of time for Cell-B and Vessel-1 with Dowtherm A, with two cooling system designs: two U-shape 1/4 inch pipes and three U-shape 3/16 inch pipes, both with an average cooling power of 1600 watt. The three pipes configuration allows a shorter cooling duration of 472 sec instead of 486 sec for the two pipes configuration. However, the two pipes configuration has lower pressure drop of 0.108 MPa, relative to 0.26 MPa of the three pipes configuration.

For all coolants, the transition from laminar to turbulent flow significantly increases the cooling power. Dowtherm A provides the highest average cooling power with the lowest required pump work.

CONCLUSIONS
A dynamic one-dimensional heat and mass transfer numerical model for closed system cylindrical sorption cell is developed and discussed. The model simulates thermal cycles of heating and cooling phases, it is governed by energy and mass equations, and a uniform inner pressure is assumed, due to slow thermal processes. In this paper, the system operates at room temperature of 300K, with initial pressure of 0.2MPa. During heating phase, three main parameters are examined for different insulation methods and HC dimensions: TESC, RATS and maximum pressure. In addition, during cooling phase an active cooling method with an inner heat exchanger is investigated, where five different coolants are tested.

The results show that the maximum pressure for each configuration is obtained at different HC dimensions. However, for all cases, the maximum TESC is obtained for a central rod HC. Moreover, for all cases, an optimal HC for the highest TESC is not the HC which provides the highest pressure in the cell. Cell-C configuration reaches the highest thermal performance; TESC and RATS; however, it achieves the lowest pressure among all cells configurations.

Cell-B reaches the highest pressure among all configurations, due to a uniform temperature distribution, however, it has the lowest TESC for all HC dimensions. Sealed Cell-C and Cell-A reach similar RATS and pressures. A correlation between RATS and the pressure is obtained, for all the test cases. Therefore, one shall conclude that a heat transfer simulation, regardless the adsorption information of the working pair, can predict the performance of a sorption system which aims for minimum or maximum pressures.

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REFERENCES