Study of Gas Drying by Adsorption on Composite Materials Using Neural Networks

RODICA DIACONESCU*, MARIUS SEBASTIAN SECULA, STELIAN PETRESCU
"Gh. Asachi" Technical University, Faculty of Chemical Engineering and Environmental Protection, Chemical Engineering Department, 71 D. Mangeron, 700050, Iasi, Romania

An artificial neural network study of gas drying by adsorption in fixed bed of composite materials is presented in this paper. The experimental investigations were carried out at two values of relative humidity and three values of air flow rate respectively. The experimental data were employed in the design of the feed forward neural networks for modeling the evolution in time of some adsorption parameters, such as adsorption rate, water concentration in the bed, water vapor concentration in air at the exit from the fixed bed, drying degree and rate respectively. Based on these adsorption parameters, two composite adsorbent materials having porous matrices were compared

Keywords: gas-drying, adsorption, neural network, mass transfer, silica gel

Recent studies on the adsorption system approach mainly the development of advanced adsorbent materials that give improved adsorption capacity and higher mass and heat transfer rates [1–6]. Comprehensive experimental studies of the physicochemical properties and some application researches of the composite adsorbents have been reported [1–6]. All their studies point out that the composite adsorbents present a higher adsorption capacity and can be regenerated at lower temperature values. However, conclusions on the feasibility of these materials for adsorption systems can only be drawn after dynamic analysis of the composite adsorbent behaviour under real operating conditions of adsorption systems.

In the last few years, neural network have attracted more and more interest as predictive models due to the fact that they are able to approximate any continuous non-linear functions [7, 8], being applied widely in the process modeling and control [9]. Thus it was concluded that the artificial neural networks (ANNs) model gives better results than regression technique for predicting results (output) from adsorption database [10]. Otherwise, ANNs offer some quite interesting possibilities for rapidly developing non-linear process model. In addition, the main feature of the neural networks - the establishment of complex relationships between data through a learning process, with no need to propose any model to correlate the desired variables - makes this technique very useful in the modeling of processes where traditional mathematical modeling is difficult or impossible.

Therefore, in this work is presented an ANNs study of gas drying by adsorption in fixed bed of composite materials with porous matrix. The experimental investigations were carried out using *LiBr*-impregnated silica gel grains of different shapes, and air at different values of the flow rate and air moisture. The experimental data were employed in the design of the feed forward neural networks for modeling the evolution in time of some adsorption parameters, such as adsorption rate, water concentration of the bed, water vapor concentration in air at the exit from the fixed bed, drying degree and rate.

Overview on artificial neural networks

Neural networks were originally inspired as being models of the biological nervous system. Thus ANNs might store experiential knowledge and make it available for use [11]. In predicting an input-output response, ANN is viewed as a "black box" due to its mathematics involved is difficult to comprehend but very simple to implement. In recent years, there has been a growing interest in the application of ANNs in chemical engineering [12-14].

The most popular neural network architecture in engineering investigations is the multilayer perceptron (MLP) [15].

An artificial neural network model that represents a *MLP* structure is written as:

$$y = f(U) = W_0 \cdot tanh(W_i \cdot U + B_i) + b_0 \qquad (1)$$

where:

y is the output of the neural network model,

U – a column vector of size p that contains the p inputs of the process;

W_0 – a row vector of size n that contains the weights of the neural network model from the hidden layer to the output;

W_i – a matrix that contains the weights of the neural network model from the inputs to the hidden layer. This matrix has n rows and p columns,;

B_i – a column vector of size n that contains the biases from the input to the hidden layer of the neural network model;

b_0 – the bias (scalar) from the hidden layer to the output of the neural network model;

$tanh(W_i \cdot U + B_i)$ - o column vector that contains the hyperbolic tangent of the elements of the vector $W_i \cdot U + B_i$ [16].

