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MATHEMATICAL MODELING OF ADIABATIC ADSORPTION

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Abstract. The application of evaporative cooling in HVAC systems has been steadily increasing over the last decades, powered by the cost reduction associated with the use of a thermal source rather than electric power. The use of evaporative cooling cycles is usually limited to climates with low average levels of relative humidity, however, the development of both liquid and solid desiccant systems has widen the range of application of such systems. Accordingly, the present work aims at developing a simple mathematical model to describe the water-vapor adsorption in a desiccant wheel, so as to evaluate the influence of the sorptive material over the coeffcient of performance of evaporative cooling cycles.
Keywords. *adsorption, desiccant cooling, evaporative cooling.*

1. Introduction

Desiccant wheels consist of a porous disc strongly impregnated with a hygroscopic material, such as silica-gel or molecular sieves. The fresh air stream is forced through the wheel, experiencing a strong decrease in its absolute humidity as it flows through micro channels. The humidity is purged out of the desiccant material by forcing a hot regeneration air stream through the wheel, as depicted in Figure 1. One of the earliest efforts of modeling air dehumidification by adsorption was made by Trelkheld and Bullock (1966) , which used a predictor corrector method to obtain silica gel equilibrium data under adsorption conditions. Maclaine-Cross and Dunkle (1982) proposed a model in which the mass and energy equations were uncoupled under some simplifying assumptions. More recently, many numerical solutions have been provided, predominantly investigating the influence of thermal resistance to heat and mass diffusion within the desiccant material (Niu et al., 2002: Pesararn, 1980; Shen and Worek, 1992). Zhang et al. (2003) proposed a “lumped-distributed” model, which considered mass and temperature distributions only in the flow direction. Their dimensional model shows reasonable agreement with experimental data, and was able to predict some interesting features such as the re-adsorption of water vapor at the beginning of the desorption period at locations far from the heat source. Accordingly, the present work uses a one-dimensional model to evaluate the influence of the adsorptive material selection over the performance of a desiccant cooling cycle.

2. Mathematical Model

Consider a single flow channel detached from the wheel, as shown in Figure (1). Some assumptions are reqired:

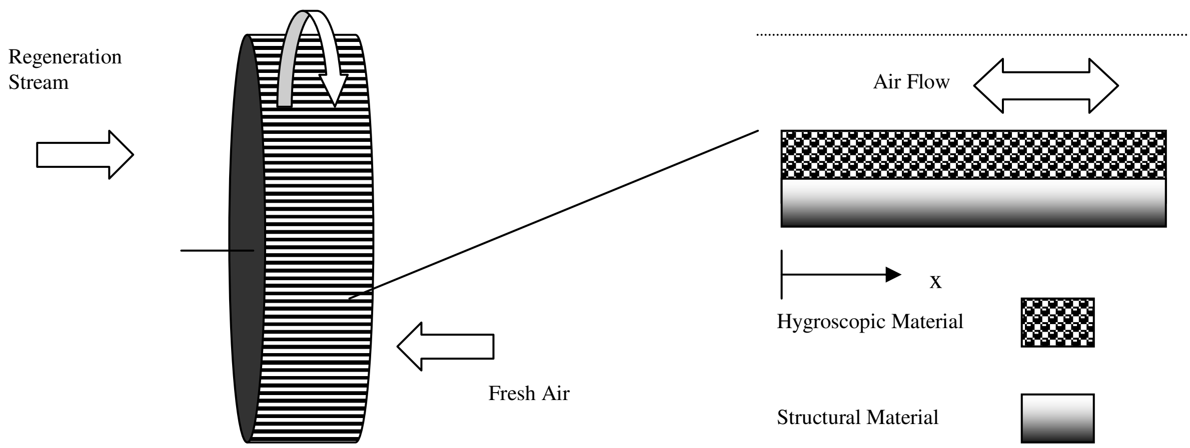

Figure 1. A typical control volume

- The channels are perfectly insulated.
- All thermo-physical properties for the fluid and the solid are considered constant.
- The flow is hydro-dynamically and thermally developed.
- Temperature and concentration distributions in the direction normal to the flow are taken to be uniform (lumped) within the channel and the solid.
- The adsorption heat is modeled as a heat source within the solid material

Based on these assumptions, the following balances are applied to elementary control volumes:

<u>Mass conservation in a control volume enclosing the channel and the solid</u>

$$\dot{m}_1\left[\frac{1}{u_1}\frac{\partial Y^*}{\partial t}+\frac{\partial Y^*}{\partial x}\right]+\frac{f\ m_w}{x_{AF}}\frac{\partial W}{\partial t}=0 \tag{1}$$

