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ON THE MODELING OF MOISTURE ADSORPTION IN A PACKED BED

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Abstract

This paper presents a mathematical model which describes process of moisture transfer from the adsorbent bed and air filtrated through the bed. The model of the packed bed column takes into consideration mass transfer in the bed as well as water diffusion and adsorption in a new composite sorbent "$CaCl_2$/alumina". The model is applied to describe evolution of vapor concentration at the exit of experimental unit for regenerating moisture in ventilation systems, which has recently been suggested, build and tested. Sorption equilibrium of water vapor on the new sorbent has been studied to be used as input parameter in the model. Good agreement between experimental and calculation data demonstrated that the model adequately reflects main physical and chemical features of the regeneration processes. Hence, it can be used for modeling a scale-up effect and for magnification of the unit from laboratory to larger size, e.g. single room, family house and large residential buildings.

Keywords: *mathematical modeling, adsorption, mass transfer, parameter identification*

1. INTRODUCTION

For countries with a cold climate the large difference between indoor and outdoor temperatures leads to large heat loses in ventilation systems, moisture freezing at the systems exit and great reduction in the indoor humidity. A new approach to regenerating moisture in ventilation systems has been proposed and tested at a laboratory scale [1-3].

Many models are used to describe mass transfer between a fixed bed of solid adsorbent and a flux of humid air that is filtrated through the bed [4, 5]. In this paper mass transfer processes in the fixed bed column are described by the convection-diffusion equation with a volume reaction which in the case is an adsorption between water and the salt confined to the pores of alumina.

2. MATHEMATICAL MODEL

The mathematical description of the mass transfer in the gas phase has the form:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial z} = D\frac{\partial^2 c}{\partial z^2} - \frac{k_1}{\varepsilon}\left[c\left(1 - \frac{c_S}{c_S^{max}}\right) - kc_S\right],$$

$$t = 0, \quad c = c_0; \tag{1}$$

$$z = 0, \quad c = c_0, \quad \frac{\partial c}{\partial z} = 0.$$

The concentration of the moisture connected with the adsorbent can be obtained from the equation:

$$\frac{\partial c_S}{\partial t} = \frac{k_1}{1-\varepsilon}\left[c\left(1-\frac{c_S}{c_S^{max}}\right)-kc_S\right], \tag{2}$$

$$t = 0, \quad c_S = c_S^0,$$

where u is the velocity distribution, c-concentration of the moisture in the gas phase, t-the time, z-axial coordinate, D-diffusivity, c_0-initial concentration, c_S-concentration of the moisture connected with the adsorbent, c_S^{max}-maximal concentration (saturation), k-volume reaction rate constant, ε-gas hold-up in the adsorption column.

The model equations (1, 2) will be solved in the time interval $\left[t_0 \le t \le t_{critical} = 5.83\,min\right]$.

The minimization of the least square function will be used for parameter identification. The problem will be solved in dimensionless form, using the characteristic scale of the process:

$$t = t_0 T, \quad c = c_{max} C, \quad c_S = c_S^{max} C_S, \quad z = lZ. \tag{3}$$

The replacement of eq. (3) in eqs. (1) and (2) leads to:

$$\frac{\partial C}{\partial T} + \frac{ut_0}{l}\frac{\partial C}{\partial Z} = Fo\frac{\partial^2 C}{\partial Z^2} - \frac{k_1 t_0}{\varepsilon}C + \frac{k_1 k t_0}{\varepsilon}\frac{c_S^{max}}{c^{max}}C_S, \tag{4}$$

$$\frac{\partial C_S}{\partial T} = \frac{k_1 t_0}{1-\varepsilon}\frac{c^{max}}{c_S^{max}}C - \frac{k_1 k t_0}{1-\varepsilon}C_S, \tag{5}$$

$$T = 0, \quad C = 1, \quad C_S = 0;$$

$$Z = 0, \quad C = 1, \quad \frac{\partial C}{\partial Z} = 0, \quad C_S = 0, \tag{6}$$

where

$$Fo = \frac{Dt_0}{l^2}. \tag{7}$$

For the long time process t_0 is very big and if divide the equation (4) by $\frac{ut_0}{l} \Rightarrow \frac{\partial C}{\partial T} \approx 0$, i.e. the process is stationary. The concentration of the moisture connected with the adsorbent (C_S) depends on time, because of that the concentration of the moisture in the gas phase (C) depends also- time is the parameter in the eq. (4).

$$\frac{\partial C}{\partial Z} = \frac{1}{Pe}\frac{\partial^2 C}{\partial Z^2} - \frac{k_1 l}{u\varepsilon}C + \frac{k_1 k l}{u\varepsilon}\frac{c_S^{max}}{c^{max}}C_S, \tag{8}$$

$$\frac{\partial C_S}{\partial T} = \frac{k_1 t_0}{1-\varepsilon}\frac{c^{max}}{c_S^{max}} C - \frac{k_1 k t_0}{1-\varepsilon} C_S, \tag{9}$$

$$T = 0, \quad C_S = 0; \tag{10}$$

$$Z = 0, \quad C = 1, \quad \frac{\partial C}{\partial Z} = 0, \quad C_S = 0,$$

where

$$Pe = \frac{ul}{D} \tag{11}$$

The parameter identification problem for the model equations (8-10) will be solved, using the real experimental data (Fig.1) [2].