First, the neural network is trained in order to calculate optimal values of the weights. When the number of data used for training is huge or the number of hidden nodes is large, then the training may take a long time. Once the network is trained, it can be tested on a different set of data than that used for training. It is a good approach to divide the given input/output data into two parts: one part (about 70%) is used for training whereas the other part usually smaller is used for testing the neural network model. The testing data set is reserved to validate the trained network [17].

Training and testing of the networks were performed by means of the *NeuroSolutions* software, using the *Marquardt* algorithm and cross validation. In the studied case, the

* *email: diac@ch.tuiasi.ro*

neural network model was determined as having four neurons in input, one hidden layer with eight neurons and one output, *MLP (4:8:1)*.

Experimental part

In the experimental investigations was used a laboratory installation consisting in an adsorption column, a wetting air column, a fan and devices for measuring and controlling temperature and air flow rate. A full description of the experimental installation employed to obtain the data needed in this study can be found in [18].

The investigations were carried out using two types of composite adsorbent materials obtained from spherical silica gel particles having a diameter of 2.57 . 10^{-3} m by impregnation with *LiBr*. The two composite materials, *MCSS2* and *MCS2*, differ by their geometrical shape, *MCSS2* having a spherical shape, while *MCS2* a non-spherical shape. Experimental investigations were performed under atmospheric pressure at an initial value of air temperature of 38°C, using wet air as gaseous phase at two values of the relative humidity: 60 and 85 %, and at several values of air flow rate: 0.3, 0.6 and 1.2 $m^3 . h^{-1}$.

The adsorption process was achieved in fixed granular bed of composite materials under dynamic regime. The geometrical parameters of the fixed adsorbent bed were 0.15 m in height and 2.95 . 10^{-2} m in diameter.

Results and discussions

In order to study the adsorption process, the water concentration in the fixed bed, *X*, water concentration of air at the fixed bed exit, C, adsorption rate, ν_a, drying degree, η_u, and drying rate, v_u, were considered as functions of type y = f (material, C^0, M_v, t), where: materials used were MCSS2 or MCS2, C^0- water vapor concentration of wet air at the entrance in the fixed bed, M_v- flow rate of the wet air and *t*- time of adsorption. These parameters are defined as follows:

$$X = \frac{\Delta m + m_0 \cdot x_0}{m_0(1 - x_0)} \tag{2}$$

where:

m_0 - mass of adsorbent bed at t = 0, kg;

Δ_m – mass of water uptake of the bed, kg;

x_o - water mass ratio in adsorbent at t = 0;

$$v_a = \rho_v \frac{dX}{dt} \tag{3}$$

where:

ρ_v - apparent density of packing, kg . m^{-3};

$$\eta_u = 1 - \frac{C}{C_0} \tag{4}$$

where:

C_o, C - water vapor concentration in gas phase at the entrance and respectively exit of the adsorbent bed, kg . m^{-3};

$$v_u = \frac{1}{V_v} \frac{dw}{dt} \tag{5}$$

where:

w – water vapor quantity removed from air flux, kg.

V - gas volume, m^3.

The 445 experimental data points corresponding to the above-mentioned variables were collected and processed. The four variables listed in the right-hand side of above equation were considered as input variables while the *X*, *C*, ν_a, h_u and v_u were considered as the output values. Thus,

Table 1
STATISTICAL CHARACTERIZATION
FOR TRAINING PHASE

Variable	*R*	*MSE*	*MAE*
X (kg/kg)	0.9967864	2.6574E-05	0.00406677
C (kg/m^3)	0.997073	2.00E-07	0.0003346
v_a (kg/m^3s^{-1})	0.988196	2.0085E-08	0.00011103
η_u	0.9982809	3.227E-13	3.9882E-07
v_u(kg/m^3s^{-1})	0.9990092	0.00011403	0.00763676

