ADSORPTION DYNAMICS IN DESICCANT DEHUMIDIFICATION COLUMN

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Abstract. *This paper presents a numerical simulation of a column packed-bed using silica gel. The simulation involves a 100 cm column containing spherical silica gel particles with an average diameter of 5 mm. The problem consists of a cylindrical column filled with uniform silica gel (desiccant material) that is initially almost dry, submitted to humid air flow with prescribed temperature, pressure, concentration and speed in the entrance of the column. A one-dimentional, transient and non-isothermal method derived from the heat and mass equations as applied to both the stream bed and the grain was used. The equations were resolved by the finite-volumes method using a full implicit scheme with a colocated arrangement. The linear systems were chosen by means of the algorithm of Thomas (TDMA). The results are presented in the form of temperature and relative humidity outlet column profiles, and the amount of adsorved mass column in relation to time. These results were shown to be physically consistent with the condition of the desired end result. The simulation showed the necessary time for column saturation and the possible time for drying, without the need for column regeneration.*

Keywords: Adsorption, Silica Gel, Desiccant, Dehumidification

1. Introdução

Adsorption is a well-known phenomenon dating back to the 18th Century, when it was observed that definitive type of coal had the capacity to hold back great amounts of water vapor and after its saturation was necessary to submit it a hot and dry air flow for regeneration of the desiccant one. Since then, diverse research comes being carried through in the development of new adsorbent materials and improvement of the involved processes of manufacture.

In the last decades, the adsorption has come to be used in diverse applications, for example, in purification processes for which a fixed-bed column filled up with desiccant material, with the purpose to remove the humidity of the adsorbate. The main used desiccant materials in the adsorption processes are: silica gel, activated alumina and zeólite.

In the adsorption processes, the choice of the desiccant material depends on the type of application to be used and on the type of used adsorbate, therefore each pair adsorbent/adsorbate has a particular behavior.

In the case of the dehumidification processes, the Silica Gel has been used as desiccant material for some time now thanks to its high performance in the removal of water vapor found in humid air in the ventilation systems of most modern buildings. Its microscopic structure with a huge external area may account for the high adsorption facility (Sun and Besant, 2005).

Packed-beds have many industrial applications, the most important of which are: air dehumidification to prevent humidity adsorption in storing hygroscopic products (pharmaceuticals, jellies, sweets, other food products and grains), the acclimatization of areas where products are vulnerable to humidity instability (such is the case of laminated glass production and soluble foods), the prevention of condensation in plastic injection moulds in industrial processes submitted to sudden cooling, and, finally among a number of other applications, the reduction of power consumption in some air-conditioner systems by diminishing the excess of condensation in coils and heat-exchangers. The low operational and initial costs constitute some of the greatest advantages that clearly justify the use of packed-beds. Another advantage lies in the fact that packed-beds do not make use of toxic gasses and may be regenerated at low temperatures with the use of solar energy.

The study of adsorption dynamics in packed-beds has been developed for some time now. Cooney (1974) conducted a numerical study of the adsorption dynamics on an adiabatic column, where the velocity within the bed and the concentration in the core of the grain were taken to be constant, analyzing as well the adsorbate found at the entrance of column, the heat and mass transfer coefficients on the surface of the grain and the adsorption heat over the dynamics of the bed. Pessaran & Mills studied humidity transfer on packed-beds both analytically (1987a) and experimentally (l987b) with a focus on water-vapor resistance in the core of the grain. Park and Knaebel (1992) calculated the dynamics of water-vapor adsorption over a silica gel fixed-bed, assessing in this way the humidity content present in the humid air that flows through the column by taking into account the constant air flow velocity and by using the of differences finite method in order to determine the adsorption rate in silica grains. San & Jiang (1994) experimented with and modeled analytically the transient response obtained from a system of double packed-beds with silica gel employed for dehumidification. Inaba and Horibe (2004) examined numerically the adsorption features within a rectangular bed with silica gel spherical particles when submitted to a humid air flow and proposed a bi-dimensional model as obtained from mass and energy consideration equations.

The present work has as its main objective the study of the dynamics of adsorption in packed-beds with the purpose of investigating heat and mass transfer via temperature profiles and adsorbed mass along the column, seeking at the same time to determine the relative humidity at the bed outlet. Its purpose is also that of investigating column saturation time and dehumidification time capacity on the packed bed without the need for regeneration.

