The influence of the reactor design in the performance of a chemisorption refrigerator

Carlos Javier Noriega Sanchez[1], Rogerio Gomes de Oliveira[2], Sérgio Colle[3]

[1]Department of Mechanical Engineering, Federal University of Santa Catarina (UFSC), Florianópolis, Brazil – noriegacarlosjavier@hotmail.com
[2] Campus Araranguá, USFC, Araranguá, Brazil – rogerio.oliveira@ararangua.ufsc.br
[3] Department of Mechanical Engineering, USFC, Florianópolis, Brazil – colle@emc.ufsc.br

ABSTRACT: We investigate the influence of the reactor characteristic in the specific cooling power, in the cooling power density and in the coefficient of performance (COP) of a chemisorption refrigerator using $SrCl_2$ compound adsorbent. The study was conducted through the simulation of a two-dimensional heat transfer mathematical model. The experimental conditions simulated were chosen according to a fractional factorial design and a central composite design. The reactor characteristics investigated were the length and thickness of the adsorption bed, the heat transfer fluid flow, the fins thickness and pitch, the type of the adsorbent, the cycle time, and the wall heat transfer coefficient. Among the above variables, the type of adsorbent was the most important one to increase the cooling power and COP. When the analysis was done considering only the consolidated adsorbent, it was possible to observe that the length of the adsorbent bed and the use of fins were not critical to the refrigerator performance. Moreover, the cooling power was negatively affected by the increase of the bed thickness and cycle time, whereas their COP was positively affected by the increase of these same variables. Such a result indicates that it is not possible to simultaneously maximize the cooling power and the COP through the manipulation of the bed thickness and cycle time. However, through the use of a central composite experimental design and contour plots, it was possible to identify conditions were both performance indicators could be simultaneously maximized.

Keywords: Adsorption, Experimental Design, Heat Exchanger, Refrigeration.

1. INTRODUCTION

The world dependence on non-renewable energy sources motivated in the last decades the study on renewable energy source, and on applications that use renewable sources and wasted energy. Such a type of study becomes even more urgent when considered that the International Energy Agency [1] estimated that the energy consumption will have an annual growth of 1,2 %

until 2035. Hence, in the last couple of years there was an increase in the studies related to sorption systems [2]. These systems can produce cooling effect using as the main source of energy a large range of heat sources, and which include solar energy and waste heat from different processes. The sorption systems comprise the aBsorption or the aDsorption machines. In the former type, both the sorptive and the sorbate are fluids, whereas in the latter type, the sorptive is a solid and only the sorbate is a fluid. The absorption technology is commercially more developed than the adsorption technology; however, the adsorption systems do not need an internal pump to circulate the sorbent, does not need rectification column, and they can be designed to operate in with a larger range of temperature sources.

Although the adsorption refrigerators can be an alternative to the mechanical compression refrigerators, the former are usually bulker and with lower coefficient of performance (*COP*) than the latter ones. The attempts to overcome these performance problems are related to the reduction of the heat and mass transfer resistance of the sorbent and to a better management of the heat used by the system [3-4]. For this reason, the proper design characteristic of the reactor that contains the adsorbent bed is critical to enhance the overall performance of the system. Hence, we study through simulation of mathematical model, the influence of certain design characteristics of the reactor on the *COP*, the specific cooling power (*SCP*) and the cooling power density (*CPD*) of an adsorption system using an adsorbent compound made with $SrCl_2$ and expanded graphite. The refrigerant was ammonia, and the adsorption capacity was described by the following reaction: $SrCl_2 \cdot 1NH_3 + 7NH_3 \Leftrightarrow SrCl_2 \cdot 8NH_3 + 7\Delta H_r$.

Where one mol of $SrCl_2$ can adsorb up to 7 moles of ammonia, and which leads to an adsorption capacity of 0.75 kg of refrigerant per kg of salt.

The mathematical model of the reactor considered two-dimensional heat transfer inside the adsorbent bed, and due to this characteristic, it enable us to verify the influence of the fins pitch and thickness and the bed length and thickness on the system performance.

