Numerical Modeling of Combined Heat and Mass Transfer in an Adsorbent Bed with Rectangular Fins

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Abstract
This paper investigates the performance of an adsorption chiller working with composite sorbent SWS-1L and driven by a low temperature heat source. A three-dimensional non-equilibrium numerical model describing the combined heat and mass transfer in the plate finned-tube heat exchanger is presented. The spatial variations of pressure and gas flow inside the adsorbent bed along with the internal and external resistances of bed particles are considered to construct a qualified model capable of investigating nearly all the system parameters with minimum restrictions. Flow patterns and pressure distributions throughout the bed are examined in detail for all cycle phases. It was found that the bed flow patterns are relatively complex for the isosteric phases due to the simultaneous occurrence of adsorption and desorption processes. Furthermore, a detailed investigation is performed for different fin heights and spaces to identify the share of each part of the system from the input energy during the heating phase.

Keywords: adsorption chiller, finned bed, porous medium, numerical modeling, mass transfer

Introduction
Adsorption chillers, known as environmentally friendly technology, have been receiving much research attention in a way to become appropriate alternatives to the CFC-based vapor-compression ones. As the main drawback of these systems is the weak conductivity of the adsorbent bed, incorporating extended surfaces is suggested to enhance the heat and mass transfer processes throughout the bed; however it is only recently that some studies considered the transient modeling of beds with extended surfaces, which are briefly discussed here.

Zhang [1] studied a 3D non-equilibrium model, considered both inter and intra particle mass transfer resistances in an adsorber incorporating axial fins. Despite the fact that the model was capable of providing detailed information about the heat and mass transfer processes through the bed very limited information is provided. Chua et al. [2] proposed a 2D model to study the transient and steady state behaviors of a finned tube heat exchanger neglecting the details of the vapor flow through two successive fin spaces. Ilis et al. [3] performed a transient two dimensional numerical study on heat and mass transfer in an annular adsorbent bed assisted with axial fins. The model was fairly simplified based on the uniform pressure approach, which neglects the convective effects of refrigerant vapour throughout the bed. Pei-zhi [4] modeled the heat and mass transfer in an adsorbent bed with annular fins using a lumped parameter method to calculate temperature variations and adsorbate distribution. Riffel et al. [5] performed a transient 2D modeling of heat and mass transfer is an adsorber with annular finned-tube. However, in their numerical modeling, an increment in the direction of heat/cooling fluid containing one fin pitch was considered and the convective effects of the working fluid in the bed were ignored. Saha et al. [6] presented a dynamic modeling of adsorption bed with annular fins based on the experimentally confirmed adsorption isotherms and kinetic data of the sorbent. The aim of the study was to analyze the performance of a new family of composite sorbents called selective water sorbents performance (SWS) in adsorption cooling systems. Niazmand and Dabzadeh [7] performed a detailed 2D numerical investigation of heat and mass transfer processes inside an adsorbent bed with annular fins. The velocity, temperature and concentration fields inside the bed are examined in detail for each process of the refrigeration cycle. Furthermore, the effects of fin spacing and height on the performance of the system are discussed. However, the input energy distributions between different parts of the system, which can provide some insight about the optimization of these systems, were not presented. Experimental investigation for an annular finned-tube adsorption chiller is presented in Reference [8]. Recently, Rezk and Al-Dadah [9] presented an empirical lumped analytical simulation model for a silica gel/water adsorption chiller with rectangular fins neglecting the spatial variations of the pressure and temperature throughout the bed.

This literature survey reveals that there is a shortage of information regarding the particulars of transfer processes associated with adsorbent beds with extended surfaces. In this paper a detailed three dimensional numerical modeling of a SWS-1L/water adsorption bed is presented. The spatial variations of pressure and gas
flow inside the bed along with the internal and external resistances of bed particles are considered. Therefore, the model can predict heat and mass transfer in beds with different particle sizes and porosities. Flow patterns and pressure distributions throughout the bed are examined in detail for all cycle phases and furthermore some considerations about the input energy distribution between different parts of the bed are given.

**Mathematical Model**

As shown in Figure 1, the adsorbent chamber consists of four basic components known as adsorbent bed, fins, metal tube and thermal fluid.