Notation

Cp	specific heat at constant pressure [J/kg K]	*Greek letters*
C_S	volumetric heat capacity of the solid [J/m³ K]	ε — bed porosity
C_m	volumetric heat capacity of the mixture [J/m³ K]	λ — thermal conductivity [W/m K]
d_p	pellet diameter [m]	ρ — specific mass [kg/m³]
D_{ef}	effective mass diffusion coefficient [m²/s]	ϕ — relative air humidity [%]
D_L	axial dispersion [m²/s]	
q	concentration in the solid phase [kg/m³]	*Subscripts*
$\bar{q}$	volumetric average concentration over pellet [kg/m³]	∞ — Relative at the ambient conditions
u	interstitial velocity [m/s]	0 — Relative at the initial condition
h	convection heat transfer coefficient [W/m² K]	e — Relative at the external surface
ΔH	heat of adsorption [J/kg]	f — Relative at the fluid phase
L	column length [m]	I — Relative at the internal surface
Nu	nusselt number	in — Relative at the column inlet
p	pressure [Pa]	p — Relative at the pellet
P	pressure [Pa]	S — Relative at the solid phase
Pr	Prandtl number	w — Relative at the column wall
r	pellet radial coordinate [m]	a — dry air
R	column radius [m]	v — water vapour
R_e	Reynolds number	m — gás (dry air + water vapour)
R_g	ideal gas constant [J/kg K]	
t	time [s]	*Superscript*
T	temperature [K}	* — Relative at the adsorption equilibrium
U_g	Overall heat transfer coefficient [W/m² K]	
x	axial coordinate in the column [m]	

2. Mathematical Modeling

The present paper is concerned with adsorption dynamics on gel silica packed-bed through which there runs a flow of humid air (dry air and water vapor); the adsorbate used to fill up the bed was found to be almost dry, a description of which is shown in Figure 1.

The governing equations used in the present work take into account the heat and mass transfer equations based on simplifying hypothesis resulting to mass diffusion model in non-isothermal grains and the adsorptive packed-bed. Due to the complexity of these equations, some simplifying hypotheses have been considered in order to facilitate the mathematical modeling, such as: (1) velocity along the column was taken as constant; (2) pressure drop along the column is negligible; (3) heat transfer within the packed bed takes place through convection, and water vapor mass diffusion; (4) the adsorbate used in the flow that runs through the packed bed has been considered to be the ideal gaseous mixture; (5) temperature and the effective mass coefficient in the grain were taken as uniform. The instantaneous equilibrium on the surface of the grain has also been considered by means of a non-linear isotherm.

In order to further simplify the numerical approach, an adsorptive bed was regarded as consisting of a horizontal column occupied by a number of control volumes, where every volume is represented by a single adsorbent

homogenous spherical grain that is submitted to a humid air flow (Figure 2). Differently, the exact packed bed representation would result exceedingly complex, requiring, as it is, unfeasible computational time in order to produce such detailed information.
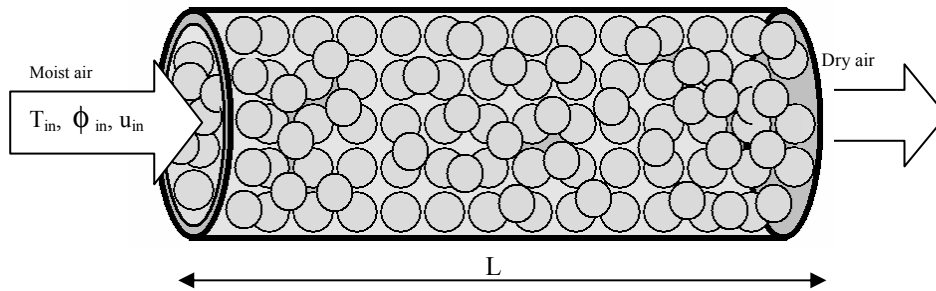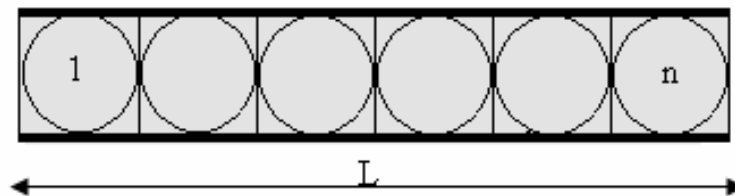

Figure 1 – Packed bed diagram

Figure 2 – Packed-bed plan considering an absorbent grain for each control volume.

