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# Sorption properties for different types of molecular sieve and their influence on optimum dehumidification performance of desiccant wheels

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#### Abstract

The sorption property data for different types of molecular sieves (synthetic zeolites) are presented in equation form. The variation of the isosteric heat of sorption with water loading is derived using Othmer's method. It is found that heat of sorption can be up to 50% greater than the latent heat of vaporization. Heat of sorption data, together with equilibrium isotherms are curve fitted and are incorporated into a numerical model of the nonlinear heat and mass transfer processes that occur in desiccant wheels. Using the numerical model, the influence of different assumptions for heat of sorption and equilibrium equation of molecular sieve on predicted optimum performance of rotary dehumidifier is evaluated.

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Keywords: Desiccant wheel; Sorption properties molecular sieves

#### 1. Introduction

Rotary dehumidifiers are used as industrial air dryers and in commercial desiccant cooling systems. The dehumidification performance of rotary regenerators largely depends on the sorption properties of porous matrix. Desiccant wheels, in which maximum moisture transfer is important, have a sorbent matrix with large moisture capacity and small heat capacity. Natural zeolites, silica gels and molecular sieves are some of different solid desiccants that have been utilized in the design of thermally activated desiccant cooling systems.

A considerable amount of research [\[1–8\]](#page-7-0) has been conducted in recent years with a purpose of modeling the simultaneous heat and mass transfer processes that occur in rotary dehumidifiers and analyzing effects of different parameters on their performance. In all of these studies, the dehumidifier has been modeled using particular sets of desiccant matrix properties. An in depth study of the effect of desiccant matrix properties on the performance of rotary dehumidifiers was presented by Jurinak et al. [\[9\]](#page-7-0). The matrix properties considered were the sorption isotherm shape, the heat of sorption, the matrix thermal capacity, matrix moisture diffusivity and sorption isotherm hysteresis. It was shown that sorption properties have a significant affect on the desiccant wheel performance.

In this paper sorption property data in equation form are presented for Type 3A, 5A and 13X molecular sieves and the influence of the equilibrium and heat of sorption property data on predicted optimum performance of desiccant wheel is evaluated numerically.

#### 2. Modeling of a rotary adiabatic dehumidifier

A schematic of a rotary adiabatic dehumidifier is shown in [Fig. 1](#page-1-0). The desiccant wheel is a rotary cylindrical wheel that consists of a large number of parallel channels. The channel walls can be coated or impregnated with a

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## <span id="page-1-0"></span>Nomenclature

- $c_s$ ,  $c_d$ ,  $c_{p_{da}}$ ,  $c_{wv}$ ,  $c_{lw}$ ,  $c_{wr}$  specific heat of support material, desiccant, dry air, water vapor, liquid water, wall  $(J/kg °C)$
- f mass fraction of desiccant material inside desiccant wheel
- h heat transfer coefficient  $(W/m^2 °C)$
- $L$  channel length  $(m)$
- Le Lewis number
- NTU number of thermal transfer units
- $P_{v}$ ,  $P_{\text{sat}}$  vapor pressure of air streams, saturation pressure (Pa)
- $T_a$ ,  $T_w$ ,  $T_{\text{reg}}$  temperature of air stream, channel wall, regeneration  $(^{\circ}C)$
- $t$  time (s)
- $W<sub>b</sub>$ ,  $W<sub>max</sub>$  moisture content of the desiccant, maximum moisture content of desiceant (kg  $H_2O/kg$  desiccant)



Fig. 1. Schematic of rotary dehumidifier.

desiccant material. The process air stream, which is supplied to a conditioned space after being dehumidified and cooled, passes through adsorption side of the desiccant wheel. The regeneration air, heated by an external heat source, passes through the regeneration side of desiccant wheel and regenerates the desiccant. Within the desiccant wheel, heat and mass transfer processes take place between the two air streams and the desiccant wheel.

