

**SIMULATION OF A SHELL-AND-TUBE HEAT EXCHANGER
FOR A SOLAR ADSORPTION CHILLER**

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ABSTRACT

This paper presents a simulation of a shell-and-tube heat exchanger as the main component (adsorber) of a 20 kW air conditioning central unit, which runs mainly on solar energy, with a complementary heat provided by gas. The proposed system is basically composed of a cold water storage tank produced by an activated carbon-methanol adsorption chiller, a hot water storage tank and a fan-coil that is a heat exchanger between the cold water and the air to be conditioned. The system's functioning is based on 2 adsorbers, operating in alternated turns, which is a shell-and-tube liquid-adsorbent heat exchanger. A transient model of the heat and mass transfers for the adsorber is proposed to optimize the adsorptive cycle. It is described on a mixed finite-difference and finite-volume method. The influences of some important design and operational parameters on the performance of the system are also studied, such as the effects of the operating temperature, the flow rate and the cycle time on the coefficient of performance.

INTRODUCTION

Solar cooling is an interesting application of solar energy because, the stranger the insolation, the greater needs for cooling. As a rule, the systems requiring thermal energy as their main power input for the production of frigorific effect are most dependable on sorption processes. This energy may come from different sources, such as: process heat, residual vapor or solar energy. One of the main advantages of such a system in relation to the conventional vapor compression system lies on its minimum use of electric energy and on its low cost of maintenance.

In the last two decades, absorption chillers, running on natural gas, have been introduced in markets all over the developed world – in the US, Japan, France, Italy, Spain and more recently in Portugal. As to adsorption systems – in spite of several studies that demonstrate their technical feasibilities –, there exist only experimental units, though stand

considerable chances of becoming economically viable, especially where thermal comfort applications are concerned.

This paper presents some of the adsorption fundamentals and also the energy equations for adsorbers using shell-and-tube heat exchanger. Then it puts forwards the simulation of a 20 kW air conditioning unit based on both the adsorption process and solar energy. Cold water is produced during night-time in an activated carbon-methanol adsorption chiller and then stored into a tank in order to supply cooling air during day-time. Solar energy is used for regenerating the adsorbent medium by means of highly efficient flat-plate collectors. Thermal energy is stored in a hot-water tank so as to feed the chiller at night. The central unit was created to provide thermal comfort to four adjoined laboratory rooms, whose total area is 110m².

ADSORPTION FUNDAMENTALS

Adsorption constitutes a solid sorption process by which the binding forces between fluid molecules (adsorbate) and the solid medium (adsorbent) derive from an electrostatic origin or from dispersion-repulsion forces. It is an exothermic process as a result of the gas-liquid phase change. The energy liberated during adsorption is called isosteric heat, and it depends on the nature of the adsorbent-adsorbate pair.

A number of state equations – known as isotherms of adsorption – are proposed. These functions correlate the temperature T , the pressure P , and the concentration of the adsorbed phase a , so that $f(T, P, a) = 0$. Dubinin and Radushkevich have proposed the micropore volume filling theory, which is related to Eucken-Polanyi potential theory. The Dubinin-Rudushkevich isotherm describes adsorption as a single type of uniform pores that is similar to Langmuir-like local isotherms in adsorption on energetically heterogeneous solids. This theory was later expanded by Stoeckli, allowing it to describe adsorption on energetically heterogeneous solids with a continuous distribution of pore sizes. Leite (1998) puts forward a detailed analysis of the thermodynamics of adsorption and its different isotherms.

In general, all microporous materials are adsorbent and are characterized by their high porosity. Their structures have pores with diameters smaller than 20 Å. The most common adsorbents are silica gel, activated carbon, zeolite and aluminas. Zeolite-water and activated carbon-methanol are one of the most adsorbent-adsorbate pairs utilized in refrigeration systems. Methanol is easily desorbed from activated carbon when heated, whereas in zeolite, the water is sustained for much longer. Thus, the activated-methanol pair is best adapted for operating cycles with small evaporating temperature variations (up to 40°C), whereas the adsorption cycles with zeolite-water pair, a larger range evaporating temperature (70°C, or more) is needed.