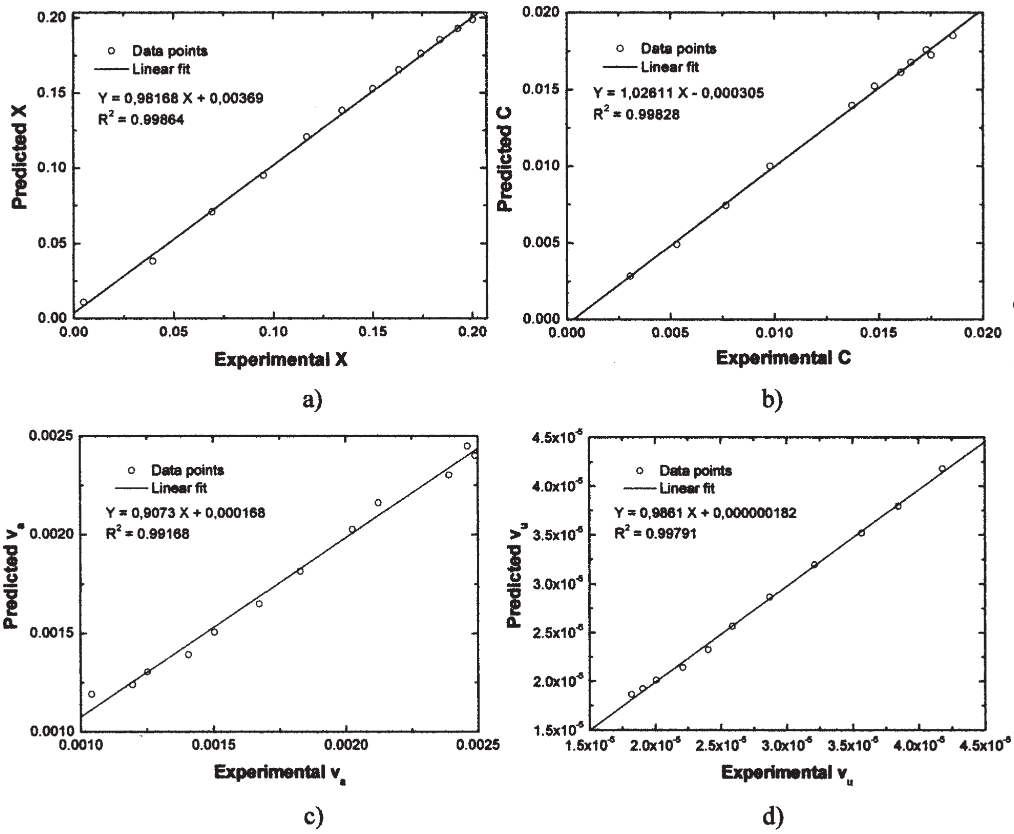
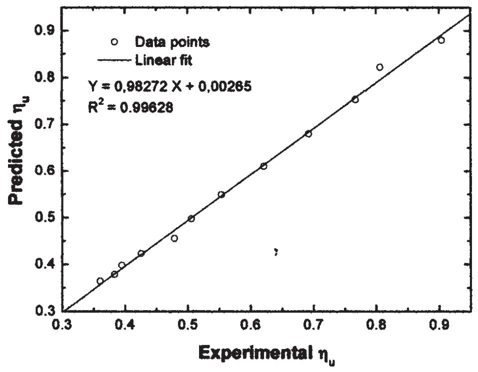


Fig. 1a-d. NN predictions (X, C, v_a, η_u and v_u) versus experimental values for several training sets: a) water concentration of MCS2 at C^0 = 0.0204 kg/m^3 and M_v = 1.2 m^3/h; b) water vapours concentration of wet air at the exit from the fixed bed of MCSS2 at C^0 = 0.0293 kg/m^3 and M_v = 0.6 m^3/h; c) adsorption rate at the exit from the fixed bed of MCSS2 at C^0 = 0.0204 kg/m^3 and M_v = 0.6 m^3/h; d) drying rate of MCS2 at the exit from the fixed bed at C^0 = 0.0293 kg/m^3 and M_v = 0.6 m^3/h



e)

Fig. 1e. NN predictions (X, C, v_a, h_u and v_u) versus experimental values for several training sets e) drying degree of MCSS2 at C^0 = 0.0293 kg/m^3 and M_v = 0.6 m^3/h

each *ANN* presents four input variables and one output variable.