![Figure 1: Adsorbent chamber basic components](image)

In order to model the transport processes through the bed, simultaneous thermal analyses of all components are required based on the following main assumptions:
- The particles in the adsorbent bed are all spherical with uniform size and porosity.
- No heat loss is considered through the chamber wall.
- The adsorbed phase is assumed to be liquid and the refrigerant vapor is considered to be an ideal gas.
- The only variable thermo physical property of the adsorbent bed elements is the density of adsorbate gas.
- The condenser and evaporator are assumed to be ideal with constant temperature during the isobaric phases.
- The mass balance equation of the refrigerant is given as:

\[
\int (\rho C_p)_{fluid} \frac{\partial T_{fluid}}{\partial t} dV + \int (\rho C_p \bar{u} T)_{fluid} dA =
- h_{fluid} A(T_{fluid} - T_{int,entrance})
\] (1)

Where the heat transfer coefficient is calculated from the following correlation [1]:

\[ N_{fl} = 0.023 Re^{0.8} Pr^{0.4} \quad \text{for cooling} \]
\[ N_{fl} = 0.023 Re^{0.8} Pr^{0.4} \quad \text{for heating} \] (2)

2. **Metal Tube**

The transient three dimensional heat transfer equation is expressed by:

\[
\int (\rho C_p)_{tube} \frac{\partial T_{tube}}{\partial t} dV = \int [h \nabla T]_{tube} dA + \epsilon \gamma Q_{tube-fin}
\] (3)

+ \gamma Q_{tube-fin}

where \( \gamma = 1 \) if the control volume has an interface with the fin, otherwise \( \gamma \) is set to zero.

3. **Fins**

Since fins are very thin, heat transfer is considered two dimensional in the plate perpendicular to the tube axis:

\[
\int (\rho C_p)_{fin} \frac{\partial T_{fin}}{\partial t} dV = \int (\lambda \nabla T_{fin}) dA - Q_{fin-tube}
\] (4)

4. **Adsorbent Bed**

The energy balance of the adsorbent bed is expressed by:

\[
\int (\rho C_p)_{bed} \frac{\partial T_{bed}}{\partial t} dV + \int \lambda (\nabla T_{bed}) dA + \int (\rho C_v \bar{u} T_{bed}) dA =
- h_{bed} A(T_{bed} - T_{int,entrance})
\]

where the heat transfer coefficient is calculated from the following correlation [2]:

\[
N_{bed} = \frac{1}{0.02628} \left( \frac{\sqrt{\frac{T_b}{M}}}{P \sigma^2 \Omega} + \frac{1}{29.905 \sqrt{\frac{T_b}{M}}} \right)
\] (10)

The refrigerant vapor superficial velocity is determined by Darcy correlation:

\[
\bar{u}_g = \frac{K_{app}}{\mu} \nabla P
\] (9)

Where the permeability of an adsorbent bed \( K_{app} \) is calculated by the following equation:

\[
K_{app} = \frac{e_b^2 d_p^2}{150(1-e_b)^2} + \frac{e_b \mu}{e_b \sigma^2 P}
\]

The equilibrium uptake at temperature \( T_b \) and the pressure \( P \). According to [6], the following correlation has been obtained experimentally for SWS-1L:

\[
w^* = \sqrt{\frac{1.6 \times 10^{-12} P \exp\left(\frac{2.78 \times 10^6}{RT_b}\right)}{1 + \left(2 \times 10^{-12} P \exp\left(\frac{2.78 \times 10^6}{RT_b}\right)\right)^{1.1}}} \] (8)

The energy balance of the adsorbent bed follows:

\[
\int (\rho C_p)_{bed} \frac{\partial T_{bed}}{\partial t} dV + \int (\rho C_v \bar{u} T_{bed}) dA =
- h_{bed} A(T_{bed} - T_{int,entrance})
\] (1)