2. EXPERIMENTAL PROCEDURE

2.1 Mathematical model

The mathematical model assumed a concentric tube reactor, as shown in Fig. 1, where the adsorbent was inside the inner tube and the heat transfer fluid flew in the channel formed between the concentric tubes. There was a hollow space in the middle of the adsorbent bed, in which the refrigerant gas could enter or leave the bed, respectively, during the adsorption and desorption periods of the cycle.

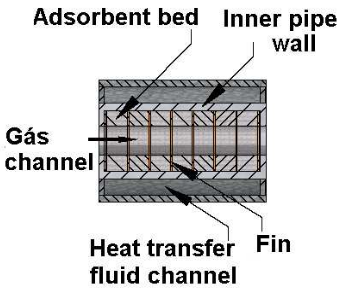

Figure 1. Reactor scheme.

The heat diffusion in the reactor bed is described by the following equation:

$$\hat{C}_B \frac{\partial T_B}{\partial t} = \lambda_B \frac{\partial^2 T_B}{\partial r^2} + \frac{\lambda_B}{r}\frac{\partial T_B}{\partial r} + \lambda_B \frac{\partial^2 T_B}{\partial z^2} + 7N_s \Delta H_r \frac{dx}{dt} \quad (1)$$

Where T_B is the adsorbent bed temperature, $\hat{C}_B$ is the adsorbent bed volumetric heat capacity, ΔH_r is the reaction enthalpy, λ_B is the effective bed thermal conductivity, N_s is the bulk molar density of salt, and x is the local reaction conversion.

The reaction rate was calculated with the following equations, respectively, in the adsorption and desorption periods:

$$\frac{dx}{dt} = k_{Ad} \exp\left(\frac{E_{Ad}}{RT_B}\right)(1-x)^{M_{Ad}}\left(\frac{P_c - P_{eq}}{P_{eq}}\right) \text{ and } \frac{dx}{dt} = k_{Ds} \exp\left(\frac{E_{Ds}}{RT_B}\right)x^{M_{Ds}}\left(\frac{P_{eq} - P_c}{P_{eq}}\right).$$

Where the subscripts *Ad* and *Ds* are respectively related to the adsorption and desorption reactions, k is the Arrhenius constant, E is the activation energy, M is an adjust factor. The value of these parameters were obtained in Huang et al. [5], P_c is the constrain pressure imposed by the evaporator or by the condenser, depending on the cycle period, and P_{eq} is the equilibrium pressure for the reaction between the salt and the refrigerant.

It was assumed that the thermal conductivity was a function of the proportion of the expanded graphite, the degree of reaction conversion and the bulk density of the expanded graphite in the composite sorbent. The value used in this work were based on experimental results with compounds that had similar bulk density, proportion of expanded graphite, and amount of ammonia adsorbed[6].

The model considered that each fin had negligible temperature gradient in the axial direction, and in the radial direction the temperature gradient was obtained with the following equation:

$$\hat{C}_{Fin}\frac{\partial T_{Fin}}{\partial t} = \lambda_{Fin}\frac{\partial^2 T_{Fin}}{\partial r^2} + \frac{\lambda_{Fin}}{r}\frac{\partial T_{Fin}}{\partial r} + \frac{1}{\varepsilon}\frac{(T_{Fin} - T_B)}{R_{ct}} \quad (2)$$

Where ε is the fin thickness and R_{ct} is the contact resistance between the bed and the pipe wall or the fin, or the contact resistance between the fin and the pipe wall.

The temperature gradient in the radial direction of the heat transfer fluid was assumed negligible, and the temperature gradient in the axial direction was obtained with the following equation:

$$\hat{C}_{Fl}\left(\frac{\partial T_{Fl}}{\partial t} + V\frac{\partial T_{Fl}}{\partial z}\right) = \frac{\pi D_W h_{cv}}{A_{Flow}}(T_W - T_{Fl}) \quad (3)$$

Where V is the fluid velocity, D_W is the pipe wall diameter, h_{cv} is the convection heat transfer coefficient, A_{Flow} is the cross-section flow area and T_W is the pipe wall temperature.