Dubinin-Astakhov equation

To describe adsorption in microporous materials with polymodal distributions, Dubinin and Astakhov (1971) have proposed an isotherm that is a log-linear form of Dubinin-Rudishkevich equation, which can be expressed as follows:

$$a = W_o \rho_l(T) \exp\left\{-D\left[T \ln\left(P_s / P\right)\right]^n\right\} \quad (1)$$

where a is the concentration (adsorbed mass per unit of adsorbent mass), W_0 is the maximum adsorption capacity (volume of adsorbate/mass of adsorbent), ρ_l is the specific mass of the liquid adsorbate, D is the “coefficient of affinity” and n is a characteristic parameter that depends on the adsorbent-adsorbate pair.

This equation has a wide field of application, and it is particularly suitable for strongly activated carbon with high pores heterogeneity. According to Passos (1986), for regenerating temperature ranging from 20 to 100°C, and for concentrations, ranging from 71 to 286 g/kg of adsorbent, a fitted curve, obtained from methanol adsorption experimental data, showed a residual error of 2.2%. These results demonstrate that this state equation is most suitable for a number of engineering applications of low-grade sources, especially those concerning solar energy.

Isosteric heat of adsorption

The energy released during the adsorption process, i.e. the isosteric heat (q_{st}) can be derived from the Gibbs’ isotherm, being reduced to a constant adsorbed mass function called isoster, which is given as follows

$$\left(\frac{\partial \ln P}{\partial T}\right)_a = -\frac{q_{st}}{RT^2} \quad (2)$$

For the saturating condition ($P = P_s$), the q_{st} term in Eq. (2) is replaced by the latent heat L . Then, the Dubinin-Astakhov equation becomes

$$\frac{\partial \ln P}{\partial T} = \frac{\partial \ln P_s}{\partial T} + \ln(P_s / P) \left\{ T^{-1} + \frac{\alpha}{nD} [T \ln(P_s / P)]^{-n} \right\} \quad (3)$$

where α is the coefficient of thermal expansion of the liquid adsorbate and it is given by $W_0 \partial \ln(\rho_l / a) / \partial T$. Integrating Eq. (3) and, after some algebraic operations, the isosteric heat of adsorption can be given as

$$q_{st} = L + RT \ln(P_s / P) + \left[\frac{\alpha RT}{nD} \right] [T \ln(P_s / P)]^{(1-n)} \quad (4)$$

Being the latent heat, the first term of Eq. (4), the other terms do correspond to the energy that most specifically concerns the adsorption binding forces. For temperature around -5°C , the value of L is about 1,200 kJ/kg. According to Srivastava and Eames (1998), the isosteric heat of adsorption for activated carbon-methanol ranges from 1,800 and 2,000 kJ/kg. So, the energy resulting from the binding forces in adsorption corresponds to something from 33% to 40% of the isosteric heat; the rest would come as a result of capillary condensation inside the micropores.

Ideal thermodynamic cycle

The adsorption refrigeration cycle consists of two well-defined stages: one is described as the adsorber cooling, with its consequent adsorption process, when the evaporation of the working fluid (the adsorbate) takes place. The other stage consists of the solid medium (the adsorbent) regeneration, when the adsorbate is desorbed and condensed

(Fig. 1a). The ideal thermodynamic cycle can be represented by two isosters (isolines with constant adsorbed phase concentration, a) and two intercalated isobars, as shown in Fig. 1b.

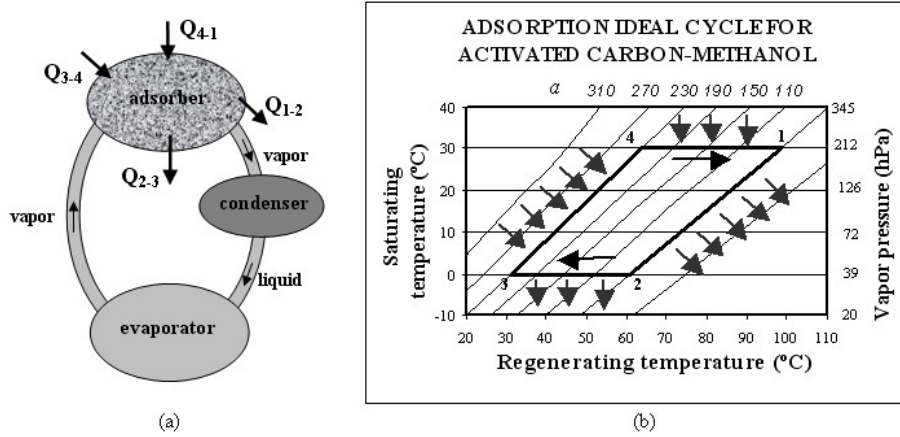


Fig. 1 - Functioning principle (a); network of isosters and ideal cycle (b).