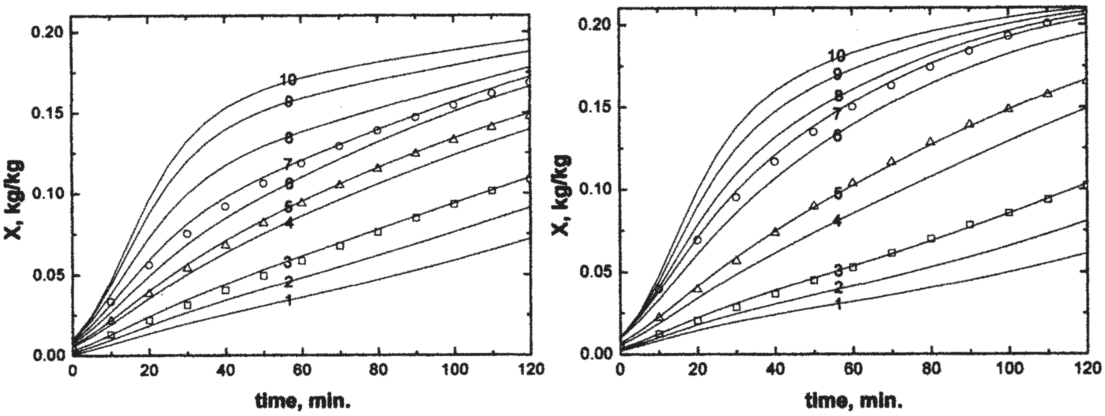
In the training phase, the statistical parameters: linear correlation coefficient (*R*), mean squared error (*MSE*) and mean absolute error (*MAE*) (table 1) indicate that the neural models describe well the adsorption process.

Several examples are presented in figure 1 that shows a comparison between experimental data and neural network predictions on training data. A good agreement is emphasized proving that the neural model has learned well the behaviour of the studied process.

The purpose of direct neural modeling lies in the obtaining the network (group of formula) describing the dependences between the experimental data defining the investigated process. The elaborated neural model was then applied for several sets of experimental data in order to generate the necessary outputs. For validation, there were used new data that were not employed in the network training. In the studied case, the network *MLP (4:8:1)*

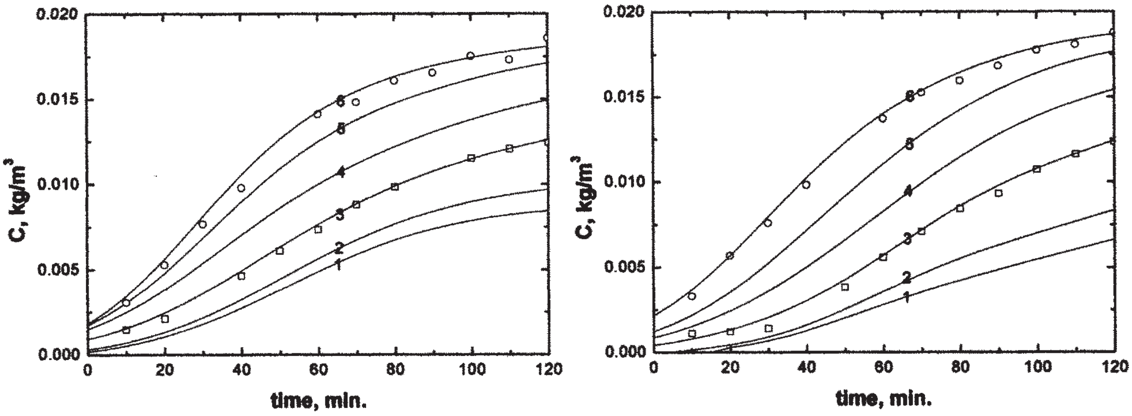
Table 2
STATISTICAL CHARACTERIZATION FOR VALIDATION PHASE OF MLP (4:8:1).

