Adsorption Analysis for Theoretical Modelling of Silica Gel Desiccant Wheels

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Abstract

Desiccant evaporative cooling system is a potential environment-friendly alternative to conventional vapour compression chillers. A desiccant wheel is the heart of this heat driven cooling system and it uses a solid desiccant for dehumidification with silica gel being most widely used. The desiccant material is coated, impregnated or formed in a place on the supporting rotor structure. The matrix consists of multiple channels in the direction of axis of rotation of the wheel. Proper design of the wheel is very important for the successful operation of the system and theoretical models are very useful tool in predicting the performance and design optimization. One of the major difficulties in numerical modelling of the desiccant wheel is the lack of knowledge of adsorption equilibrium of porous medium.In this paper, adsorption equilibria of the silica gel is studied and the different theories existing to characterize the adsorption process and different equations for prediction of adsorption equilibria are compared and used in a theoretical model predicting the wheel performance. The results of the different models are compared with experimental data and conclusions are drawn.

1. Introduction

Desiccant/evaporative cooling systems offer a potential environmental-friendly alternative to conventional vapor compression chillers. They operate on an open heat-driven cycle consisting of a combination of a dehumidifier, a sensible heat exchanger and evaporative coolers. In this environment friendly system, dehumidification of air is done at first using a desiccant wheel to very low humidity levels so that evaporative cooling can be employed effectively to reduce the temperature of air.

A desiccant wheel is the heart of the heat driven cooling system and it uses a solid desiccant for dehumidification. The desiccant material is coated, impregnated or formed on the supporting rotor structure. The matrix consists of multiple channels in the direction of axis of rotation of the wheel. The wheel constantly rotates through two separate air streams, the supply air which is dried by the desiccant and hot regeneration air which reactivates the desiccant. The regeneration and supply air sides are separated by clapboard. The matrix of of most of desiccant whee are of sinusoidal shape.

2. Transport Phenomenon in a Desiccant Wheel

The adsorption of water vapor from air involves many physical processes which offer resistances to vapor transfer from the gas phase to the solid phase. These heat resistances in this hygroscopic matrix can be categorized into two groups namely the gas side and the solid side resistances. The gas side resistance is the resistance of vapor transport from bulk gas to surface of the solid desiccant whereas the solid side resistance is resistance for transport of the adsorbed molecules into the pore structure of

the desiccant material from the surface of the desiccant [1]. The gas side resistance is mainly attributed to convective heat and mass transfer between the air and desiccant. Solid side resistances are due to heat conduction and mass diffusion within the desiccant.

To develop a heat and mass trasfer model of a desiccnat wheel, differential equations that represent these transport mechanisms, will generally be set up to describe a single desiccant coated flow channel, traversing through the respective supply and regeneration air streams in a 360 degree circular path. To relate the humidity ratio of air with water content of desiccant, the adsorption eqilibruim relationship which determines the amount of moisture that is adsorbed by the desiccant is used.

3. Review of Adsorption equilibrium theories

There are several theories existing to characterise the adsorption process. The main theories are Henry's law, Langmuir's theory, Gibb's theory and Adsorption potential theory.

3.1 Henry's Law

According to this law, concentration of absorbed phase and fluid phase are directly proportional and constant of proportionality is called Henry's constant. But there was no accepted value of this constant and it doesn't seem to be valid for most of the porous substance. This law is applicable only at uniform surface and observed only at sufficiently low concentration [2].

3.2 Langmuir theory of mono layer adsorption

This theory is the most common model which bases the concept of adsorption as surface phenomenon with single layer of adsorbate, i.e. mono layer adsorption. It equates the rate of adsorption with rate of desorption to form the equilibrium relationship.

$$X = a.b.P/(1 + aP) \tag{1}$$
, where X is mass of water vapor adsorbed per unit area, P being the equilibrium pressure and a and b are constants.
It is the best one parameter isotherm, but ignores adsorbent-adsorbate interaction and effects of temperature [3]. This theory is good for relatively low pressure and non-porous adsorbents. It fails with silica gel, since it is highly porous and occupancy of multi layer adsorptions [4].