Where the heat transfer coefficient is calculated from the following correlation [1]:

\[ N_{fl} = 0.023 Re^{0.8} Pr^{0.4} \quad \text{for cooling} \]
\[ N_{fl} = 0.023 Re^{0.8} Pr^{0.4} \quad \text{for heating} \] (2)
Combining Darcy’s law, Eq. 9, with the mass balance, Eq. 6, results in the following equation for the pressure distribution throughout the bed:

\[ \int_{\text{cv}} \frac{d\rho}{dt} \, dA = \int_{\text{cv}} \left( \frac{\rho_{\text{app}} K}{\mu} \nabla \cdot \mathbf{v} \right) \, dA - \int_{\text{cv}} \rho_{\text{app}} \frac{\partial w}{\partial t} \, dA \]

(11)

The equation of state is used to evaluate the density of the refrigerant vapor in desorbed phase:

\[ P = \rho_{\text{g}} R \frac{T_b}{M} \]

(12)

The performance of adsorption chillers is mainly evaluated based on the coefficient of performance (COP), and specific cooling power (SCP), defined as:

\[ \text{COP} = \frac{Q_{\text{evap}}}{Q_{\text{heating}}} \]

(13)

\[ \text{SCP} = \frac{Q_{\text{evap}}}{m_b \times t_{\text{cycle}}} \]

(14)

In which \( Q_{\text{heating}} \) is the total supplied heat to the adsorbent bed by the thermal fluid during one cycle and \( Q_{\text{evap}} \) is the produced cooling energy in the evaporator calculated according to:

\[ Q_{\text{evap}} = \int_{\text{adsorption}} \dot{m}_{\text{g}} L_e \, dt \]

(15)

where \( L_e \) is the latent heat, which is estimated by [10]:

\[ L_e = 1000 \times 2406 - 2.493 \times (T_{\text{evap}} - 273.15 - 40.0) \]

(16)

To reduce the computational cost and due to the symmetry, it is assumed that the section of the heat exchanger shown in Figure 2 can be used to reasonably predict the performance of the whole set if appropriate boundary conditions are applied. The described equations are numerically solved by a finite-volume technique using forward differencing scheme for unsteady terms and central differencing scheme for both of the diffusion and convective ones. The resulting discretized equations are solved using an alternating direction implicit (ADI) method and the tri-diagonal solver algorithm.

Figure 2: A magnified view of the control volumes in all different domains

Numerous grid independency tests have been performed in search for the optimum number of grid points. In this study, employing 16 control volumes in \( x \) direction, 16 control volumes in \( y \) direction, 8 grids between fins and 3 grids in radial direction of the tube, produces reasonably grid independent results for the base case (fin spacing of 6 mm and height of 28 mm). Two different time steps are employed for the isosteric and isobaric phases due to the relatively rapid variations of the parameters in isosteric phases. It can be shown that adopting 0.04 second for isosteric phases and 0.4 second for isobaric ones provides reasonable time accurate results.

It must be emphasized that the duration of isobaric heating and cooling phases are determined based on the occurrence of a certain level of the average adsorbed amount. The values of \( w_{\text{max}} \) and \( w_{\text{min}} \) are chosen according to the 20% of the maximum and minimum possible bed absorbed amount at the pressure of evaporator and condenser and at the temperature of cooling and heating thermal fluid, respectively. Moreover, two cycles are required for the cyclically steady state conditions to be established.

For validation of the numerical scheme, a comparison has been made with the experimental data of Restuccia et al. [11]. A pack of finned stainless steel tubes is used as the heat exchanger with composite sorbent SWS-1L and water as the working pair similar to what is used in the present study. The experiments were carried out at the standard conditions of a sorption air conditioner at the low desorption temperature of about 90 ºC. All relevant specifications of the experimental set up can be found in Restuccia et al. [11]. In Figure 3 the time variations of the mean bed temperature in the experimental set up has been compared with its corresponding temperature in the numerical counterpart. Reasonable agreement between the results is an indication of the proper mathematical modeling and the accuracy of the numerical scheme despite the fact that heat exchanger geometry is different from that of present study because the governing equations, mathematical modeling, and numerical procedure are basically identical.