Type of composite material	*C^0 (kg/m^3)*	*M_v m^3/h*	*Time (min)*	*y_{exp}*	*y_{RNA}*	*Relative error (%)*
			y= X(kg/kg)			
MCSS2	0.0204	0.3	30	0.03100408	0.03200937	3.24
MCSS2	0.0204	0.6	10	0.02143944	0.02349927	9.61
MCSS2	0.0204	0.6	120	0.14768898	0.14827194	0.39
MCSS2	0.0204	1.2	30	0.07530076	0.07140914	5.17
MCSS2	0.0293	0.6	30	0.07050647	0.07917837	12.30
MCSS2	0.0293	0.6	120	0.18916776	0.1894523	0.15
MCS2	0.0204	0.3	80	0.06982745	0.07192511	3.00
MCS2	0.0204	0.6	20	0.03930279	0.03990419	1.53
MCS2	0.0204	0.6	90	0.13902848	0.13721384	1.30
MCS2	0.0204	1.2	30	0.09502154	0.09313494	1.98
MCS2	0.0293	0.6	10	0.02706771	0.02858971	5.62
			y=C(kg/m^3)			
MCSS2	0.0204	0.3	20	0.00069	0.000666	3.49
MCSS2	0.0204	0.6	30	0.003421	0.003098	9.42
MCSS2	0.0204	0.6	90	0.010337	0.010358	0.20
MCSS2	0.0204	1.2	40	0.008914	0.009474	6.29
MCSS2	0.0293	0.6	50	0.011987	0.012226	1.99
MCS2	0.0204	0.3	20	0.000737	0.00078	5.74
MCS2	0.0204	0.6	40	0.0023	0.002832	23.14
MCS2	0.0293	0.6	50	0.011102	0.011499	3.57
			$y=v_a$ (kg/m^{3}s^{-1})			
MCSS2	0.0204	0.3	20	0.00130835	0.00130366	0.36
MCSS2	0.0204	0.6	50	0.00202584	0.00199108	1.72
MCSS2	0.0204	1.2	50	0.00216652	0.00204628	5.55
MCSS2	0.0204	1.2	110	0.0011114	0.00117679	5.88
MCSS2	0.0293	0.6	40	0.00281367	0.00280621	0.26
MCS2	0.0204	0.3	40	0.00108633	0.00109998	1.26
MCS2	0.0204	0.3	120	0.0011256	0.00098696	12.32
MCS2	0.0204	0.6	120	0.00108633	0.00114995	5.86
MCS2	0.0293	0.6	70	0.00202869	0.00208225	2.64
			$y=\eta_u$			
MCSS2	0.0204	0.3	40	0.96759664	0.96597353	0.17
MCSS2	0.0204	0.3	110	0.81693629	0.81636601	0.07
MCSS2	0.0204	0.6	60	0.64072105	0.63865406	0.32
MCSS2	0.0204	0.6	120	0.39297243	0.39564014	0.68
MCSS2	0.0204	1.2	70	0.34280927	0.3312629	3.37
MCSS2	0.0293	0.6	30	0.73861956	0.74573901	0.96
MCS2	0.0204	0.3	30	0.96306266	0.96453906	0.15
MCS2	0.0204	0.3	120	0.85460247	0.88570731	3.64
			$y= v_u$ (kg/m^{3}s^{-1})			
MCSS2	0.0204	0.3	40	$3.2959 \cdot 10^{-5}$	$3.2435 \cdot 10^{-5}$	1.59
MCSS2	0.0204	0.6	50	$2.5143 \cdot 10^{-5}$	$2.4472 \cdot 10^{-5}$	2.67
MCSS2	0.0204	1.2	60	$1.3884 \cdot 10^{-5}$	$1.4662 \cdot 10^{-5}$	5.61
MCSS2	0.0204	1.2	100	$8.9423 \cdot 10^{-5}$	$8.7876 \cdot 10^{-5}$	1.73
MCSS2	0.0293	0.6	70	$2.5101 \cdot 10^{-5}$	$2.4667 \cdot 10^{-5}$	1.73
MCS2	0.0204	0.3	30	$3.3072 \cdot 10^{-5}$	$3.2567 \cdot 10^{-5}$	1.53
MCS2	0.0204	0.6	50	$2.8977 \cdot 10^{-5}$	$2.7421 \cdot 10^{-5}$	5.37
MCS2	0.0293	0.6	20	$4.1805 \cdot 10^{-5}$	$4.0026 \cdot 10^{-5}$	4.26