<u>Mass conservation in a control volume enclosing the solid</u>

$$\frac{f\ m_w}{x_{AF}\ y_{AF}}\frac{\partial W}{\partial t}=2h_y\left(Y^*-Y_w^*\right) \tag{2}$$

<u>Energy conservation in a control volume enclosing the channel and the solid</u>

$$\dot{m}_1\left[\frac{1}{u_1}\frac{\partial H_1}{\partial t}+\frac{\partial H_1}{\partial x_A}\right]+\frac{m_w}{x_{AF}}\frac{\partial H_w}{\partial t}=0 \tag{3}$$

<u>Energy conservation in a control volume enclosing the channel</u>

$$\frac{\dot{m}_1}{y_{AF}}\left[\frac{1}{u_1}\frac{\partial H_1}{\partial t}+\frac{\partial H_1}{\partial x}\right]=2h_y\left(Y_w^*-Y^*\right)\frac{\partial H_1}{\partial Y}+2h\left(T_w-T_1\right) \tag{4}$$

Defining the following non-dimensional parameters,

$$x^*=\frac{2h\,y_{AF}\,x}{\dot{m}\left(\frac{\partial H_1}{\partial T_1}\right)} \tag{5}$$

$$t^*=\frac{2\ h\,y_{AF}\,x\ t_B}{m_w C_{WR}} \tag{6}$$

after extensive algebra, equations (1)-(4) can be written as

$$\frac{\partial Y^*}{\partial x^*}=Y_w^*-Y^* \tag{7}$$

$$\frac{\partial W}{\partial t^*}=\lambda_2\left(Y^*-Y_w^*\right) \tag{8}$$

$$\frac{\partial T_1}{\partial x^*}=T_w-T_1 \tag{9}$$

$$\frac{\partial T_w}{\partial t^*}=\left(T_1-T_w\right)+\lambda_1\left(Y^*-Y_w^*\right) \tag{10}$$

in which

$$\lambda_2=\frac{C_{wr}}{f\left(\frac{\partial H_1}{\partial T_1}\right)} \tag{11}$$

$$\lambda_1 = \frac{\left(\frac{\partial H_1}{\partial Y} - \frac{1}{f}\frac{\partial H_w}{\partial W}\right)}{\left(\frac{\partial H_1}{\partial T_1}\right)} = \frac{Q}{\left(\frac{\partial H_1}{\partial T_1}\right)} \tag{12}$$

Q is the heat of adsorption, given by [8],

$$Q = h_v\left(1.0 + 0.284e^{-10.28W}\right) \tag{13}$$

and the specific enthalpy of the air H_1 can be written as

$$H_1 = aT_1 + Y^*\left(d + cT_1\right) \tag{14}$$

where

$$a = 1.0046465\, KJ / Kg\ ^\circ C$$
$$d = 2467.4304\, KJ / Kg$$
$$c = 1.8837122\, KJ / Kg\ ^\circ C$$

There are four equations to be solved (7-10), and five unknowns, T_1, T_w, W, Y_1 and Y_w. We have now four equations (6) to (9) and five unknowns, Y^*, Y, W, T_1 and T_w. The missing equation is the adsorption isotherm, which relates the humidity content of the hygroscopic material, its temperature and the absolute humidity of the air layer in equilibrium with the solid,

$$W = W\left(T_w, Y_w^*\right) \tag{15}$$

with boundary conditions are given by

$$T_1(0,t^*) = T_{h\,in} \qquad ,0 < t^* < P_h^* \tag{16}$$

$$Y_1(0,t^*) = Y_{h\,in} \qquad ,0 < t^* < P_h^* \tag{17}$$

$$T_1(x_f^*,t^*) = T_{c\,in} \qquad ,P_h^* < t^* < P^* \tag{18}$$

$$Y_1(x_f^*,t^*) = Y_{c\,in} \qquad ,P_h^* < t^* < P^* \tag{19}$$

and the periodicity conditions are given by

$$T_{wc}(x^*,P^*) = T_{wh}(x^*,0) \tag{20}$$

$$W_c(x^*,P^*) = W_h(x^*,0) \tag{21}$$

The adsorption isotherm (Eq.15) is specific for each hygroscopic material. Czachorsy and Wurm (1997) suggest that although the humidity content W is a function of both temperature and relative humidity of the air layer, its dependence on the later is much stronger than on the former. Accordingly, a variety of adsorptive materials can be represented by