2.2 Mass diffusion model for non-isotherm grains

The mathematical model proposed is made up of mass diffusion equation and energy conservation equation:

$$\frac{\partial q}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 D_{ef} \frac{\partial q}{\partial r}\right) \tag{1}$$

$$C_S \frac{\partial T_S}{\partial t} = \frac{6\,h_P}{d_P}\left(T_f - T_S\right) + \left(-\Delta H\right)\frac{\partial \bar{q}}{\partial t} \tag{2}$$

The average quantity of adsorbed water is calculated by means of the following equations

$$\bar{q} = \frac{3}{R_P} \int_0^{Rp} q(r,t)\,r^2\,dr \tag{3}$$

Initial conditions and boundary of equations (1) and (2) are:

$$t < 0: \qquad q(r,t) = q^*(p_0, T_0); \qquad T_S(t) = T_0 \qquad para \qquad 0 \leq r \leq R_P \tag{4}$$

$$r = 0: \qquad \frac{\partial q(r,t)}{\partial t} = 0 \qquad para \qquad t > 0 \tag{5}$$

$$r = R_P: \qquad q(r,t) = q^*(p, T_S) \qquad para \qquad t > 0 \tag{6}$$

2.3 Adsorbed packed-bed model

Mass transfer equation for calculating the mixture:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial}{\partial x}\left(u\,\rho_m\right) = -\frac{1-\varepsilon}{\varepsilon} \frac{\partial \bar{q}}{\partial t} \tag{7}$$

Mass transfer equation for calculating water vapor:

$$\frac{\partial \rho_v}{\partial t} + \frac{\partial}{\partial x}(u\,\rho_v) = \frac{\partial}{\partial x}\left(D_L\,\frac{\partial \rho_v}{\partial x}\right) - \frac{1-\varepsilon}{\varepsilon}\,\frac{\partial \overline{q}}{\partial t} \tag{8}$$

Axial dispersion coefficient for humid air flow in the adsorption of the packed bed is expressed by the following equation (Ruthven, 1984):

$$D_L = \gamma_1\,D_m + \gamma_2\,2\,R_p\,u \tag{9}$$

Energy balance equation for column adsorption:

$$\frac{\partial}{\partial t}\left(C_M\,T_f\right) + \frac{\partial}{\partial x}\left(C_M\,u\,T_f\right) = \frac{\partial}{\partial x}\left(\frac{\lambda_f}{cp_f}\,\frac{\partial T_f}{\partial x}\right) + \frac{6\,h_p}{d_p}\,\frac{(1-\varepsilon)}{\varepsilon\,cp_f}(T_s - T_f) + \frac{2U_g(T_\infty - T_f)}{\varepsilon\,R_i cp_f} \tag{10}$$

$$p_v = \rho_v\,R_g\,T_f \tag{11}$$

$$C_M = \rho_m\,cp_m \tag{12}$$

The initial and boundary conditions are:

$$t < 0: \quad \rho_v(x,t) = \rho_0\,; \quad \rho_m(x,t) = \rho_0\,; \quad T_f(x,t) = T_0 \qquad \text{for} \quad 0 \le x \le L \tag{13}$$

$$x = 0: \quad \rho_v(x,t) = \rho_{vin}\,; \quad \rho_m(x,t) = \rho_{min}\,; \quad T_f(x,t) = T_{in} \qquad \text{for} \quad t \ge 0 \tag{14}$$

$$x = L: \quad \frac{\partial \rho_v(x,t)}{\partial t} = 0\,; \quad \frac{\partial \rho_m(x,t)}{\partial t} = 0\,; \quad \frac{\partial T_f(x,t)}{\partial t} = 0 \qquad \text{for} \quad t \ge 0 \tag{15}$$

2.3.1 Determining the wall heat transfer coefficients

The resistance to heat transfer on the column wall may be represented by the addition of the internal, external resistances and the wall resistances (Ruthven, 1984). The equation to describe the heat transfer coefficient on the wall may be expressed as follows:

$$U_g = \frac{1}{\frac{1}{h_i} + \frac{R_i}{\lambda_w}\,ln\left(\frac{R_e}{R_i}\right) + \frac{R_i}{R_e}\,\frac{1}{h_e}} \tag{16}$$