Applying mass and energy conservation laws to an infinitesimal control volume within a channel of the desiccant wheel, the following set of governing equations in non-dimensional form can be obtained (Golubovic and Worek [\[5\]\)](#page-7-0):

$$
\frac{\partial W_{\mathbf{b}}}{\partial \tau} = \beta_3 (Y_{\mathbf{a}} - Y_{\mathbf{w}}) \tag{1}
$$

$$
\beta_4 \frac{\partial T_{\mathbf{w}}}{\partial \tau} = \beta_5 (Y_{\mathbf{a}} - Y_{\mathbf{w}}) + (T_{\mathbf{a}} - T_{\mathbf{w}}) \tag{2}
$$

$$
\frac{\partial Y_{\rm a}}{\partial \zeta} = \beta_6 (Y_{\rm w} - Y_{\rm a}) \tag{3}
$$

$$
\frac{\partial T_a}{\partial \zeta} = \beta_7 (T_w - T_a) \tag{4}
$$

$$
dY_{w} = \beta_1 dT_{w} + \beta_2 dW_{b}
$$
 (5)

- $u$  velocity of air stream  $(m/s)$
- $Y_a$ ,  $Y_w$  humidity ratio of air stream, equilibrium humidity ratio of air at the surface between air stream and desiccant material (kg  $H_2O/kg$  desiccant)
- z space coordinate (m)

## Greek symbols

- $\delta$  half of the height of channel (m)
- $\lambda$  wall thickness (m)
- $\rho_{da}$ ,  $\rho_w$  density of air stream, density of the wheel  $(kg/m^3)$

#### Subscripts

- ads adsorption
- des desorption
- pain, paout process air inlet, process air outlet

The non-dimensional time and the non-dimensional length in above equations are equal to:

$$
\tau = \frac{h}{\rho_{\rm w} \lambda c_{\rm wr}} t \tag{6}
$$

$$
\zeta = \frac{h}{\rho_{\text{da}} u \delta c_{p_{\text{da}}}} z = \text{NTU} \left(\frac{z}{L}\right) \tag{7}
$$

The coefficients in Eqs.  $(1)$ – $(5)$  are defined as

$$
\beta_1 = \frac{\partial Y_{\rm w}}{\partial T_{\rm w}}, \quad \beta_2 = \frac{\partial Y_{\rm w}}{\partial W_{\rm b}}, \quad \beta_3 = \frac{c_{\rm wr}}{fLec_{p_{\rm da}}},
$$
\n
$$
\beta_4 = \frac{(1 - f)c_s + fc_{\rm d} + fc_{\rm lw}W_{\rm b}}{c_{\rm wr}},
$$
\n
$$
\beta_5 = \frac{Q}{Lec_{p_{\rm da}}}, \quad \beta_6 = \frac{1}{Le}, \quad \beta_7 = \frac{1}{1 + Y_{\rm a} \frac{c_{\rm wx}}{c_{p_{\rm da}}}}
$$
\n(8)

This set of governing equations, Eqs.  $(1)$ – $(5)$ , is subject to a following boundary and initial conditions.

Adsorption side

$$
Y_{a}(\tau, 0) = (Y_{a})^{\text{inlet}}_{\text{ads}} = \text{const.}, \quad T_{a}(\tau, 0) = (T_{a})^{\text{inlet}}_{\text{ads}} = \text{const.},
$$
  
\n
$$
W_{b}(0, \zeta) = W_{b}^{\text{des}}(\Delta \tau_{\text{des}}, NTU_{\text{des}} - \zeta),
$$
  
\n
$$
T_{w}(0, \zeta) = T_{w}^{\text{des}}(\Delta \tau_{\text{des}}, NTU_{\text{des}} - \zeta)
$$
\n(9)

Desorption side

$$
Y_{\rm a}(\tau,0) = (Y_{\rm a})_{\rm des}^{\rm inlet} = \text{const.}, \quad T_{\rm a}(\tau,0) = (T_{\rm a})_{\rm des}^{\rm inlet} = \text{const.},
$$
  
\n
$$
W_{\rm b}(0,\zeta) = W_{\rm b}^{\rm ads}(\Delta \tau_{\rm ads}, N T U_{\rm ads} - \zeta),
$$
  
\n
$$
T_{\rm w}(0,\zeta) = T_{\rm w}^{\rm ads}(\Delta \tau_{\rm ads}, N T U_{\rm ads} - \zeta)
$$
\n(10)

A finite-difference method, Golubovic and Worek [\[5\]](#page-7-0), is used to solve this set of non-linear governing equations.

<span id="page-2-0"></span>

Fig. 2. Schematic of experimental setup.