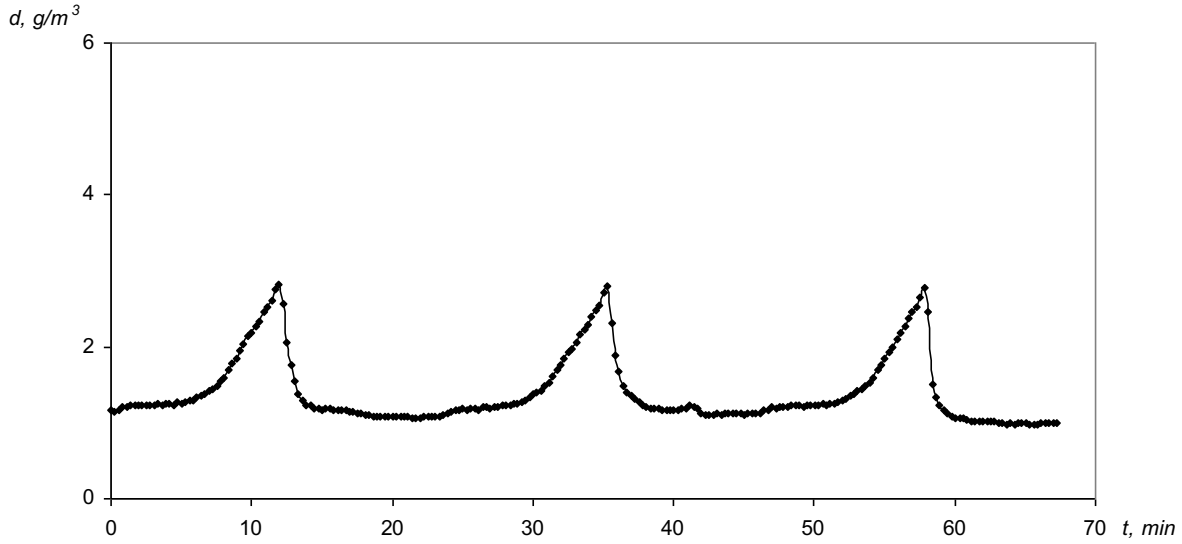


Fig. 1 Evolution of absolute humidity $d\left(g/m^3\right)$ as function of time t.

For model parameters identification the least square function is used.

$$F = \sum_{i=1}^{N}\left[C(t_i) - C_{exp}(t_i)\right]^2, \tag{12}$$

where $t_i\left(i = 1,...,N\right)$ are the times in which the concentration of the moisture in the gas phase is quantified.

The determination of the model parameters was made by minimization of (12) using the procedure *fminsearch* of MATLAB 7.5.

As a result was obtained:

$$k_1 = 0.0084\, s^{-1},\ k = 0.0388,\ \varepsilon = 0.0098\ \frac{m^3}{m^3},\ \frac{c_S^{max}}{c_S} = 3.6829,\ F = 2.5379.10^{-5} \qquad (13)$$

A comparison of the calculated concentration of the moisture in the gas phase (using the parameter values) with the experimental data is given in Fig. 2.