According to Ruthven, the internal convection coefficient may be expressed by the equation:

$$Nu_i = \frac{h_i D_i}{\lambda_f} = 0.813\,Re^{0.19}\,e^{-6\,dp\,/\,Di} \tag{17}$$

As for the external convection coefficient, forced convection conditions were adopted, and the convection coefficient was then obtained by the equation (18), as suggested by Incorpera and De Witt (2002).

$$Nu_e = \frac{h_e D_e}{\lambda_{air}} = 0.193\,Re^{0.618}\,Pr^{1/3} \tag{18}$$

3. Numerical Treatment

The governing equations (1), (7), (8) and (10), subjected to the following initial conditions (4-6), and of the boundary (13-15) were expressed via finite volumes methods with an entirely implicit formulation and with co-localized arrangements (Maliska, 1995). The Upwind interpolation scheme was used so as to avoid the properties in the control volumes interfaces.

Equations (1), (7), (8) and (10) were integrated into both space and time by means of the Upwind scheme from which the following equation was obtained:

$$A_p \varphi_P = A_e \varphi_E + A_w \varphi_W + B \tag{19}$$

Where φ may represent q, ρ_v, ρ_m and T_f, depending on the required equation. The equations obtained in this way are one-dimensional forming as a result a three-dimensional matrix.

The system's solution procedure will be iterative, resolving one equation at a time at every time instance. In order to elucidate the system of linear equations provided by equation (19), Thomas' algorithm was used (TDMA), Maliska (1995).

The following convergence criterion was used to interrupt the iterative process:

$$\left| \frac{\phi_P^{k+1} - \phi_P^k}{\phi_{max} - \phi_{min}} \right| \leq 10^{-5} \tag{20}$$

Where $\left| \phi_{max} - \phi_{min} \right|$ represents the maximum and minimum variations of the fluid phase obtained after a n-iterations. Another iteration will be required as long as such condition is not verified.

4. Numerical results

The adsorbent properties (Silica Gel Sorbead type C) used in the simulation were derived from Santos (2005) and Andrade Filho (2001) as shown in Table 1. These were the parameters studied: temperature and humidity profile at the column outlet, the adsorbate velocity and the amount of adsorbed mass at different places along the column.

Table 1 – Data used in the simulation (Santos, 2005 and Andrade Filho, 2001).

Parameter	Symbol	Value
Particle radius	R_p	0.5 mm
Column length	L	1 m
Column inner radius	Ri	2 cm
Initial temperature	T_0	305 K
Adsorbate velocity	u	1 e 1.5 m/s
Effective diffusion coefficient	D_{ef}	5×10^{-10} m^2/ s
Axial dispersion	D_L	Eq. (9)
Adsorption heat	ΔH	3×10^6 J/kg
Bed porosity	ε	0.4
gás constant	R	461.52 J/kgK
Adsorbent density	ρ_s	1270 kg/m^3
Surrounding temperaure	T_∞	305 K
Specific heat	Cp_S	1074 J/kgK
Overall heat transfer coefficient [W/m^2 K]	U_g	Eq. (16)

Figure 3 shows adsorbed mass profiles for specific points along the packed bed when relative humidity and temperature at the column inlet are equal to 73% and 32º C, respectively. These profiles reveal that the grain closer to the column inlet – represented by the first volume control – achieves its saturation state much faster and in sequential form in relation to other control volumes as the front mass penetrates the column until it achieves complete saturation. This happens so because the mass transfer zone reaches the first grains at the same time it cools them. Here the maximum adsorbed mass for this particular type of silica gel under such conditions corresponds to approximately 330g of vapor/kg silica, and the saturation time is approximately 24 hours.