# 3. Sorption data for different types of molecular sieves

To study the equilibrium capacity of desiccant material at various temperatures and humidities, the design of the typical test system is shown in Fig. 2. The desiccant is placed in the sampler holder and it is first dried by inserting the sample holder into the setup and running dry air through the sample until equilibrium is reached (i.e., the sample weight becomes independent of time). This typically takes about one day. The sample holder is removed from the setup and weight is recorded using single-pan analytical balance that typically has an accuracy of  $\pm 0.0001$  g. The inlet and outlet air temperatures as well as the temperature of the sample are monitored and the dewpoint of the inlet and outlet air stream is measured. After the drying is complete, the sample is allowed to cool, weighed and then the adsorption process is started.

For adsorption measurements near room temperature, a bubbler is used to give saturated air which is mixed with heated air to obtain the required inlet moisture and temperature conditions. For adsorption measurements well above room temperature, a steam generator is used to provide steam which is mixed with heated dry air to produce the desired inlet temperature and humidity conditions. The sample weight is measured on hourly basses until is no longer dependent on time. After the equilibrium is reached, the sample weight and temperature as well as inlet air sensible and dew point temperatures are recorded. The equilibrium data used in this study are given in Refs. [\[12,13\]](#page-7-0).

### 4. Heat of sorption

The adsorption of water on a solid desiccant is a spontaneous, exothermic process. When desiccants, including molecular sieves, adsorb water vapor, heat is generated. This heat is equal to the latent heat of evaporation plus an additional amount of heat due to a change in the surface energy of the desiccant material. This additional heat is called the integral of wetting and the total heat generated during adsorption is called the heat of sorption.

For solid desiccant materials for which sorption process is reversible, the Clausius–Clapeyron equation can be used to calculate the heat of sorption from vapor pressure data. Othmer [\[10\]](#page-7-0) was the first to suggest a correlation between

vapor pressure and latent heat data. This work was extended by Close and Banks [\[11\]](#page-7-0) and resulted in Eq. (11) that relates the vapor pressure, concentration and temperature data to the heat of sorption. This equation has been obtained by assuming that the gas mixture behaves as ideal gas and that surface effects in the desiccant material are negligible.

$$
\left(\frac{\partial \ln P_{\rm v}}{\partial \ln P_{\rm sat}}\right)_{W_{\rm b}} = \frac{q_{\rm s}}{h_{\rm fg}}\tag{11}
$$

Eq. (11) relations the vapor pressure data and the heat of sorption along a line of constant desiccant material moisture content. It establishes that if the equilibrium moisture uptake of a desiccant material is known at different desiccant material temperatures and vapor pressures, the ratio of heat of sorption to the latent heat of evaporation can be determined.

[Fig. 3,](#page-3-0) obtained by using experimental data from [\[12,13\],](#page-7-0) shows relation between natural logarithm of equilibrium partial vapor pressure and natural logarithm of saturation vapor pressure for three different types of molecular sieves. Lines of constant water uptake are given in [Fig. 3](#page-3-0). It can be seen that the ratio of heat of sorption to the latent heat of evaporation does not depend on the temperature of the desiccant. It only depends on water uptake of desiccant material.

The ratio  $\left(\frac{\partial \ln P_{\rm v}}{\partial \ln P_{\rm sat}}\right)$  $W_{\rm b}$  is equal to the slope of a curve in [Fig. 3](#page-3-0) for a constant desiccant material water uptake,  $W<sub>b</sub>$ . By determining the slopes of the curves given in [Fig. 3,](#page-3-0) the relation between ratios of heat of sorption to the latent heat of evaporation as a function of moisture uptake for three different types of molecular sieves were determined. These results are shown in [Fig. 4](#page-4-0). From [Fig. 4](#page-4-0) it can be observed that heat of sorption can be 50% greater than the latent heat of evaporation for the molecular sieves considered here.

The results, given in [Fig. 4](#page-4-0) were curve fitted. A coefficient of determination  $r^2$  is used as parameter that indicates a quality of the curve fit. The coefficient of determination is defined as

$$
r^2 = 1 - \text{SSE} / \text{SSM} \tag{12}
$$

In Eq. (12) SSE is the sum of the squares about the mean and SSM is the sum of squared errors (residuals). A high  $r^2$  value, greater than 0.95, is needed for good representation of the data. In our case, all equations obtained by curve fitting the data obtained from [Fig. 3](#page-3-0) have an  $r^2$  greater than 0.99.