The convection heat transfer coefficient depended on the type of flow, i.e, completely developed laminar flow, completely developed turbulent flow or entrance region flow. The values were calculated as indicated in the literature [7-10]

The equation were solved with the initial conditions as $T_B = T_{Fin} = T_W = T_0$ and $x = 0$.

The following boundary conditions were assumed in the radial direction:

$$\left.\frac{\partial T_B}{\partial r}\right|_{r@gas.channel} = \left.\frac{\partial T_{Fin}}{\partial r}\right|_{r@gas.channel} = 0,\ \left.\lambda_B\frac{\partial T_B}{\partial r}\right|_{r@pipe.wall} = \frac{(T_B - T_W)}{R_{ct}} \text{ and } \left.\lambda_B\frac{\partial T_{Fin}}{\partial r}\right|_{r@pipe.wall} = \frac{(T_{Fin} - T_W)}{R_{ct}}.$$

In the axial direction, the following boundary conditions were used:

$$\left.-\lambda_B\frac{\partial T_B}{\partial z}\right|_{z@fin} = \frac{(T_{Fin} - T_B)}{R_{ct}} \text{ and } \left.T_{Fl}\right|_{z=0} = T_{In}.$$

Where T_{In} is the set-up fluid heat sink or heat source temperature, respectively, in the adsorption and desorption periods of the cycle.

The model was numerically solved with an implicit finite difference scheme and with the following assumptions: (1) the heat transfer fluid jacket was insulated; (2) the gas channel in the bed centre had a diameter of 10 mm; (3) the evaporator pressure was 0,4 MPa and in the condenser pressure was 1,2 MPa; (4) industrial oil was assumed as heat transfer fluid, and its properties were obtained in the literature [11]; (5) the set-up heat transfer fluid temperature in the adsorption period was 30 °C, whereas in the desorption period it was 140 °C; (6) the mass transfer resistance was assumed negligible, according to the results obtained by Lu et al. [12] and Han and Lee[13].

2.2 Performance indicators

The performance indicators for the adsorption refrigerator studied were the *COP*, the specific cooling power (*SCP*) and the cooling power density (*CPD*). The *COP* is related to the first law efficiency of the machine, and it is expressed as the ratio between the cooling capacity of the machine (Q_e) and the heat consumed by the machine during the regeneration period of the cycle (Q_r). The *SCP* is related to the cooling power of the machine per mass unit of adsorbent, whereas *CPD* is related to the cooling power of the machine per volume of reactor. The following equations were used to calculate the *COP*, the *SCP* and the *CPD*:

$$COP = \frac{Q_e}{Q_r}\,,\; SCP = \frac{Q_e}{m_{Ads}\,\Delta t/2} \text{ and } CPD = \frac{Q_e}{\forall_{Reactor}\,\Delta t/2}$$

$$Q_e = \sum_{i=0}^{\Delta t/2} 7 M_{NH3} \forall_B N_s \left[h_{vl} - Cp_{NH3}\left(T_{Cn} - T_{Ev}\right)\right]\frac{dx_i}{dt} \text{ and } Q_r = \dot{m}_{Fl}\sum_{i=0}^{\Delta t/2}\left(T_{In.i} - T_{Out.i}\right)$$

Where m_{Ads} is the mass of adsorbent inside the reactor, $\Delta t/2$ is the length of the adsorption or the desorption period of the cycle, $\forall_{Reactor}$ is the reactor volume, not including the volume of the heat transfer fluid jacket, M_{NH3} is the molar mass of ammonia h_{vl} is the vaporization enthalpy of ammonia, Cp_{NH3} is the specific heat of liquid ammonia, T_{Cn} is the condensation temperature, T_{Ev} is the evaporation temperature, T_{In} is the inlet heat transfer fluid temperature, T_{Out} is the outlet heat transfer fluid temperature and $\dot{m}_{Fl}$ is mass flow of the heat transfer fluid.