The temperature profiles along the packed bed as represented in Figure 4 show two stages. In the first stage, temperature rises rapidly till it gets to its maximum level within the profile. In the second stage, however, it gradually drops off till the inlet temperature is achieved. The temperature is entirely related to the adsorbed mass once first grains adsorption takes place very fast. As adsorption is an extremely high exothermic reaction, an enormous heat production does occur. This heat is then dragged on by the adsorbate that flows along the bed in such a fashion that fluid temperature rises fast during the first stage. Maximum temperature is approximately 57ºC, and saturation time is the same as that shown in Figure 3.
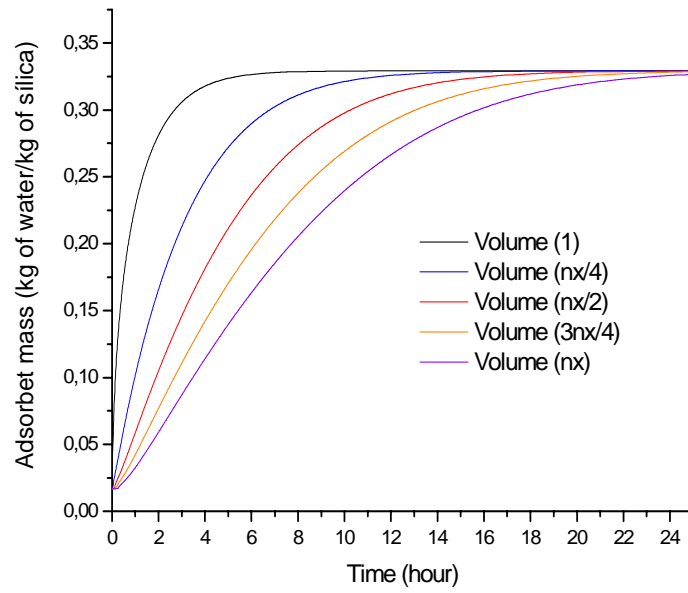
Figure 3: Adsorbed mass (u=1.5 m/s, UR$_\infty$= 73%, T$_\infty$=32ºC, D$_{ef}$= 1.34x10^{-10} m^2/s).
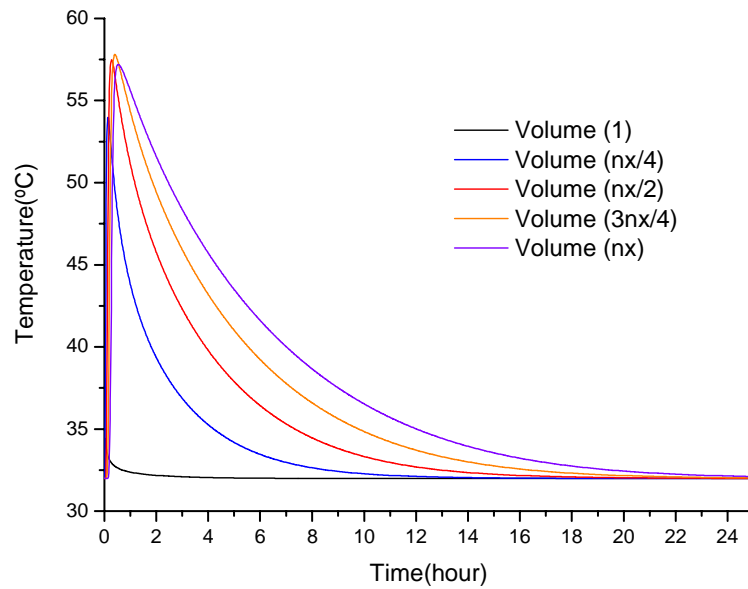
Figure 4: Temperature profile (u=1.5 m/s, UR$_\infty$= 73%, T$_\infty$=32ºC, D$_{ef}$= 1.34x10^{-10} m^2/s).
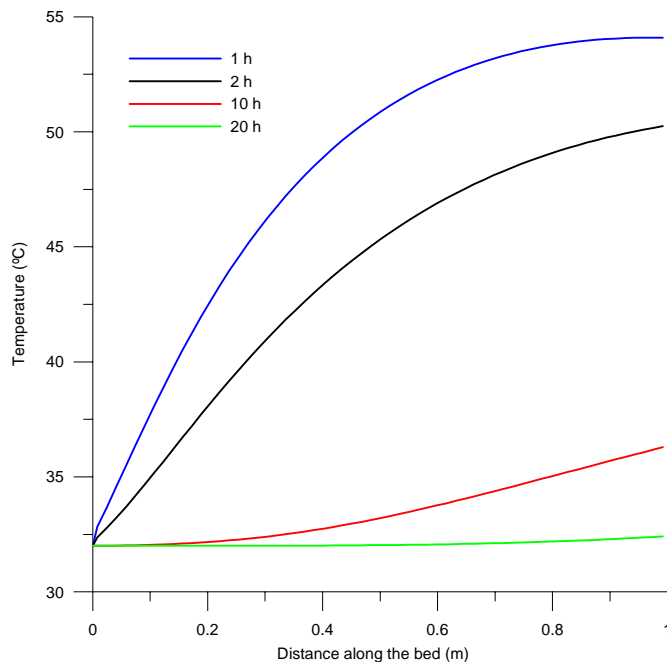
Figure 5: Temperature profile along the bed (u =1.5 m/s, UR_∞= 73%, T_∞=32ºC, D_{ef}= 1.34x10^{-10} m^2/s).