$$\frac{W}{W_{\max}} = \frac{1}{(1 - R + \frac{R}{\phi_w})} \tag{22}$$

In which the separation factor R characterizes a particular adsorbent material. The pressure of saturated water vapor given by

$$P_{ws} = \exp\left(23.196 - \frac{3816.44}{T_w - 46.13}\right) \tag{23}$$

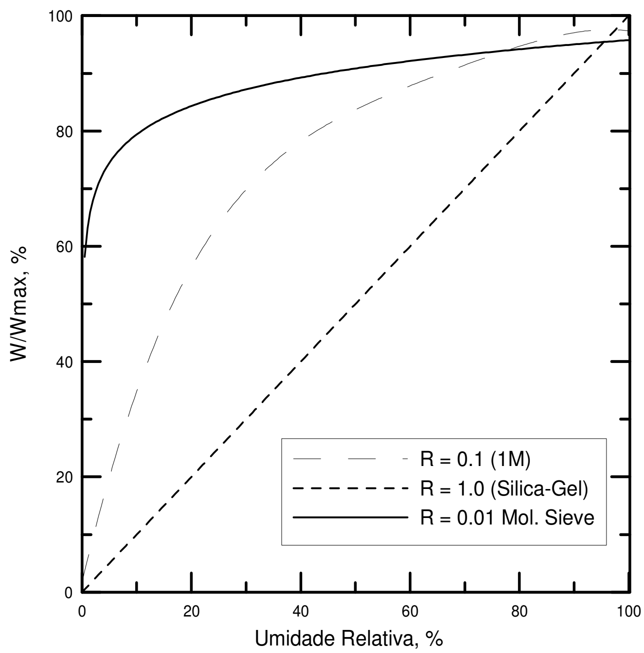

Figure 2. Typical isotherm shapes

and the absolute humidity given by

$$Y_w^* = \frac{0.62188\, p_w}{p_{atm} - p_w} = \frac{0.62188\phi_w}{\dfrac{p_{atm}}{p_{ws}} - \phi_w} \tag{24}$$

The problem now consists of equations (7-17). Identical equations are written for the regeneration period, in which the water vapor is removed from the desiccant material. The boundary conditions for the flow are given by

$$T_1(0,t^*) = T_{h\,in} \qquad ,0 < t^* < P_h^* \tag{25}$$

$$Y_1(0,t^*) = Y_{h\,in} \qquad ,0 < t^* < P_h^* \tag{26}$$

$$T_1(x_f^*,t^*) = T_{c\,in} \qquad ,P_h^* < t^* < P^* \tag{27}$$

$$Y_1(x_f^*,t^*) = Y_{c\,in} \qquad ,P_h^* < t^* < P^* \tag{28}$$

and the periodicity conditions are given by

$$T_{wc}(x^*,P^*) = T_{wh}(x^*,0) \tag{29}$$
$$W_c(x^*,P^*) = W_h(x^*,0) \tag{30}$$

The periodic nature of the problem implies an iterative procedure. Both initial distributions of temperature and humidity within the solid are guessed, and equations (7), (8), (9) and (10) assume the form of tridiagonal matrices, as a result of the discretization using the finite-volume technique (Patankar, 1980), with a fully implicit scheme to represent the transient terms. By the end of the cycle, both calculated temperature and moisture fields are compared to the initially guessed fields. If there is a difference in any nodal point bigger than convergence criteria established for temperature and moisture content,

$$Crit.\ \ Conv._{temp} = \frac{T_w(x,0) - T_w(guess)(x,0)}{T_w(x,0)} \tag{31}$$

$$Crit.\ \ Conv._{mass} = \frac{W(x,0) - W(guess)(x,0)}{W(x,0)} \tag{32}$$

The procedure is repeated, using the calculated fields as new guesses for the initial distributions. Since the control-volume regime is periodic, the inlet of enthalpy must equal the average outlet enthalpy, as required by the heat and mass balance error,

$$HMBE = \frac{\dot{m}_h\, h_{hi} + \dot{m}_c\, h_{ci} - (\dot{m}_h \frac{1}{p_h}\int_0^{p_h} h_{ho}\, dt^* + \dot{m}_c \frac{1}{p_c}\int_0^{p_c} h_{co}\, dt^*)}{\dot{m}_h\, h_{hi} + \dot{m}_c\, h_{ci}} \tag{33}$$

3. Results

Consider the schematic of a desiccant cooling system, shown in Figure (3). Ambient air is successively forced through a desiccant (where it is dried and heated) and pre-cooled in a regenerator, before its cooled in a evaporative device and meets the temperature and humidity room conditions.