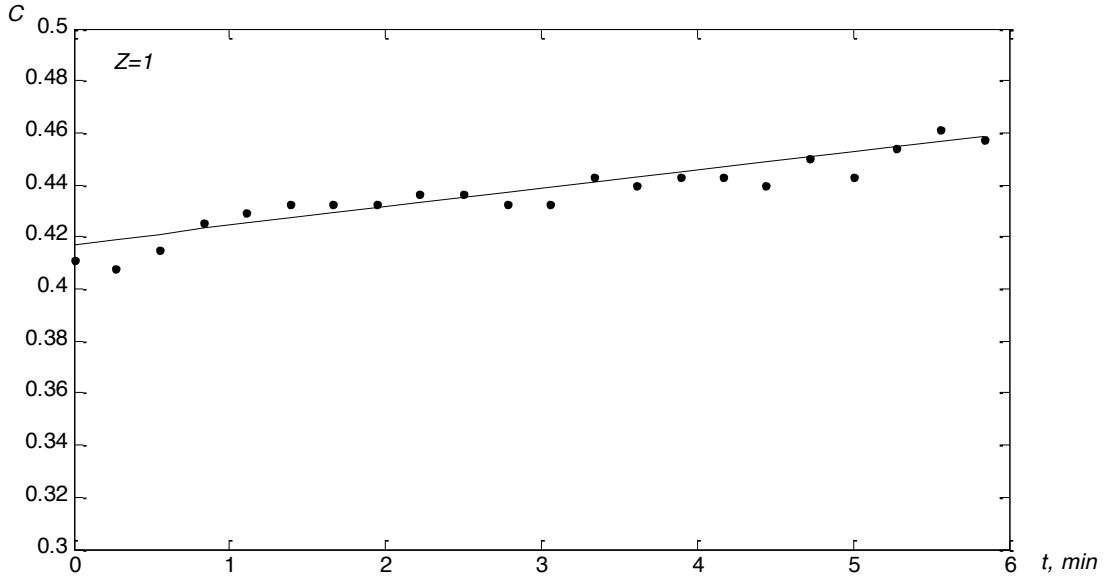


Fig. 2**.** Comparison of the calculated values and experimental data for dimensionless concentration of the moisture in the gas phase (C)

From the model equations (4-6), with the calculated values of the parameters, could be determined the evolution of concentration of the $CaCl_2$ in the solid phase as function of time $C_S = f(t)_{Z=1}$ (Fig.3), and the evolution of concentration of the moisture in the gas phase $C = f(Z)_{t=t_{critical}}$ and of concentration of the $CaCl_2$ in the solid phase $C_S = f(Z)_{t=t_{critical}}$ as function of column height (Figs. 4, 5).

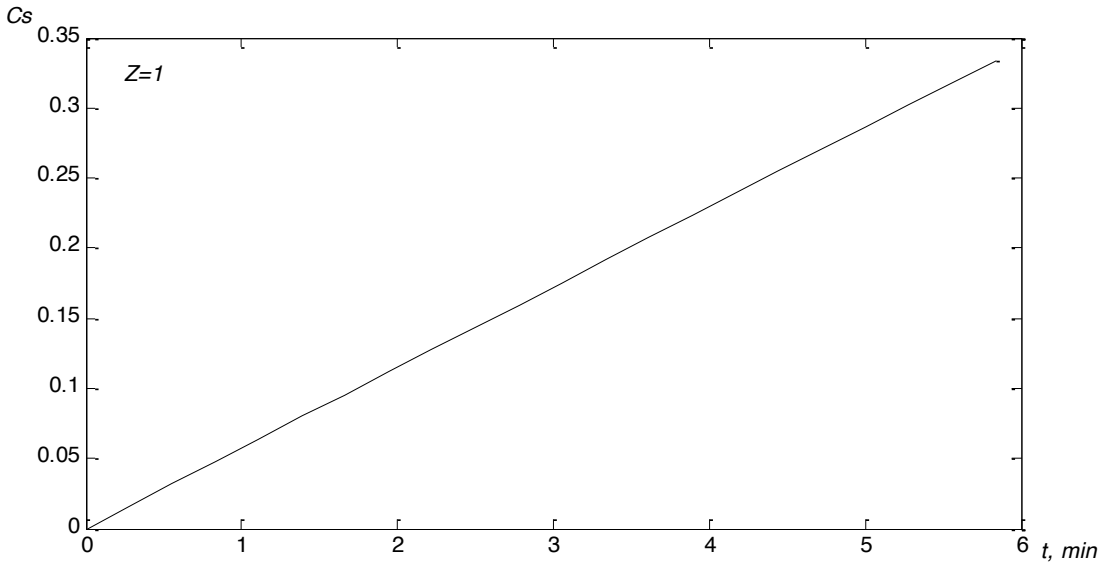


Fig. 3 Evolution of concentration of the $CaCl_2$ in the solid phase as function of time $C_S = f(t)_{Z=1}$