For 3A molecular sieve and 5A molecular sieve, the ratio of heat of sorption and latent heat of evaporation can be represented as

$$
\frac{Q}{H_{\text{fg}}} = a + b \cdot W_{\text{b}} + c \cdot W_{\text{b}}^2 + d \cdot W_{\text{b}}^3 + e \cdot W_{\text{b}}^4 + f \cdot W_{\text{b}}^5 + g \cdot W_{\text{b}}^6 + h \cdot W_{\text{b}}^7 \tag{13}
$$

where Eq. (13) is valid for equilibrium moisture content in the range  $0.02 \leq W_{\rm b} \leq 0.2$ .

<span id="page-3-0"></span>

Fig. 3. Ratio of equilibrium vapor pressure and saturation vapor pressure: (a) molecular sieve 3A; (b) molecular sieve 5A; (c) molecular sieve 13X.

For 13X molecular sieve and the equilibrium moisture content in the range  $0.02 \leq W_b \leq 0.25$ , the best fit is given by Eq. (14)

$$
\frac{Q}{H_{\text{fg}}}=a+b\cdot W_{\text{b}}+c\cdot W_{\text{b}}^{2.5}+d\cdot W_{\text{b}}^{0.5}+e\cdot \exp(-W_{\text{b}}) \quad (14)
$$

The coefficients for Eqs. [\(13\) and \(14\)](#page-2-0) are given in [Table 1.](#page-4-0)

<span id="page-4-0"></span>

Fig. 4. Ratio of heat of sorption and latent heat of evaporation for different types of molecular sieve.

Table 1 Heat of sorption equation coefficients

Coefficients	Molecular sieve 3A Eq. $(13)$	Molecular sieve 5A Eq. $(13)$	Molecular sieve 13X Eq. $(14)$
$\overline{a}$	1.3993	1.674	11.31
h	17.9948	$-17.633$	$-4.652$
$\mathcal{C}$	$-900.9695$	599.92	$-17.999$
$\overline{d}$	18006	$-9995.5695$	$-2.123$
$\ell$	$-191104$	85259.204	$-9.647$
	1143703	$-357042$	
g	$-3665594$	573693	
h	4879165		

#### 5. Equilibrium equation

Equilibrium equations for three different types of molecular sieves are obtained by curve fitting experimental data obtained from [\[12,13\]](#page-7-0). For all curve fits  $r^2$  is greater than 0.99.

For 3A molecular sieve, for a range of equilibrium moisture uptake of  $0.05 \leq W_b \leq 0.223$ , the following equation was used to fit the data:



$$
RH = \frac{a+b \cdot T_w + c \cdot T_w^2 + d \cdot W_b + e \cdot W_b^2 + f \cdot W_b^3}{1+g \cdot T_w + h \cdot W_b + i \cdot W_b^2 + j \cdot W_b^3} \tag{15}
$$

For 5A molecular sieve, for  $0.05 \leq W_b \leq 0.16$ , the following equation was used to fit the data:

$$
RH = \frac{a + c \cdot T_w + e \cdot W_b + g \cdot T_w^2 + i \cdot W_b^2 + k \cdot T_w \cdot W_b}{1 + b \cdot T_w + d \cdot W_b + f \cdot T_w^2 + h \cdot W_b^2 + j \cdot T_w \cdot W_b}
$$
\n(16)

and for  $0.16 \leq W_b \leq 0.21$ , the following equation is used:

$$
RH = \frac{a + b \cdot T_w + c \cdot T_w^2 + d \cdot W_b + e \cdot W_b^2 + f \cdot W_b^3}{1 + g \cdot T_w + h \cdot T_w^2 + i \cdot T_w^3 + j \cdot W_b}
$$
(17)

For 13X molecular sieve, for  $0.05 \leq W_b \leq 0.25$ , the following relation was used to fit the data

$$
RH = \frac{a+b \cdot T_w + c \cdot T_w^2 + d \cdot T_w^3 + e \cdot W_b}{1 + f \cdot T_w + g \cdot W_b + h \cdot W_b^2 + i \cdot W_b^3}
$$
(18)

Coefficients given in Eqs.  $(15)$ – $(18)$ , can be found in Table 2.