3.3 Gibb's theory

This theory is formed based on ideal gas laws and assumes that adsorbate is microscopic and bi dimensional. With volume of bulk phase replaced with area and the pressure is replaced with spreading pressure, equations of state with moles of adsorbate, area, spreading pressure and adsorbed phase concentration are used with Gibb's equation.

This theory designates adsorption is the density gradient of fluid at a surface and excess density is called as the Gibb's adsorption. The absolute adsorption is the total number of molecules adsorbed on the layer and it is a function of temperature, pressure (or density) and composition. At low vapor pressures, the difference between absolute and Gibb's (excess) adsorption is negligible.

3.4 Adsorption potential theory

This was proposed by Polanyi and Dubinin and is based on pore-filling model [4]. This thermodynamic approach considers adsorbate as fluid phase and is more suitable for micro porous materials. It has been extended by several investigators and theory still subject of further investigation mainly by statistical mechanics and computational methods.

In this theory, adsorbate is considered as a fluid phase in which is excreted to external forces of atoms and molecules located on the surface of a sorbent material. General condition for thermodynamic equilibrium for such phase against gaseous sportive phase is give by

$$\mu_a - \varphi = \mu_f - 0 \qquad (3)$$

where μ_a is the chemical potential of the adsorbate phase, μ_f is the chemical potential of sportive phase and φ is the mechanical potential per unit mass of forces acting near the surface of the sorbent. By assuming ideal gas, this can be approximated to

$$\varphi = RT\, ln(p_s(T)/p) \qquad (4)$$

where $p_s(T)$ indicates the saturation pressure of sportive medium at temperature T.

Assuming the portion of the micro pore filled with adsorbed molecules to be a function of φ, it can be written as

$$W = W_0\, exp\,(-(\alpha\,\varphi)^N), \qquad (5)$$

where W_0 indicating total volume of pore. This can be simplified to

$$W = W_0 exp\,[-[\alpha\,R\,T\,ln(p_s(T)/p)]^N\,] \qquad (6)$$

This is the generalized version of Dubinin - Radushkevich Adsorption Isotherm[5].

3.5 Empirical and semi empirical equilibrium relationships

Due to complexity in structure of practical solids, fundamental isotherms cannot describe the process. So for actual solid, ideal solid theories are initially used then it is developed to an empirical or semi empirical equation.

3.5.1 Freundlich Equation

According to this equation the uptake of water in silica gel can be expressed by

$$w = w_0 \left(\frac{p(T_w)}{p(T_s)}\right)^{1/n} \qquad (7)$$

with w is defined as the mass of water adsorbed to mass of silica gel; w_0 and n are constants determined by experiment data fitting process T_w and T_s are the temperatures of water vapour and silica gel respectively; $p(T_w)$ and $p(T_s)$ are the corresponding saturation vapour pressure at T_w and T_s.

The values of these constants for water silica gel pair are $w0 = 0.444$ and $n=1.342$[6].

3.5.2 Modified Freundlich Equation

According to this equation the uptake of water in silica gel can be expressed by

$$w = A(T_s) . \left[\frac{p(T_w)}{p(T_s)}\right]^{B(T_s)} \tag{8}$$

$$A(T_s) = A_0 + A_1 T_s + A_2 T_s^2 + A_3 T_s^3 \qquad B(T_s) = B_0 + B_1 T_s + B_2 T_s^2 + B_3 T_s^3$$

Where constants; A_0, A_1, A_2, A_3, B_0, B_1, B_2, B_3 are the constants determined by a fitting process with experimental data[6].

The values of these constants for water silica gel pair are $A_0 = -14.2904$, $A_1 = 0.1546$ K^{-1}, $A_2 = -5.5498x$ 10^{-4}, $A_3 = 6.7512x10^{-7}$ K^{-3}, $B_0 = 36.1487$, $B_1 = -0.382$ K^{-1}, $B_2 = 1.3016x10^{-2} K^{-2}$, $B_3 = -1.4150x10^{-6} K^{-3}$.

3.5.3 Dubinin- Astakhov (DA) Equation

This equation expresses the uptake of adsorbate as

$$w = w_0 \exp\left(-k \left(\ln \frac{p(T_s)}{p(T_w)}\right)^n\right) \tag{9}$$

where x_0, k and n are the constants determined by the fitting process with experiment data[6].
The values of these constants for water silica gel pair are $w_0 = 0.348$, $n=1.609$, $k= 0.019$.