![Figure 3: Comparison between numerical and experimental time variations of the bed mean temperature](image)

All related bed specifications and chamber working conditions are listed in Table1.
Table 1: Parameters value and modeling conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Inlet cold water temperature</td>
<td>( T_{\text{cooling}} )</td>
<td>K</td>
<td>303.15</td>
</tr>
<tr>
<td>Inlet hot water temperature</td>
<td>( T_{\text{heating}} )</td>
<td>K</td>
<td>358.15</td>
</tr>
<tr>
<td>Evaporator temperature</td>
<td>( T_{\text{cond}} )</td>
<td>K</td>
<td>303.15</td>
</tr>
<tr>
<td>Condenser temperature</td>
<td>( T_{\text{evap}} )</td>
<td>K</td>
<td>283.15</td>
</tr>
<tr>
<td>Adsorbent mean density</td>
<td>( \rho_b )</td>
<td>kg m(^{-3})</td>
<td>650</td>
</tr>
<tr>
<td>Specific heat of adsorbent</td>
<td>( C_{pb} )</td>
<td>J kg(^{-1}) K(^{-1})</td>
<td>924</td>
</tr>
<tr>
<td>Adsorbent thermal conductivity</td>
<td>( \lambda_b )</td>
<td>W m(^{-1}) K(^{-1})</td>
<td>0.2</td>
</tr>
<tr>
<td>Heat of adsorption</td>
<td>( \Delta H )</td>
<td>J kg(^{-1})</td>
<td>( 2.76 \times 10^6 )</td>
</tr>
<tr>
<td>Inner diameter of the tube</td>
<td>( D_i )</td>
<td>mm</td>
<td>10.92</td>
</tr>
<tr>
<td>Outer diameter of the tube</td>
<td>( D_o )</td>
<td>mm</td>
<td>12.7</td>
</tr>
<tr>
<td>Fin thickness</td>
<td>( F_T )</td>
<td>mm</td>
<td>0.2</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>( d_p )</td>
<td>mm</td>
<td>0.2</td>
</tr>
<tr>
<td>Porosity of the particle</td>
<td>( \rho )</td>
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</tr>
<tr>
<td>Porosity of the bed</td>
<td>( \varepsilon_b )</td>
<td></td>
<td>0.36</td>
</tr>
</tbody>
</table>

**Results and Discussion**

Adsorption chillers go through isosteric and isobaric heating and cooling processes in their thermodynamic cycle. In the isosteric heating phase hot water passes through the metal tube and a strong desorption occurs specially around the tube, which leads to the formation of local high pressure region and the generation of a radial vapor flow through the bed as shown in Figure 4(a). In contrast, adsorption process still occurs in the upright corner part of the bed, which can be attributed to the simultaneous effects of following factors: (1) it takes longer time for heat to defuse to this region, which is farthest from the heated surfaces, (2) this region has adsorbed much less adsorbate gas in the previous phase and (3) the chamber pressure rises due to the vapor accumulation which acts in favor of adsorption in this region. Adsorption around the upright corner of the bed also creates a local region of low pressure, which causes the flow of vapor from disrobing areas of the bed and also from the chamber to this region. Fins enhance the heat and mass transfer through the bed considerably as indicated in Figure 4(b). Relatively strong desorption occurs in the regions close to the fin surfaces as compared to the core region. It is notable that no adsorption happens around this region of the bed and the desorbed vapor inter the chamber increasing its pressure.

When the chamber pressure reaches to the condenser pressure, the condenser valve is opened and the isobaric heating phase begins. The heat transfer to the bed continues and the desorbed vapor leaves the chamber.
toward the condenser to keep the chamber pressure constant. Typical vapor velocity filed and its pressure contours are plotted in Figure 5(a). There is a continuous flow of the desorbed vapor towards the chamber during this phase. Similarly, the region between the two fins in the $x$-$z$ plane as shown in Figure 5(b) indicates an almost parallel flow with uniform velocity profile.

After reaching a given level of desorption, the isosteric cooling phase begins. In this phase all connecting valves are closed and due to the adsorption process, the chamber pressure reduces until reaching the evaporator pressure. The velocity field and pressure contours are plotted in Figure 6(a) for the same bed cross section as previous figure. In isosteric phase, the adsorbent close to the solid walls cools down by the tube cooling fluid flow and the adsorption process starts, which in turn generates local low pressure regions and causing a strong vapor flow towards the metal tube surface. A local high pressure region around the upright corner is detected where the vapor flows toward the chamber indicating that desorption process still continues there. This flow pattern can be attributed to the relatively low heat transfer rate to this area resulting in a lower desorption level in the previous phase and also the reduction of the chamber pressure as the result of strong adsorption in regions close to the metal tube. In Figure 6(b) the effect of fins are more considerable in the adsorption process. The strong adsorption close to the fin surfaces reduces the pressure along these surfaces as compared to the central section, where the velocity field is also weaker.