# 6. Results and discussion

In this section, differences in desiccant wheel performance using the equilibrium and heat of sorption equations presented in past literature for molecular sieves with those using sorption property equations developed and presented in this paper are evaluated. Adequacy of different assumptions for equilibrium equation and the heat of sorption of molecular sieve is determined.

All results are obtained for an inlet process air temperature of 35  $\degree$ C, the inlet humidity ratios of both air streams are 0.014 kg  $H_2O/kg$  of dry air, the absolute pressure of both air streams is 1 bar and the Lewis number is assumed to be 1. The non-dimensional channel length, as determined by Eq. (7) is 18.5. This is a typical range of nondimensional lengths for desiccant wheels as presented by Zheng et al. [\[6\]](#page-7-0). Also, the wheel is split equally between the process and regeneration stream. This makes the nondimensional time period for adsorption and the nondimensional time period for regeneration to be the same and are equal to half of the total non-dimensional time.



Table 3 Comparison of optimum points for different sets of sorption data,  $T_{\text{reg}} = 110 \text{ °C}$ 

Sorption property data	Total optimal non-dimensional time, $\tau_{\rm opt}$	Exit process air temperature, $\circ$ C	$(Y_{pa_{in}} - Y_{pa_{out}})/$ $Y_{\text{pa}_{in}}, \%$
Molecular sieve 3A	179	82.6	72.1
Zheng et al. $[6]$ Jurinak et al. [9]	238 324	74.5 70.8	69.1 76.2

# 6.1. Comparison of desiccant wheel performance using different sets of sorption property data

Upon reviewing previous work on simulating desiccant and energy wheels performances, two sets of sorption property data for molecular sieves can be found. Both sets of data assume the heat of sorption is equal to the latent heat, Zheng et al. [\[6\]](#page-7-0) and Jurinak and Mitchell [\[9\]](#page-7-0). Only difference is in equilibrium equation. Jurinak and Mitchell [\[9\]](#page-7-0) suggested an equilibrium relation for molecular sieves in the form of

$$
RH = (W_b/W_{\text{max}})/(1 + 50 \cdot (1 - W_b/W_{\text{max}})] \tag{19}
$$

and Zheng et al. [\[6\]](#page-7-0) suggested equilibrium equation in form

$$
RH = R \cdot (W_b / W_{\text{max}}) / [1 - (1 - R) \cdot (W_b / W_{\text{max}})] \tag{20}
$$

The term  $R$  in Eq. (20) is constant and is called the "separation factor''. Many times the separation factor is set equal to 0.01 for molecular sieves. Both Eqs. (19) and (20) assume that the relative humidity of water vapor in equilibrium with desiccant material does not depend on temperature of desiccant material only on its water uptake.

In Table 3, with  $T_{\text{reg}} = 110 \degree C$ , the optimal performances of a desiccant wheel obtained using different sets of sorption property data for molecular sieves are compared. It can be seen that predictions of optimum percentages of initial mass of water vapor removed from process air stream in the desiccant wheel are different and strongly depend on the set of sorption property data used. In the case of desiccant wheel with molecular sieve type 3A, using sorption property data for molecular sieve from literature would lead to 3–4% lower or higher prediction of optimum percentage of initial mass of water vapor removed from process air stream pending on the set of sorption property data used. Also, there is significant difference in optimal non-dimensional time (i.e., the optimal rotational speed) when different sets of heat of sorption and equilibrium equation are used. This can lead to a significant degradation in performance of a desiccant wheel that has type 3A molecular sieve if these wheels are operated at these falsely obtained non-dimensional times, as shown in Table 4.

At very high regeneration temperatures,  $T_{reg} = 170 \degree C$ , the optimal dehumidification performances predicted using

#### Table 4

Performance of desiccant wheel with molecular sieve 3A at non-optimum rotational speeds,  $T_{\text{reg}} = 110 \text{ °C}$ 

Sorption property data	Total optimal Exit process $(Y_{pa_{in}} - Y_{pa_{out}})$ non-dimensional air temperature, $Y_{\text{na}}$ , % time, $\tau_{\text{opt}}$	$^{\circ}C$	
Molecular sieve 3A 179		82.6	72.1
Molecular sieve 3A	238	78.2	67.7
Molecular sieve 3A	324	69.4	54.7

Table 5

Comparison of optimum points for different sets of sorption data,  $T_{\text{res}} = 170 \text{ °C}$ 

Total optimal non-dimensional time, $\tau_{\text{opt}}$	Exit process air temperature, ℃	$(Y_{pa_{in}} - Y_{pa_{out}})/$ $Y_{\text{pa}_{\text{in}}}, \, \frac{0}{0}$
389	88.8	93.9
432 450	78.1 76.9	91.1 92.2

different sets of sorption property data differ less than in case when regeneration temperature is equal to  $110^{\circ}$ C. These results are given in Table 5. The optimal non-dimensional times (i.e., optimal rotational speeds) are still noticeably different, however operating the desiccant wheel with type 3A molecular sieve at optimum non-dimensional times obtained using sets of sorption property data from literature cause only small degradation in performance, Table 6.