3.5.4 Toth Equation

According this empirical equation, the uptake of adsorbate can be expressed as

$$w = \frac{K_o \exp\left(\frac{\Delta H_{ad}}{R.T}\right) P}{\left\{1 + \left[\frac{K_o}{q} \exp\left(\frac{\Delta H_{ad}}{R.T}\right).P\right]^t\right\}^{1/t}} \tag{10}$$

where K_o, q, and t are constants; ΔH_{ad} is the isosteric heat of adsorption , R is the universal gas constant and T is the temperature in Kelvin. For water- silica gel pair $K_0 = 7.3x10^{-13}$ kg/(kgPa); $t=12$; $q=0.45$ kg/kg[7].

3.5.5 Boelman Equation

This equation used for adsorption chiller modeling by Wang et al. in adsorption chiller modeling [8].

$$w = 0.346 \left(\frac{p(T_w)}{p(T_s)}\right)^{1/1.6} \tag{11}$$

This quite similer to the Freaundlich equation with diffrence in conatants.

3.7 Comparisons of Equilibrium relationships for water-silica gel pair

Figure 1 shows the variation of the water vapor uptake of at various relative humidity air at 300K calculated using different relationships.
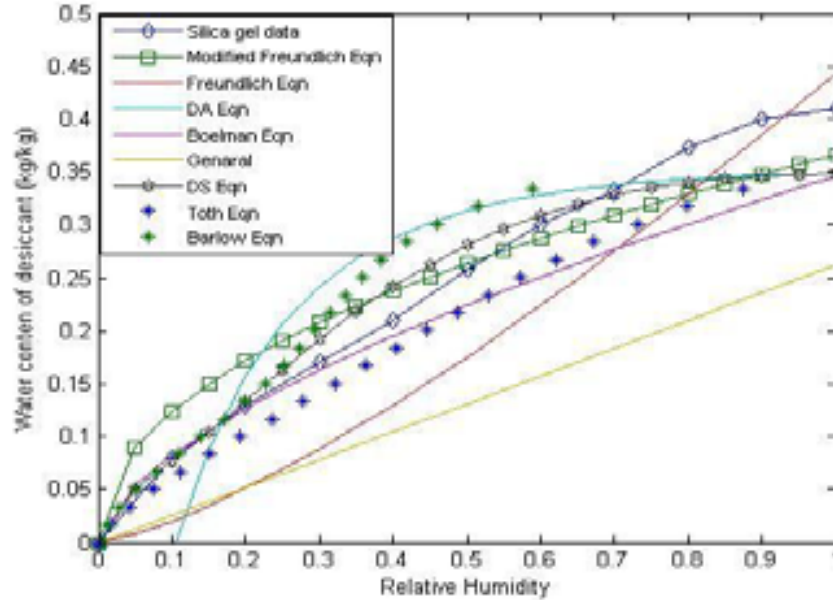

Fig 1 : Comparison of uptake at 300K for different relationships

It is obvious from the graph that at this temperature of the desiccant, Modified Freundlich equation, Peasaran's equation, Barlow's equation, Toth equation and Boelman equation have almost similar variations for water uptake at different values of relative humidity of air.

4. Review of Equilibrium relationships used in silica gel desiccant wheel models.

The review different models available in the literature shows that different equilibrium relationships are used in desiccant wheel modeling with no emphasis placed on the selection of the relationship. In most of the models, water content of the desiccant is expressed as function of relative humidity only. A few models the water content of the desiccant is taken as function of both relative humidity and temperature of air.Table 1 shows the different equilibrium relationships used in desiccant wheel modeling. Here Wd, Td and ψ are desiccant water content, temperature and relative humidity of air respectively. It is obvious that most widely used relationship is the isotherm equation of Pesaran.