Figure 5 shows the temperature profiles for along the column at distinct time intervals (period). One can easily see that the maximum temperature is found at the first hour, and it comes probably as a result of the fast adsorption creating in this way isotherm heat which propagates all along the column. As the front mass spreads, there occurs a fall in temperature at all instants until the whole column attains thermal balance, which for this configuration may take about 24 hours. It results that the outlet temperature is equal to the inlet temperature.
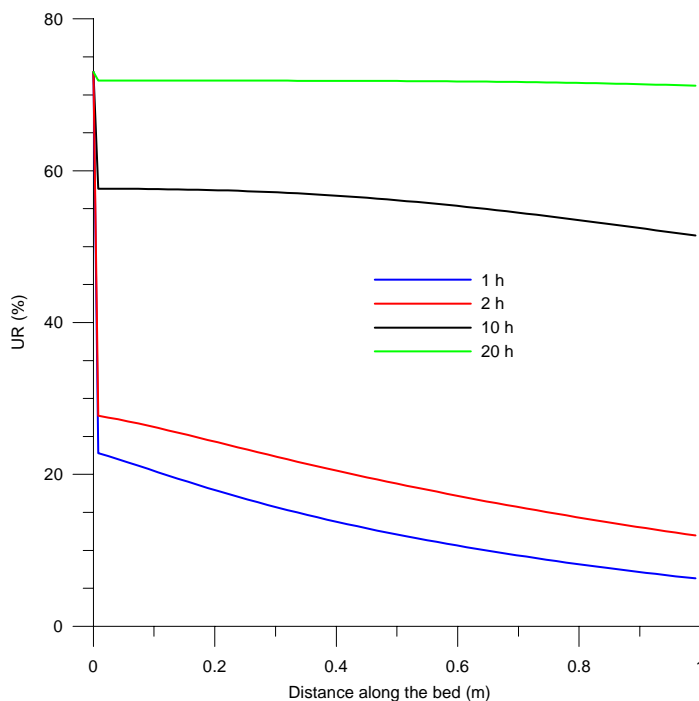

Figure 6: Relative humidity profile along the bed (u =1.5 m/s, UR_∞= 73%, T_∞=32ºC, D_{ef}= 1.34x10^{-10} m^2/s).

Figure 6 shows a decrease in relative humidity along the adsorbent bed during the first few hours of the simulation process. As the time interval gets longer, the bed is deprived of its capacity to retain the water vapor found in humid air until complete saturation of silica grains that permeate the bed takes place. Along the first centimeters of the column

length, one notices that for every time interval, there occurs an abrupt drop in relative humidity. This is accounted for the fact that the bed presents at the outset very low relative humidity, and on getting into contact with the humid air flow (around 73%) it adsorbs the water vapor present in the air very fast. As the grain loses its adsorption capacity due to its saturation state, this difference tends to decrease to the point at which the air humidity at the bed inlet equals to that of the bed outlet.

5. Conclusions

The present work investigated numerically the adsorption dynamics within packed bed by applying a number of heat and mass transfer equations. To calculate the heat and mass transfer equations, a computational code based on the finite volumes method was used. The numerical results obtained for the specified conditions at the entrance (inlet) revealed that complete column saturation occurs when the last volume attains its saturation state. Both temperature and relative humidity profiles did reveal themselves to be physically consistent with Park and Knaebel's experimental data (1992). The column saturation time was approximately 24 hours. Moreover, the humidity content was observed to be around 50% within a period of 10 hours; that is an excellent dehumidification period for which no regeneration process had been used. The research will continue with the construction of a packed-bed prototype at the Solar Energy Laboratory.

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7. Acknowledgements

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