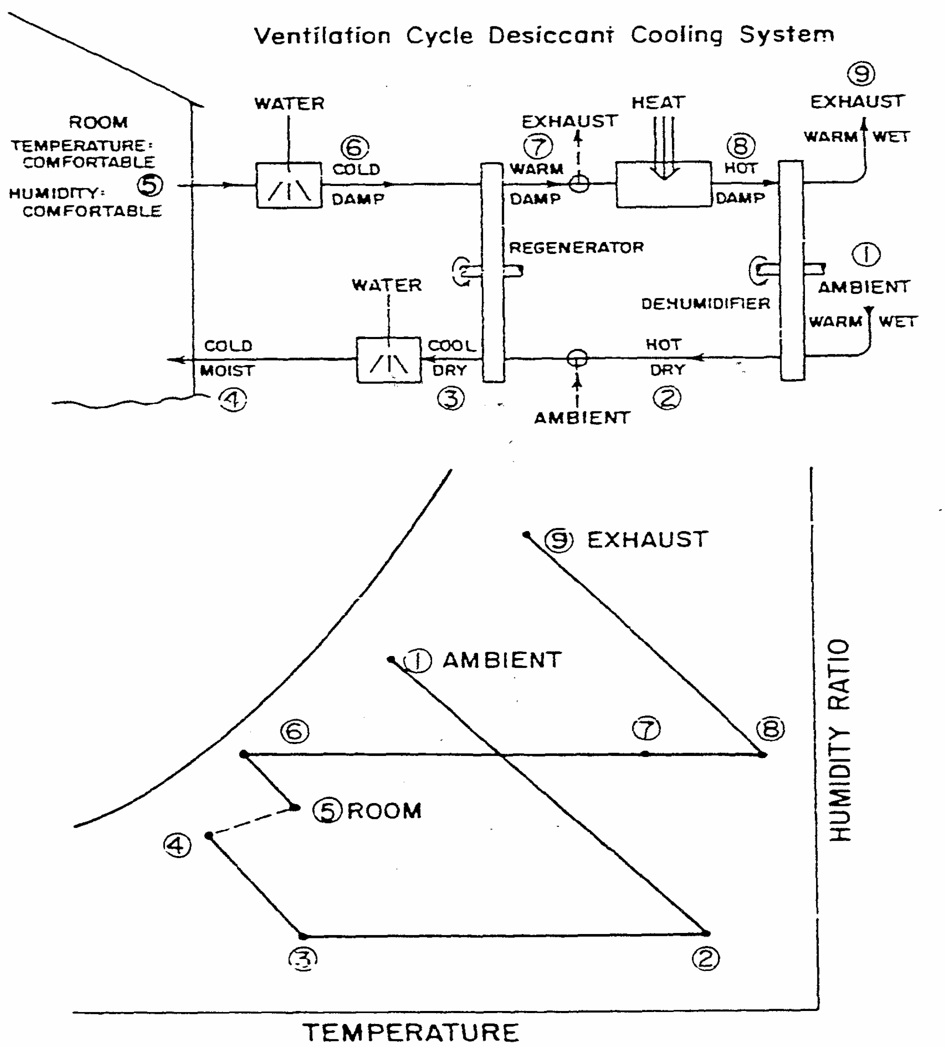

Figure 3. Desiccant cooling system: ventilation cycle

Return air is further cooled in an evaporative device, before it is successively forced through the regenerator, a heat source and the desiccant wheel. If the coefficient of performance is to be considered, it will be necessary to also model and simulate the evaporative process, which is outside the scope of the present work. However, this can be avoided by noting that the regeneration heat may be expressed by

$$\dot{Q}_{REG} = \dot{m}_h C_p (T_8 - T_7) \tag{34}$$

whereas the thermal load may be expressed by

$$\dot{Q}_L = \dot{m}_c (h_5 - h_4) \approx \dot{m}_c (h_5 - h_3) \tag{35}$$

in which the approximation is carried out by noting that process 3-4 is isenthalpic. From Figure (3)

$$T_5 \approx T_3 \tag{36}$$

This procedure is suggested by Van Den Bulk et al. (1992), also certified by experimental data. Therefore,

$$\dot{Q}_L = \dot{m}_c h_{fg} (Y_5 - Y_3) \tag{37}$$

Dividing (37) by (24),

$$COP = \frac{\dot{Q}_L}{\dot{Q}_{REG}} = \frac{\dot{m}_c h_{fg} (Y_5 - Y_3)}{\dot{m}_h C_p (T_8 - T_7)} \tag{38}$$