The adsorber cooling corresponds to the isosteric process 1-2, depending on the ambient conditions. This process continues until the adsorber pressure reaches its minimum value (point 2), when it becomes equal to the evaporator pressure. At this point, the adsorption process starts and prolongs until its temperature reaches the minimum value (point 3). Then, the adsorber is heated, corresponding to another isosteric process (3-4), until its pressure reaches a maximum value (point 4). Desorption starts at this point, and goes on until the adsorber temperature reaches its maximum value (point 1), completing, in this way, the cycle.

ENERGY EQUATIONS

The energy equations related to the adsorber, which will be given next, correspond to a multi-tubular system, whose outer surface exchanges heat with the water coming from the hot storage tank or from the water supply network, depending on the stage of the cycle. The adsorbent occupies an annular space delimited by the wall of the tube and a metal screen through which the adsorbate flows.

Heat transfer in the adsorbent medium

For the heat transfer in the adsorbent medium, the following assumptions have been considered: (a) the pressure is uniform; (b) the heat conduction is only unidirectional (radial); (c) the adsorbent-adsorbate pair is treated as a continuous medium in relation to thermal conduction; (d) the convective effects and pressure drops are negligible. The heat transfer in the adsorber component can be expressed separately by two equations: one for the adsorbent, and the other for the wall of the tubes. In the case of the former, we have

$$\left[\rho_1 (Cp_1 + aCp_2) \right] \frac{\partial T}{\partial t} = k \nabla^2 T + q_{st} \rho_1 \frac{\partial a}{\partial t} \quad (5)$$

with

$$\frac{\partial a}{\partial t} = \left(\frac{\partial a}{\partial T} \right)_{\ln P} \frac{dT}{dt} + \left(\frac{\partial a}{\partial \ln P} \right)_T \frac{d \ln P}{dt} \quad (6)$$

where Cp is the specific heat (indices 1 and 2 refer to the adsorbent and the adsorbate, respectively), ρ the specific mass and k , the conductivity of the adsorbent. Equation (6) represents the kinetics of adsorption. After some algebraic operations, we obtain

$$\frac{da}{dt} = b \left[\frac{d \ln P}{dt} - \frac{q_{st}}{RT^2} \frac{dT}{dt} \right] \quad (7)$$

with

$$b = a n D T^n \left(\ln \frac{P_s}{P} \right)^{n-1} \quad (8)$$

The da/dt term depends on the process that occurs in the adsorber. In the case of an isosteric process it is null and $b q_{st}/RT^2 dT/dt$ for adsorption or desorption process. Then, the energy equation for the adsorbent can be written as

$$\left[\rho_1 (Cp_1 + a Cp_2) + \frac{u b \rho_2 q_{st}^2}{RT^2} \right] \frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial r^2} + \frac{1}{r} \frac{\partial T}{\partial r} \right) \quad (9)$$

where u is a function of the process, 0 for isosteric and 1 for adsorption or desorption process. The condition in the interface between the adsorbent material and the adsorbate circulation tube comprise the adiabatic boundary condition

$$\left(\frac{\partial T}{\partial r} \right)_{r=r_0} = 0 \quad (10)$$

The other boundary condition is in the interface between the adsorbent and the wall of the tubes. To solve the Eq. (9), the temperature on the wall of the tubes is considered known, recalculated for each simulation step by the following energy equation

$$m_t Cp_t \frac{\partial T_t}{\partial t} = N \pi L [h d_i (T_t - T) + h_{sh} d_o (T_t - T_w)] \quad (11)$$

where m_t is the tube mass, N is the number of tubes, L is the tube length, d_i and d_o are the inlet and the outlet diameters, respectively, T_t is the tube temperature, T_w is the mean water temperature, h is the conductance at the interface tube/adsorbent, and h_{sh} is heat coefficients on the external surfaces of the tubes (on the shell side).

SIMULATION

As described, the adsorber is a component that includes a liquid-adsorbent shell-and-tubes heat exchanger. The choice of the geometric configuration was based on practical aspects, such as the simplicity of the manufacturing technology employed, and the required number of tubes, which depends on the amount of adsorbent they can hold. Thus, the chosen exchanger was that of a single pass, with a square arranged tube bank. Segmental baffles were installed on the shell in order to enhance turbulence in the water flow around the tubes. More details can be found out on Leite et al. (2006).