Table 1: Equlibrium relationships used in silica gel desiccant wheel models

Author	Isotherm Equation	Remarks
A.A Pesaran [1]	$\psi = 0.0078 - 0.05759W_d + 24.16554W_d{}^2 - 124.47W_d{}^3 + 204.226\ W_d{}^4$	Isotherm equation of Pesaran
X.J. Zhang et al.[9]	$\psi = 0.0078 - 0.05759Wd + 42.16554Wd^2 - 124.78Wd^3 + 204.226\ Wd^4$	Isotherm equation of Pesaran

C.R . Ruivo et al. [10]	$Wd = 0.77 * \psi - 0.37 * \psi^2$	Derived from Isotherm equation of Pesaran
L.Z. Zhang et al.[11]	$Wd = f * Wmax/(1 - C + \dfrac{C}{\psi})$	General Isotherm
J. D. Chung et al.[12]	$\psi = 0.0078 - 0.05759W_d + 24.16554W_d{}^2 + 124.47W_d{}^3 + 204.226\,W_d{}^4$	Isotherm equation of Pesaran
K. Tsutsui et al [13]	$\psi = [0.616238\,Wd + 16.7916Wd^2 - 74.34Wd^3 + 116.68\,Wd^4\,]/\left[1 - \dfrac{Td - 40}{300}\right]$	Equilibrium Equation of Barlow
P. Stabat et al.[14]	$\psi = C_1 * W_d + C_2 W_d{}^2$	Isotherm equation of Mathiprakasam et al.
F.E . Nia et al.[15]	$Wd = 0.106 \exp\left[-\left(\dfrac{-R\,Td\,\log\psi}{8590}\right)^2\right] + 0.242 \exp\left[-\left(\dfrac{-R\,Td\,\log\psi}{8590}\right)^2\right]$	Equilibrium equation of G. Steich

5. Desiccant wheel Modelling Governing Equations

Following assumptions are made to develop the mathematical model.

1. All the flow channels have uniform coating of the adsorbent silica gel are identical and sinusoidal. For simplicity it is divided into two equal sections: the dehumidification section and the regeneration section.
2. It is assumed that the movement of the wheel is so slow that the rate of mass and energy variation due to air flow in the circumferential direction can be neglected.
3. Heat conduction and mass diffusion in the gas side are negligible and only convective heat and mass transfer takes place in the gas.
4. There are no radial or circumferential temperature or moisture content gradients in the matrix.
5. The matrix's thermodynamic properties and the mass and heat transfer coefficients are constant.
6. The air flow is assumed to be purely axial in direction and laminar and the mass flow rate and velocity are constant for both the supply and regeneration streams.
7. Lewis number for the flow is assumed to be equal to 1.

With these assumptions, the mass and energy balance equations for the air and desiccant control volumes i.e. CV1 and CV2 can be derived.Here Yg, Tg, Yd and Td are humidity ratio and temeparture of air in the air and desiccnat control volumes..

Mass balance in CV1
$$\frac{1}{u_g} * \frac{\partial Y_g}{\partial t} + \frac{\partial Y_g}{\partial x} = \frac{4\,\beta}{u_g\,D_h}\left(Y_d - Y_g\right) \tag{12}$$
Energy balance in CV1
$$\frac{1}{u_g} * \frac{\partial T_g}{\partial t} + \frac{\partial T_g}{\partial x} = \frac{4\alpha}{u_g\,D_h\,c_{pg}}\left(T_d - T_g\right) \tag{13}$$
Mass balance in CV2
$$\rho_g \frac{\partial Y_d}{\partial t} + \rho_d \frac{\partial W_d}{\partial t} = \rho_g\,D_a \frac{\partial^2 Y_d}{\partial t^2} + \rho_d\,D_s \frac{\partial^2 W_d}{\partial t^2} + \frac{\beta \rho_g P_{in}}{A_d}\left(Y_g - Y_d\right) \tag{14}$$
Energy balance in CV2

$$\rho_d \; c_t \frac{\partial T_d}{\partial t} \;\; = \;\; \lambda_d \;\; \frac{\partial^2 T_d}{\partial x^2} + \;\; \frac{\alpha P_{in}}{A_d}(T_g - T_{d)} + \;\; q_a \rho_d \;\; \frac{\partial W_d}{\partial t} \hspace{2cm} (15)$$

To solve these equations, auxiliary equations of relative humidity expressed in terms of humidity ratio, hydrailic diameter of channel geometry, Nusselt and Lewis number expressions are needed.These expresions are given in the previous work of authors[16].