Figures (4) and (5) show the influence of the selection of the adsorptive material over the coefficient of performance COP. Figure (4) shows that for a moderate regeneration temperature, 1M and silica-gel exhibit similar behaviors, far more efficient than molecular sieve (R = 0.01) . This is consistent with the fact that stronger adsorbents such as molecular sieve also require a higher regeneration temperature to purge out the humidity and complete the cycle. For a higher regeneration temperature, (Figure (5), 1M exhibits a better performance when compared to silica-gel (R =1,0) and molecular-sieve.

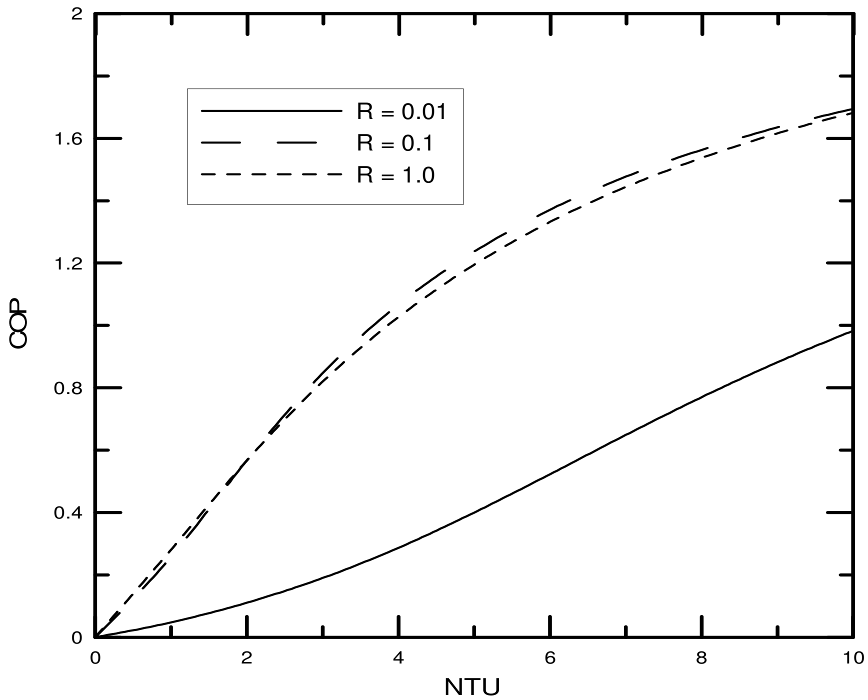

Figure 4. Influence of adsorptive material, T_{hi} = 80°C

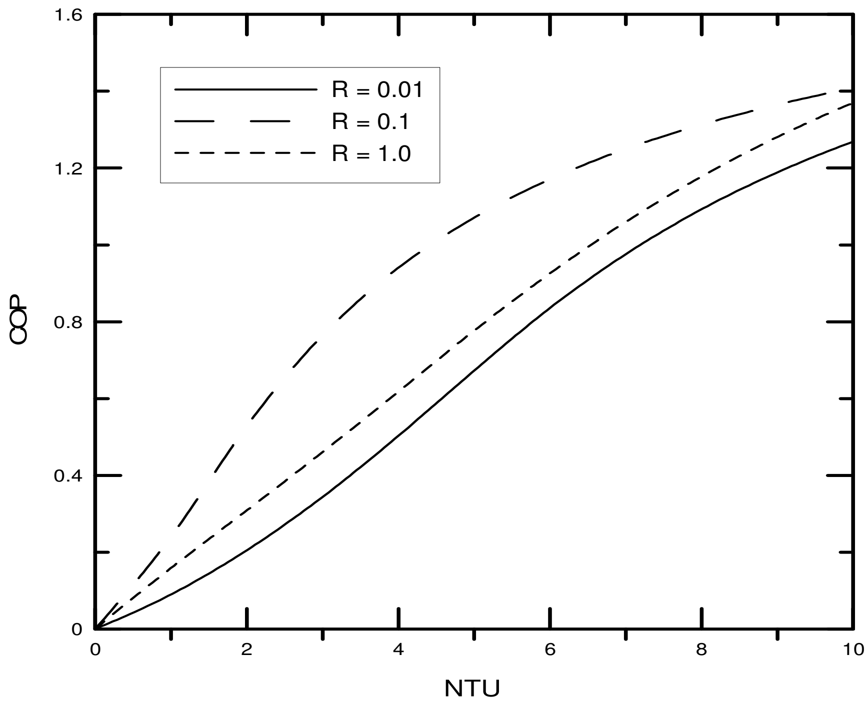

Figure 5. Influence of adsorptive material, T_{hi} = 120°C

4. Conclusion

A mathematical model for a rotary dehumidifier was developed and solved, and the influence of the adsorptive material over the coefficient of performance of a desiccant cooling cycle has been evaluated. A preliminary analysis revealed that silica-gel and moderate adsorbent (1M) exhibit better performances than molecular sieves for low regeneration temperatures. For higher temperatures, a balance between silica-gel and molecular sieve properties is required, if better performances of the desiccant cooling cycles are to be attained. This reinforces the need of a computational code as an important aid to the HVAC designer.

5. Nomenclature

a	=	Constant
c	=	Constant
d	=	Constant
f	=	desiccant mass fraction
h	=	Convective heat transfer coefficient (KJ/m^2s)
h_y	=	Convective mass transfer coefficient (Kg/m^2s)
h_v	=	Heat of vaporization (KJ/Kg)
H	=	Enthalpy of air (KJ/Kg)
$\dot{m}$	=	Air mass flow rate (kg/s)
m	=	Mass of the wall (Kg)
P	=	Period of revolution (s)
P_{atm}	=	Atmospheric Pressure (Pa)
P_{ws}	=	Saturation Pressure (Pa)
Q	=	Heat of Adsorption (KJ/Kg)
t	=	Time (s)
T	=	Temperature (°C)
u	=	Air flow velocity (m/s)
W	=	Humidity content within the desiccant (kg/kg)
x	=	Coordinate (m)
X_{AF}	=	Length of the wheel (m)