In order to create a reliable and efficient simulation of this kind of exchanger, a good understanding of both the flow and the temperature field is required. However, the geometry and the complexity to describe it analytically made the simulation necessary. One way to simplify it is the use of the overall heat transfer coefficients (h_{sh}). Such information can be obtained through either experimental analysis (Bell, 1963; Halle et al., 1984; Pletcher and Andrews, 1994) or through simple calculation methods.

Shell-and-tube heat exchanger

An energy balance was made for each baffle (finite volume method), as described in the following equations for the first, the last and the intermediary baffle, respectively.

$$M_w \frac{dT_0^w}{dt} = \frac{kS}{Cp_w} \frac{(T_1^w - T_0^w)}{\Delta x} + \frac{US_L}{Cp_w} (T_{amb} - T_0^w) + m_w (T_{in} - T_0^w) + \frac{h_{sh} S_{tub}}{Cp_w} (T_0^t - T_0^w) \quad (12)$$

$$M_w \frac{dT_n^w}{dt} = \frac{kS}{Cp_w} \frac{(T_{n-1}^w - T_n^w)}{\Delta x} + \frac{US_L}{Cp_w} (T_{amb} - T_n^w) + m_w (T_{n-1}^w - T_n^w) + \frac{h_{sh} S_{tub}}{Cp_w} (T_n^t - T_n^w) \quad (13)$$

$$M_w \frac{dT_i^w}{dt} = \frac{kS}{Cp_w} \frac{(T_{i-1}^w + T_{i+1}^w - 2T_i^w)}{\Delta x} + \frac{US_L}{Cp_w} (T_{amb} - T_i^w) + m_w (T_{i-1}^w - T_i^w) + \frac{h_{sh} S_{tub}}{Cp_w} (T_i^t - T_i^w) \quad (14)$$

where S is the effective surface through which the water flows (at the center of the shell), S_L is the lateral surface, S_{tub} is the external surface of the tubes, T^w is the water temperature (indices 0, i and n refer to the first, the intermediate and the last node, respectively), T^t is the temperature of the tube, T_{amb} is the ambient temperature, M_w is the mass of water, m_w is the mass flow of water and Δx is the distance between two nodes.

To solve the system of equations formed by Eq. (1), (4), (9), (11), (12), (13) and (14), all flow and porous medium properties must be known, especially k , h and h_{sh} . According to Guillemint et al. (1987), for the AC-35 activated carbon: $k = 0.19$ W/mK and $h = 16.5$ W/m²K. The methodology for obtaining h_{sh} is given in a previous paper (Leite et al., 2006).

RESULTS

The chosen operating conditions are those typical of an air conditioning cycle (T_{ev} 10°C, T_{con} 30°C): inlet temperature of the heat transfer fluid is 105°C at 1 kg/s, condensation pressure of 250 hPa, evaporation pressure of 40 hPa and ambient temperature of 25°C. To facilitate the presentation, all the parameters were expressed dimensionless, using the maximum values of each unity as reference.

The first simulation results shown the time response of the adsorbers (cycle time), or else, how is the dynamic behavior of the shell-and-tube exchanger as adsorber. The evolution of the outlet water temperature (T_w), the mean adsorbate temperature (T) and the mass of adsorbent (m_{me}) is plotted on Fig. 2. The next graphic, Fig. 3, shown the total heat exchanged with the water Q_w , the cooling power Q_f , the coefficient of performance COP (ratio of Q_f to Q_w), the heat of desorption Q_{des} and the sensible heat of the refrigerant Q_{me} and of the adsorbent Q_{ca} . The difference between the Q_w and the summarized Q_{ca} , Q_{me} and Q_{des} is a heat loss to the ambient and other losses inside the exchanger. It is in the order of 20.85 MJ or 35% of the cooling power. To resume, before 90 minutes, 52 kg of methanol are desorbed

with a total heat consumed of 90.76 MJ (Q_w). The others maximum values were: $P = 250$ hPa, $T = 105^\circ\text{C}$, $m_{me} = 72$ kg, $Q_f = 81.3$ MJ, $Q_{des} = 52,64$ MJ, $Q_{ca} = 17$ MJ and $Q_{me} = 0,21$ MJ.

The influence in the COP, past 1 hour, of the hot water flow rate, m_w , and the inlet water temperature, T_{in} , is shown in Fig. 4. The dimensionless T_{in} represents a temperature from 45 to 105°C. It can be seen that an increase in the water flow and in the inlet temperature rises the performance, however an increment higher than 0.2 kg/s do not represent higher COP. The inflection of the curve of the T_{in} shows the beginning of the adsorption process, in ca. 60°C.