6. Results

The governing equations are solved using COMSOL modelling software and results of outlet humidity ratio and temperature of air obtained for different equilibrium relationships. These results are compared with experimental data of Brillhart [17]. Figure 2 and 3 show the comparison of these result with experimental data. It is clear that for most of the relationships give generally similar results as that of experiment, but at many points there is significant deviation from the experimental data.
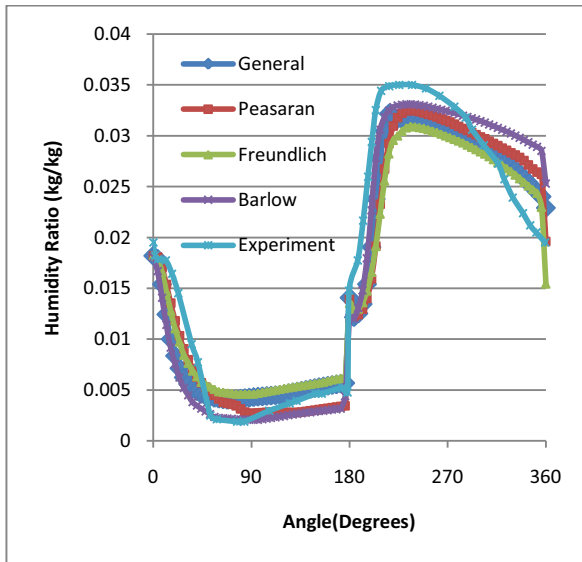

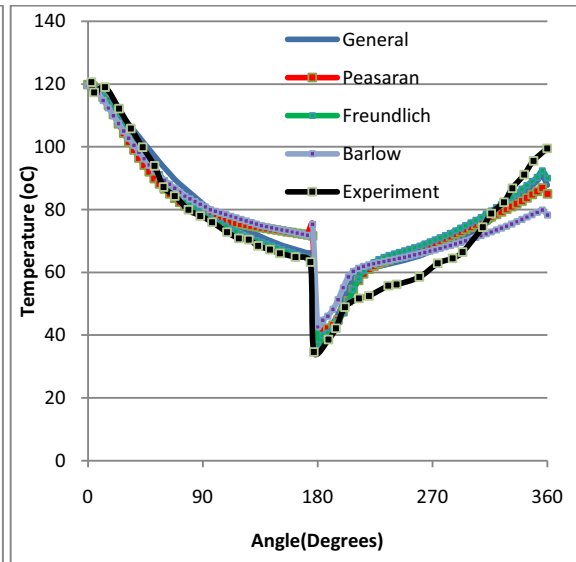| Fig 2 : Variation of outlet humidity ratio of air. | Fig 3 : Variation of Outlet temperature of air. |

7. Conclusions

Table 2: Comparison of outlet values for different models

Equilibrium relationsip used	Average outlet humidity ratio (kg/kg)	Percentage variation from experimrntal results (%)	Average outlet temperature (^{o}C)	Percantage variation from experimrntal results(%)
General	0.005998	-16.52	87.11	+4.38
Peasran's Isotherm	0.00551	-23.31	85.95	+2.99
Fraeundlch Eqn.	0.006858	-4.50	84.75	+1.54
Barlow's equation	0.004351	-39.44	87.28	+4.57

Adsorption phenomenon and different equilibrium relationships are for silica gel- water pair is studied. Due to complexity in structure of silica gel, fundamental isotherms cannot describe the process. So empirical or semi empirical equations are used. Review of literature of different equilibrium relationships used in the silica gel desiccant wheel modeling shows that isotherm relation which express the water content of deciccnat as funtion of the relative humidity of air is widely used with the isotherm equation of Pesaran being the most common one. A heat and mass trensfer model of silica gel desiccant wheel is deveoped and different isothem equations are used and results are compared. Table 2 shows that Freundlich equations has better accuracycompared to other relaltionships.This can attributed to that fact that it is based on not only relative humidity, but also temperature of air.It is clear that since adsorption is a dynamic process, emphasis should be placed on the selection of relationship to get wider range of results. For an accurate model, an equilibium relation expressing the water content of deciccant as a funtion of the relative humidity and temperature of air will be more suitable.

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