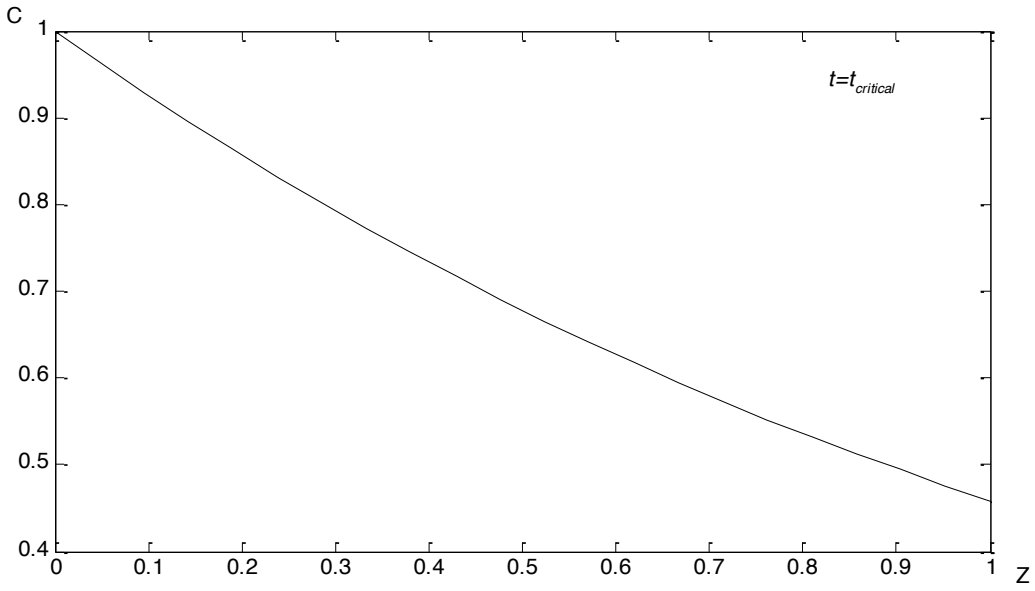


Fig. 4 Evolution of concentration of the moisture in the gas phase as function of column height $C = f(Z)_{t=t_{critical}}$

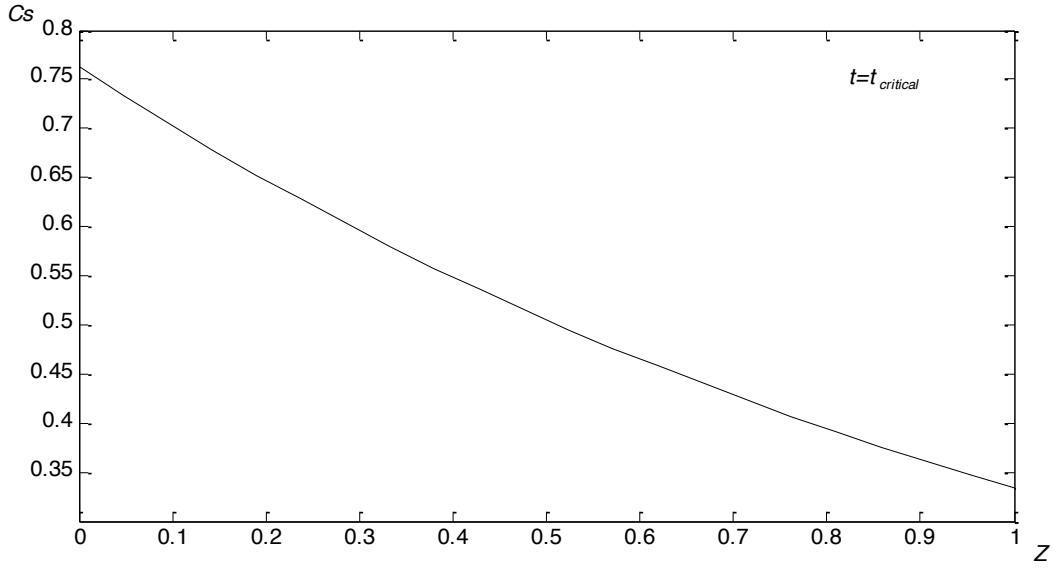


Fig. 5 Evolution of concentration of the $CaCl_2$ in the solid phase as function of column height $C_S = f(t)_{Z=1}$

3. CONCLUSION

The method is tested on moisture adsorption modeling in a packed bed. The results obtained are in a good agreement with the experimental data.

From the model equations could be determined the evolution of concentration of the $CaCl_2$ in the solid phase as function of time $C_S = f(t)_{Z=1}$, and the evolution of concentration of the moisture in the gas phase $C = f(Z)_{t=t_{critical}}$ and of concentration of the $CaCl_2$ in the solid phase $C_S = f(Z)_{t=t_{critical}}$ as function of column height.

The next step is to solve the model equations for entire time period of the adsorption process and to calculate the parameter values.

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NOMENCLATURE

c	concentration of the moisture in the gas phase, [kmol/m^3]
c_S	concentration of the $CaCl_2$ in the solid phase, [kmol/m^3]

c_0	inlet concentration of the moisture in the gas phase, [kmol/m^3]
c_S^0	initial concentration of the $CaCl_2$ in the solid phase, [kmol/m^3]
k	equilibrium constant
k_1	mass transfer coefficient, [s^{-1}]
u	velocity distribution in the column, [m/s]
D	diffusivity of the water in the gas phase, [m^2/s]
l	column height, [m]
ε	gas hold-up in the adsorption column, [m^3/m^3]
t	time, [s]
z	axial coordinate, [m]
N	Number of the experimental data
F	Least square function
Fo	Fourier' number
Pe	Peckle' number

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