2.3 Experimental design and simulation conditions

The mathematical model was solved in a set of experimental conditions where the values of the independent variables varied according to a fractional factorial design (*FFD*) [14]. Such a procedure was used to access which was the effect of each independent variable in the *COP*, in the *SCP* and in the *CPD*. The value of each independent variable was codified as -1 and as +1, and the independent variables assumed a value related to one of these levels in each experimental condition. The number of experimental conditions necessary to identify the effects in a *FFD* was equal to 2^{k-r}, where k is the number of independent variables and r is the resolution of the design. Tab. I shows the 8 independent variable used in the *FFD*, which had a resolution equal to four. Hence, the number of experimental conditions necessary to identity the effects were 16. The outer radius of the reactor was the variable that represented the influence of the bed thickness.

A positive effect indicates that the change in the value of the independent variable from its level -1 to its level +1 increases the response variable, whereas a negative effect indicates the opposite.

Although a level of confidence of 95 % is usually employed to ensure that a response is statistically significant, we assumed that an effect was statistically significant if the confidence level was above 90 %. This was done because in the *FFD* with resolution equal to four, the main effects are mixed with third order interaction effects, and the use of a level of confidence of 95 % could exclude the possibility that some variables are indeed important to the system performance.

Once we identified which were the variables with statistical significant effects, we conducted other simulations on the experimental conditions indicated by a central composite design (*CCD*). The latter design had 2^k experimental conditions, plus experimental conditions in the central and star points (α)[14]. The experiments in the central point correspond to the operation conditions in which the codified value of all independent variables was equal to 0. In this case, no independent variable with discrete value, as the type of adsorbent, were tested.

Table I. Independent variables and their levels in the *FFD*.

Variable	Level -1	Level +1
Outer radius of the bed [mm]	16.70	36.51
Heat transfer fluid flow [L/min.]	61.70	1750
Bed length [mm]	250	750
Cycle time [min.]	30	60
Type of adsorbent	Powder	Consolidated
Fin pitch [mm]	10	30
Fin thickness [mm]	0.25	0.45
Contact thermal resistance [m^2.K/W]	10^{-3}	10^{-2}

The code number for the star points (α) depends on the number of independent variables, and on the number of times that each experimental condition was repeated. For a *CCD* with no repetition $\alpha = \left(2^k\right)^{1/4}$ [14].

The conduction of the experiments according to the *CCD* allowed us to obtain the coefficients of a 2° order polynomial model that where used to create surface responses and contour plots, which were used to maximize simultaneously different performance indicators, as the *COP* and the *CPD*. The simultaneous maximization was possible to be done by visual inspection of the contour plots, and occurred at the operation conditions in which the value of the dependent variables DV_x made the result of the following equations equal.

$$DM_{V1} = \frac{DV_1 - DV_{1\min}}{DV_{1\max} - DV_{1\min}} \times 100\% \text{ and } DM_{V2} = \frac{DV_2 - DV_{2\min}}{DV_{2\max} - DV_{2\min}} \times 100\% .$$

Where DM_x is the percentage increase of the dependent variable DV_x above its minimum value in the contour plot. A DM_x equal to 100 % implies that the dependent variable reached its maximum value on the operation conditions presented in the contour plot.

3. RESULTS

According to the results presented in Tab. II, the independent variables that have the highest influence on the indicators of performance are the cycle time and the type of the adsorbent.

Considering the results of the 16 experimental conditions of the *FFD*, it was observed that the use of consolidated adsorbent instead of powder adsorbent decreased in the mean, the SCP in 93.6 W/kg, but increased the CPD in 37.23 kW/m^3 and the COP in 0.107.

Because the type of the adsorbent had a far higher influence on the performance indicators, we conducted a second *FFD*, in which only the consolidated adsorbent was used. The values of the conditions -1 and +1 for the other variables were the same as those presented in Tab. I, except for the fin pitch and the heat transfer fluid flow. In the second *FFD*, the fin pitch level -1 corresponded to the absence of fin, whereas the level +1 corresponded to a 10 mm pitch. The fluid flow was reduced in 20 times because from the first set of experiments, we identified that it would be necessary about 20 reactors to achieve a cooling power of 1 TR, which was the rated cooling power to be achieve by the small size machine. Moreover, the fin thickness was not included in the second *FFD* because this was the variable with the smallest influence on the performance of the machine.