Therefore, at lower regeneration temperatures, around 110  $\degree$ C, it is important to use sorption property data for particular type of molecular sieve when optimizing the performance of desiccant wheel. Using incorrect sorption property data for molecular sieves in general can lead to error in prediction of optimum dehumidification performance and optimum rotational speed which as result can lead to serious degradation in dehumidification performance of desiccant wheel. At higher regeneration temperatures, around  $170^{\circ}$ C, using sorption property data for molecular sieves in general still leads to an error in the prediction of optimum rotational speed but this does not lead to noticeable degradation in desiccant wheel performance.

Table 6

Performance of desiccant wheel with molecular sieve 3A at non-optimum rotational speeds,  $T_{\text{reg}} = 170 \text{ °C}$ 

Sorption property data	Total optimal Exit process non-dimensional air temperature, $Y_{\text{pa}_{\text{in}}}$ , % time, $\tau_{\text{opt}}$	°C	$(Y_{\text{pa}_{\text{in}}} - Y_{\text{pa}_{\text{out}}})/$
Molecular sieve 3A	389	88.8	93.9
Molecular sieve 3A	432.	87.7	93.3
Molecular sieve 3A	450	86.9	92.4

# <span id="page-6-0"></span>6.2. Effect of equilibrium equation dependence on temperature of desiccant material on predicted performance of desiccant wheel via computer simulation

A common practice in the field of numerical modeling of desiccant wheel performance is to represent the equilibrium equation with one experimentally generated equilibrium isotherm. This is done because to experimentally generate several equilibrium isotherms at different descant material temperatures would require substantial time. As result of this assumption certain error in prediction of desiccant wheel dehumidification performance is generated. The magnitude of this error and a way to minimize it can be observed from Tables 7 and 8. These tables are obtained by assuming that equilibrium equation of molecular sieve type 3A can be represented by individual equilibrium isotherm. The heat of sorption used is equal to heat of sorption of molecular sieve type 3A presented in this paper.

It can be seen from Table 7,  $T_{reg} = 110 \degree C$ , that using an individual equilibrium isotherm instead of equilibrium equation in full form leads to under prediction of optimum dehumidification performance of desiccant wheel. This under prediction of optimum percentage of initial mass of water vapor removed from process air stream is significant and can be between 5.2% and 11.3% pending on equilibrium isotherm. However, the higher the temperature of desiccant material for which equilibrium isotherm is obtained the smaller the under prediction of optimum dehumidification performance. In the case of higher regeneration temperatures (i.e.,  $T_{\text{reg}} = 170 \text{ °C}$ ) Table 8 shows the under prediction of optimum dehumidification performance is still present. Only this under prediction, between 3.9–5.4% which depends on the equilibrium isotherm, is smaller when compared to under prediction at lower regeneration temperatures. Therefore, influence of molecular

Table 7 Influence of different equilibrium isotherms on optimum desiccant wheel performance,  $T_{\text{reg}} = 110 \text{ °C}$ 



Table 8

Influence of different equilibrium isotherms on optimum desiccant wheel performance,  $T_{\text{reg}} = 170 \text{ °C}$ 

Equilibrium isotherm, $\mathrm{C}$	Total optimal non-dimensional time, $\tau_{\text{opt}}$	Exit process air temperature. $\circ$ C	$(Y_{pa_{in}} - Y_{pa_{out}})/$ $Y_{\text{pa}_{\text{in}}}, \, \frac{0}{0}$
110	343	87.6	88.5
140	361	85.7	89.3
170	375	84.0	90.0

sieve 3A temperature on its equilibrium and on the prediction of optimum desiccant wheel performance is significant and cannot be neglected.