The final phase is the isobaric cooling phase, where the chamber valve to evaporator is opened and the refrigerant vapor is adsorbed by the bed. As shown in Figure 7(a), due to the cooling effects, a rather strong rate of adsorption occurs throughout the bed and mostly in regions where cooling is stronger. Adsorption also forms a relatively strong pressure gradient that facilitates the flow of the refrigerant vapor to the farthest region from the chamber in the left side of the bed. At the end of this phase, the amount of adsorbed water in the upper right part of the bed is less than the other parts due to its higher temperature, which in turn makes this region to adsorb refrigerant in the subsequent isosteric heating phase as mentioned earlier.

Figure 7(b) shows that adsorption occurs uniformly as the vapor flows from the chamber towards the metal tube in the passage formed by the fins. Continuous reduction in the length of the velocity vectors is an indication of the continuous adsorption through this section of the bed. Similar flow patterns can be observed at other times during this phase.

One of the important parameters in the design of the heat exchangers for the adsorption cooling systems is the geometric specifications including fins dimensions and spacing, which directly affects the performance of the system. COP variations with fin height and spacing can be comprehended easily using the energy sharing between different parts of the system. Figure 8 demonstrates the distribution of the supplied thermal energy between the adsorbent bed, fins, metal tube and thermal fluid, and the required desorption heat for different fin height and spacing. Obviously, except for the desorption heat, the transferred energy to all other
parts of the system are essentially considered as a waste, since, in the cooling phases, the added heat to these parts must be removed without any direct contributions to the desorption process and the resulting cooling power. Figure shows that as the fin height increases at a fixed fin spacing, the share of input energy for the desorption process increases significantly, which means the wasted energy in the cycle reduces and therefore, the COP increases considerably. Figure 8 also indicates that fin spacing variations at a given fin height slightly affect the useful share of the desorption heat, which also reflects in the slight variations of the COP with the fin spacing.

**Figure 8**: Distribution of the supplied thermal energy between different parts of the system including the: adsorbent bed (1); fins (2); metal tube (3); thermal fluid (4); and desorption heat (5) during heating phases

**Conclusions**
In this paper, a three-dimensional model has been developed for predicting the dynamic performance of an intermittent adsorption cycle working with the composite sorbent SWS-1L and water. In particular, the model includes the extended surfaces to enhance the transfer characteristics of the adsorption bed known for the relatively low thermal conductivity. Taking into account both the internal and the external mass transfer resistance among the adsorbent particles the vapor flow patterns and pressure distributions throughout the bed are examined for all cycle phases. It was found that the bed flow patterns are relatively complex for the isosteric phases due to the simultaneous occurrence of adsorption and desorption processes. Furthermore, a detailed investigation of the share of each part of the system from the input energy during the heating phase is presented for different fins height and spacing. It was found that COP increases as the bed height increases, while it is less sensitive to the fins spacing.

**List of Symbols**

- $E_a$: Activation energy (Jkg$^{-1}$)
- FH: Fin Height (m)
- FS: Fin space (m)
- $R$: Gas constant (Jkg$^{-1}$K$^{-1}$)
- $M$: Molar mass (kgmol$^{-1}$)
- $Pr$: Prandtl number
- $D_{\infty}$: Pre-exponent constant of surface diffusivity (m$^2$s$^{-1}$)
- $P$: Pressure (Pa)
- $Re$: Reynolds number
- $R_u$: Universal gas constant (Jmol$^{-1}$K$^{-1}$)
- $u$: Velocity (m s$^{-1}$)

**Greek symbols**

- $O$: Collision integral
- $\sigma$: Collision diameter for Lennard-Jones potential (A)
- $\mu$: Viscosity (Pa s)
- $\lambda$: Thermal conductivity (W m$^{-1}$K$^{-1}$)

**Subscripts**

- $a$: Adsorbate
- $b$: Adsorbent
- $g$: Vapor

**References**