Table II. Effect of 8 independent variables on the performance indicators.

Variable	SCP [W/kg]	CPD [kW/m^3]	COP [-]
Mean value	181.43	26.47	0.111
Outer radius of the bed	-11.48	2.13	0.065*
Heat transfer fluid flow	8.59	2.32	0.002
Bed length	1.59	0.89	0.001
Cycle time	-61.74*	-7.09*	0.026*
Type of adsorbent	-93.60*	37.23*	0.107*
Fin pitch	-10.29	-2.09	-0.001
Fin thickness	0.49	-0.96	-0.003
Contact thermal resistance	-11.86	-3.994	-0.006

From the results of the second *FFD* presented in Tab. III, it was possible to observe that the heat transfer fluid flow had a statistically significant positive effect on all performance indicators, whereas the thermal resistance had the opposite behaviour. The increase of the bed length and the use of fins did not have statistically significant effects, which is an indication that these variables are not critical to the performance of the system. Hence, if the machine uses consolidated adsorbent, the use of fins is not necessary, and the bed can be designed to be long, with about 75 cm in length. The results of Tab. III also indicated that the increase of the bed radius (i.e. thickness) and cycle time had a negative influence on the cooling power of the system, but a positive effect on the COP. Hence, it is not possible to optimize the cooling power and the COP simultaneously in respect to these two variables. However, through the superposition of contour plots, which were draw from the results of the *CCD*, it was possible to identify a range of values for these variables were both the COP and the cooling power could be simultaneously maximized.

Table III. Effect of 6 independent variables on the performance indicators.

Variable	SCP [W/kg]	CPD [kW/m^3]	COP [-]
Mean value	110.68	39.40	0.147
Outer radius of the bed	-35.01*	-5.40*	0.042*
Heat transfer fluid flow	25.93*	9.76*	0.017*
Bed length	-10.84	-4.37	-0.008
Cycle time	-22.46*	-7.89*	0.043*
Fins	12.09	3.15	0.004
Contact thermal resistance	-22.46*	-8.07*	-0.015

The Fig. 2 shows the contour plots for the *CPD* and the *COP* as function of the cycle time and outer radius of the bed, for three different heat transfer fluid flow. It is possible to see in

* Statistically significant with 90% confidence.

the hatched area of Fig. 2.1 that the *COP* and the *CPD* are on the fifth level above its minimum if the cycle time is 32 minutes, the outer radius is 32 mm and the heat transfer fluid flow is 24 L/min. At these same conditions, except that the fluid flow is to 45 L/min (Fig. 2.2), the *COP* and the *CPD* can reach values within their sixth level. When the fluid flow rises to 66.4 L/min. (Fig. 2.3) the simultaneous maximization occurred at the same value of outer radius, however at lower cycle time of 30 minutes. The contour plots also showed that it was possible to keep the value of the *CPD* within the same level but increase one level for the COP, when the fluid flow was 24 L/min. and 66.4 L/min. Hence, for the studied case, a reactor with an outer diameter of 32 mm operating under a cycle time of 36 minutes would lead to COP between 0.15 and 0.18 and a CPD between 42 and 48 kW/m^3, depending on the heat transfer fluid flow.