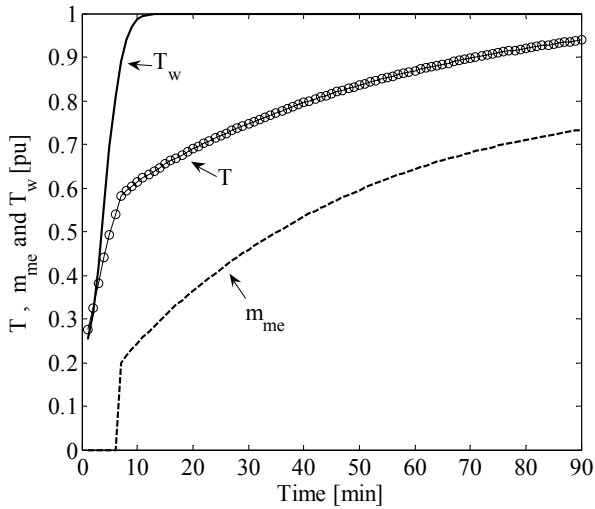


Fig. 2– Time response of T , m_{me} and T_w

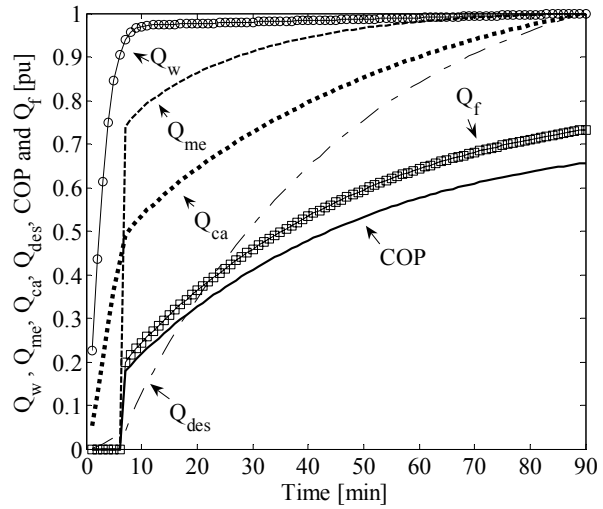


Fig. 3 – Time response of Q_w , Q_{me} , Q_{ca} , Q_{des} , Q_f and COP

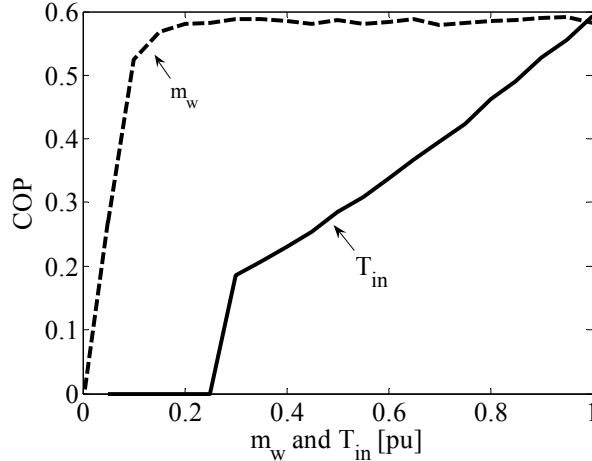


Fig. 4 – Effects of the hot water flow rates m_w and hot water inlet temperatures T_{in}

The COP presented in Fig. 3 and 4 was instantly calculated, but a great loss is not yet considered; the energy necessary to heat the remained cold water (inside the adsorber) in the beginning of the first cycle of the day. The shell-and-tube exchanger holds a great volume of water, in this case, 500 kg. It represents a loss of 168.2 MJ that muss be divided by the number of daily cycles, in this case, 10 cycles. The maximum COP falls from 0.65 to 0.55.

FINAL REMARKS

It was presented a description of the mathematical models to simulate the dynamic behavior of the shell-and-tube exchanger as an adsorber. The one-dimensional energy balance equations have been written, using the mixed finite-difference and finite-volume formulation.

The simulation results show that the system performance is strongly dependent on the operating conditions such as the operating temperatures, flow rates and cycle times. The performance of this exchanger is mostly influenced by the cycle time; it needs long time of operation, resulting lower specific cooling power. This is due to its great volume of water inside the shell. For the present application, other faster exchangers (compacts) are under study to build a comparison and find out the most suitable exchanger.

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