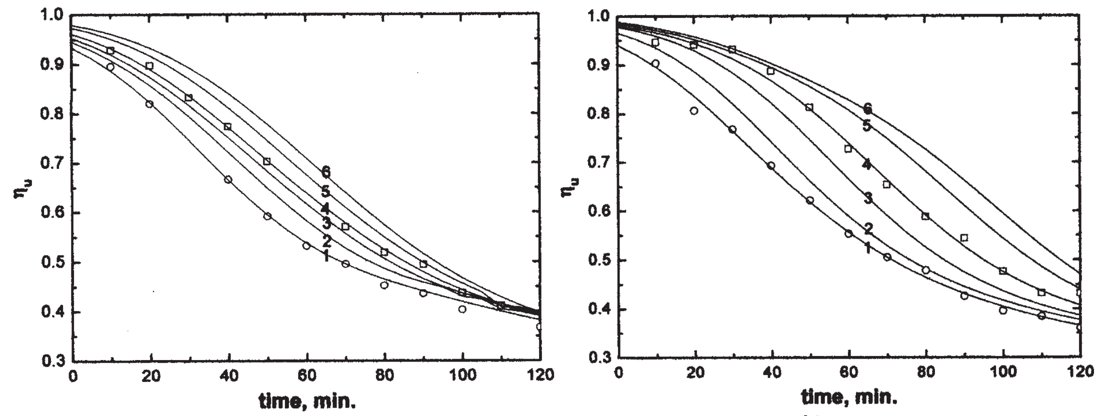
a) b)

Fig. 2. Neural networks predictions (solid line) and experimental data (□ - M_v = 0.3 m^3/h, Δ - M_v = 0.6 m^3/h, O - M_v = 1.2 m^3/h) for water concentration in MCSS2 (a) and MCS2 (b) respectively, at C^0 = 0.0204 kg/m^3 and: 1- M_{vv} = 0.1 m^3/h ; 2 - M_v = 0.2 m^3/h ; 3 - M_v = 0.3 m^3/h; 4- M_v = 0.5 m^3/h ; 5 - M_v = 0.6 m^3/h, 6 - M_v = 0.9 m^3/h ; 7 - M_v = 1.2 m^3/h; 8 - M_v = 1.5 m^3/h; 9 - M_v = 1.8 m^3/h and 10 - M_v = 2 m^3/h.



a) b)

Fig. 3. Neural networks predictions (solid line) and experimental data (□ - C^0 = 0.0204 kg/m^3, O - C^0 = 0.0293 kg/m^3) for water vapor concentration of wet air at the exit from the fixed bed of MCSS2 (a) and MCS2 (b) respectively, at M_v = 0.6 m^3/h and: 1 - C^0 = 0.015 kg/m^3; 2 - C^0 = 0.017 kg/m^3; 3 - C^0 = 0.0204 kg/m^3; 4 - C^0 = 0.023 kg/m^3; 5 - C^0 = 0.026 kg/m^3 and 6 - C^0 = 0.0293 kg/m^3.



a) b)

Fig. 4. Neural networks predictions (solid line) and experimental data (□ - C^0 = 0.0204 kg/m^3, O - C^0 = 0.0293 kg/m^3) for the drying degree corresponding to MCSS2 (a) and MCS2 (b) respectively, at M_v = 0.6 m^3/h and: 1 - C^0 = 0.015 kg/m^3; 2 - C^0 = 0.017 kg/m^3;3 - C^0 = 0.0204 kg/m^3; 4 - C^0 = 0.023 kg/m^3;5 - C^0 = 0.026 kg/m^3 and 6 - C^0 = 0.0293 kg/m^3.

received inputs unemployed in the training process and generated output values. The achieved results are presented in table 2.