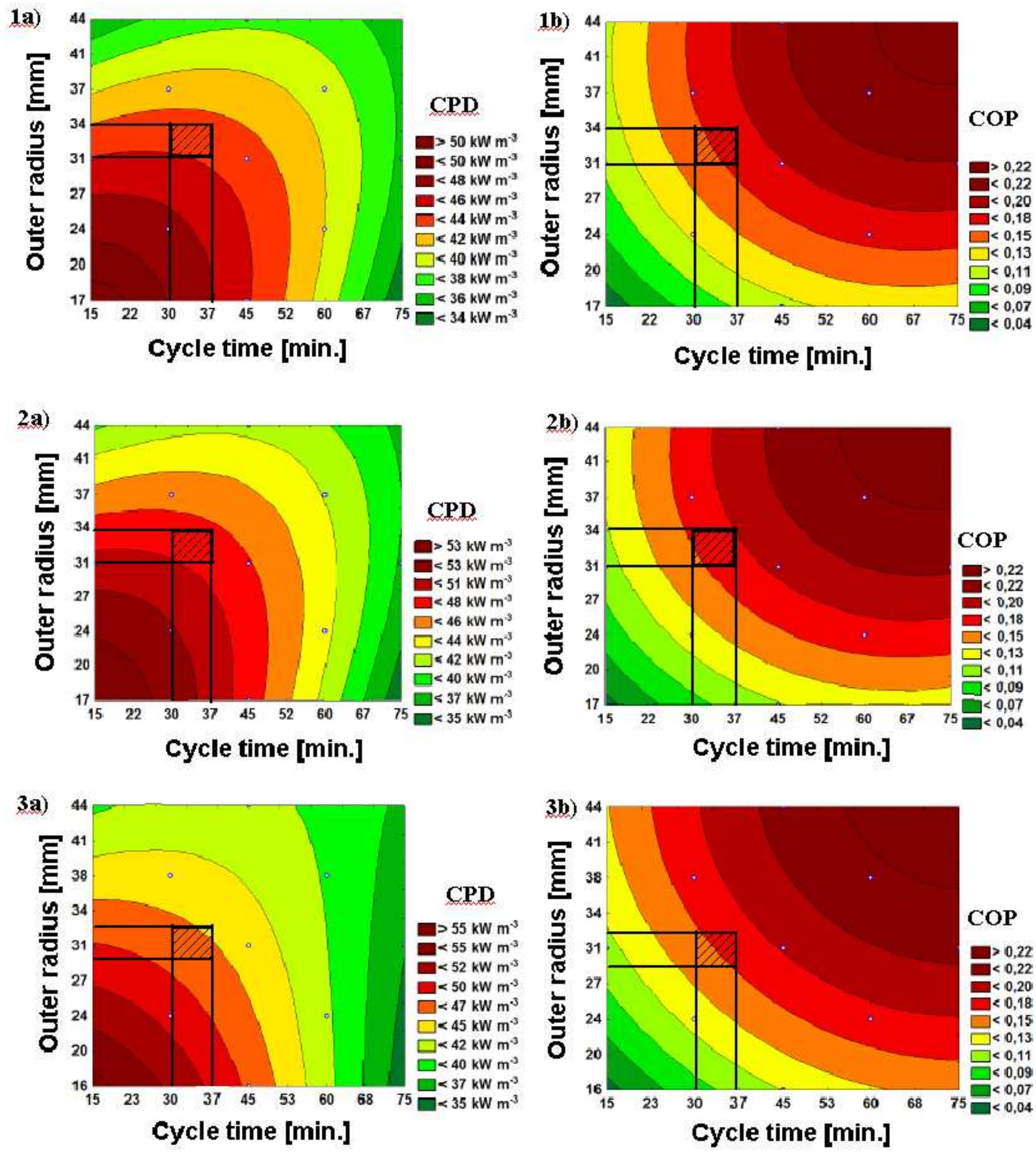

Figure 2. Contour plots of performance indicators as function of outer radius and cycle time with heat transfer fluid flow at (1) 24 L/min, (2) 45 L/min and (3) 66.4 L/min. Performance indicator equal to (a) CPD and (b) COP.

Higher values for the *COP* or for the *CPD* could be obtained, but this would imply that one of these variables would have a larger reduction from the maximum value.

4. CONCLUSIONS

The result of the experiments showed that the use of fins and the length of the adsorbent bed are not criticals to the performance of the machine when the reactor is filled with consolidated adsorbent. Moreover, the variables with the highest influence of the system performance were the bed thickness and cycle time. The increase of these variables decreases the cooling power but increase the COP; hence, it is not possible to optimize both performance indicators regarding these two variables. However, through the use of superposed contour plots, it was possible to find operation regions were both variables were simultaneously maximized.

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