Y	=	Absolute Humidity (kg vap/kg air)
Y_{AF}	=	Flow channel width (m)

Greek letters

λ_1 Dimensionless auxiliary parameter
λ_2 Dimensionless auxiliary parameter
ϕ_w Relative humidity of air layer in equilibrium
ε Effectiveness

Subscripts

w wall
hi hot inlet
ho hot outlet
ci cold inlet
co cold outlet
h hot period
c cold period
1 air

6. References

Bullock, C.E., 1965, "Dehumidification of Moist Air by Adiabatic Adsorption", M.Sc. Thesis, Mechanical Engineering Department, University of Minnesota.

Czachorsy, W., Wurm, J., 1997, "Evaluation of Desiccant and Heat Exchange Matrices", Gas Research Institute, GRI-97/0148, Des Plaines, Illinois.

Kays, W.M.; London, A.L., , 1984, "Compact Heat Exchangers" 3rd ed., McGraw-Hill, New York.

Maclaine-Cross, I.L.; Banks, P.J**.**, 1972**,** "Coupled Heat and Mass Transfer in Regenerators", *International Journal of Heat and Mass Transfer*, vol. (15).

Majumdar, P., 1998 "Heat and Mass Transfer in Composite Desiccant Pore Structures For Dehumidification", *Solar Energy*, vol.(62), pp. 1-10.

Niu, J.L.; Zhang, L.Z., 2002, "Effects of Wall Thickness on Heat and Moisture Transfer in Desiccant Wheels For Air Dehumidification and Enthalpy Recovery", *International Communications In Heat and Mass Transfer*, vol. (29), pp. 255-268.

Patankar, S., 1980, "Numerical Heat Transfer and Fluid Flow", Hemisphere Publishing Co., Boston.

Pesaran, A.A., Mills, A.F., 1987, "Moisture Transport in silica Gel Packed Beds-Part I", International Journal of Heat and Mass Transfer (30), pp. 1051-1060.

Shen, C.M.; Worek, W.M., 1992, "The Effect of Wall Conduction on the Performance of Regenerative Heat Exchangers", Energy, vol. 17, No.12.

Zhang, X.J., Dai, Y.J., Wang, R.Z.; "A Simulation Study of Heat and Mass Transfer in a Honeycomb Structure Rotary Desiccant Dehumidifier" Applied Thermal Engineering No.23, pp. 989-1003, 2003.

Zheng, W.; Worek, W.M**.,** 1993, "Numerical Simulation of Heat and Mass Transfer Processes in a Rotary Dehumidifier", *Numerical Heat Transfer,* A, vol.23.

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