# 6.3. Effect of different heat of sorption assumptions for molecular sieves on desiccant wheel predicted performance

In the literature two heat of sorption equations are suggested for molecular sieves. One assumes that heat of sorption is equal to the latent heat, Zheng et al. [\[6\]](#page-7-0) and Jurinak and Mitchell [\[9\].](#page-7-0) Another, Simonsen and Besant [\[2\]](#page-7-0), assumes the heat of sorption in form

$$
Q = \left[1 + (h_{\text{max}}^* - 1)\left(1 - \frac{W_{\text{b}}}{W_{\text{max}}}\right)^{\lambda}\right] \cdot H_{\text{fg}} \tag{21}
$$

In the above equation  $h_{\text{max}}^* = 3$  and  $\lambda$  is equal to either 2 or 5. It can be observed that all these equations for molecular sieve heat of sorption are quite different. If heat of sorption equations, from the literature, are used in computer code to predict dehumidification performance of desiccant wheel that has molecular sieve type 3A as desiccant material certain error in predicted performance is generated. This is given in Tables 9 and 10. These tables are obtained by using equilibrium equation for molecular sieve type 3A, Eq. [\(15\).](#page-4-0) Only, Table 9 is obtained for  $T_{\text{reg}} = 110 \degree \text{C}$  and Table 10 for  $T_{\text{reg}} = 170 \degree \text{C}$ . From Tables 9 and 10 it can

Table 9

Table 10

Influence of different heat of sorption equations on optimum desiccant wheel performance,  $T_{\text{reg}} = 110 \text{ °C}$ 

Heat of sorption equation	Total optimal non-dimensional time, $\tau_{\rm opt}$	Exit process air temperature, $Y_{\text{pa}_{\text{in}}}, \frac{\ }{\ }$ $\rm ^{\circ}C$	$(Y_{\text{pa}_{\text{in}}} - Y_{\text{pa}_{\text{out}}})/$
Simonsen and Besant et al. [2], $\lambda = 2$	172	85.9	66.4
Simonsen and Besant et al. [2], $\lambda = 5$	170	88.8	59.4
Jurinak et al. [9]	186	79.4	75.3
Molecular sieve 3A, Eq. (13)	179	82.6	72.1

Influence of different heat of sorption equations on optimum desiccant wheel performance,  $T_{\text{reg}} = 170 \text{ °C}$ 



<span id="page-7-0"></span>be seen that heat of sorption equations from the literature are inadequate and they generate errors in the predicted optimum dehumidification performance of desiccant wheel when molecular sieve type 3A is used as desiccant material. Only in the case when heat of sorption is assumed to be equal to the latent heat and  $T_{reg} = 170 \degree C$ , [Table 10](#page-6-0), error is negligible and the assumption appears to be valid. These errors are significant and should be avoided by using suggested heat of sorption for molecular sieve type 3A. This also is valid for other two types of molecular sieve presented in this paper.

## 7. Conclusions

The sorption properties for 3A, 5A and 13X molecular sieves are obtained and presented in equation form. The heat of sorption for each material is obtained using Othmer's method. It is found that heat of sorption for molecular sieves can be up to 50% greater than latent heat of evaporation and the ratio of heat of sorption to the latent heat of evaporation only depends on moisture uptake of the desiccant material.

The heat of sorption and equilibrium data were implemented in numerical simulation code for simulation of nonlinear heat and mass transfer processes that take place in the desiccant wheel. It was found that at lower regeneration temperatures, around 110  $\degree$ C, it is important to use sorption property data for particular type of molecular sieve when numerically optimizing the performance of desiccant wheel. Using sorption property data for molecular sieves in general can lead to error in prediction of optimum rotational speed which as result can lead to serious degradation in dehumidification performance of desiccant wheel. At higher regeneration temperatures, around  $170^{\circ}$ C, using sorption property data for molecular sieves in general still leads to an error in the prediction of optimum rotational speed, however it does not lead to noticeable degradation in desiccant wheel performance.

The influence of molecular sieve temperature on the equilibrium equation and its effect on the performance of desiccant wheel is significant. Assuming the equilibrium equation does not depend on temperature of desiccant material will lead to under prediction of desiccant wheel dehumidification performance. Also, the heat of sorption equations for molecular sieves presented in literature in most cases inadequately represent heat of sorption equations for three different types of molecular sieve considered in this paper.

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