The good results obtained in the validation stage allow the utilization of the neural model in order to perform predictions corresponding to other operating conditions than the experimental ones. In this way, there were considered both types of composite materials, the two values of C^0 (table 2), air flow rate and time were varied from *0.1 m^3/h* to *2 m^3/h*, respectively, from *0* to *120 min.* with a 5 min. step. Thus, a high number of data (approximately 5000) were generated and employed in order to describe the adsorption process on the used composite material on a range wider than that experimentally investigated as presented in figures 2-6.

In figure 2 are shown the neural network predictions for water concentration in both composite materials as function of time, maintaining the same air moisture at the entrance of the fixed bed, at several values of the air flow rate.

As it can be seen, water concentration in adsorbents increases in time, while increasing of air flow rate

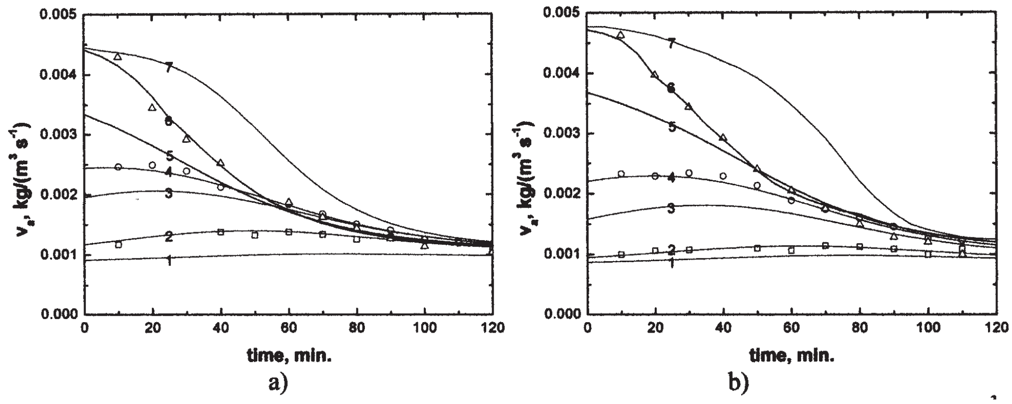


Fig. 5. Neural networks predictions (solid line) and experimental data (□ - M_v = 0.3 m^3/h, Δ - M_v = 0.6 m^3/h, O - M_v = 1.2 m^3/h) for adsorption rate corresponding to MCSS2 (a) and MCS2 (b) respectively, at C^0 = 0.020452 kg/m^3 and different values of M_v: 1- M_v = 0.1 m^3/h ; 2 - M_v = 0.3 m^3/ ; 3 - M_v = 0.5 m^3/h ; 4 - M_v = 0.6 m^3/h, 5 - M_v = 0.9 m^3/h ; 6 - M_v = 1.2 m^3/h; 7 - M_v = 1.4 m^3/h.

accelerates the adsorption process. Though both composite adsorbents behave almost similarly at low air flow rate values, *MCS2* shows rather better adsorption characteristics for water vapours at high values of the air flow rate.

In figures 3 and 4 are described the variations in time of water vapor concentration of wet air at the exit from the fixed bed and drying degree at several values of air moisture.

Water vapor concentration of wet air at the exit from the fixed bed increases in time and at high values of air moisture. This is due to a higher driving force of adsorption process. On the contrary, the drying degree decreases in time and with lower values of air moisture.

In figure 5 are depicted the time dependences of adsorption rate for both composite adsorbents corresponding to several values of air flow rate.

Increasing air flow rate leads to higher adsorption rates, which is due to weaker resistances to the external mass transfer.

In figure 6 are compared the evolutions in time of the drying rate for both composite adsorbents at two values of water vapor concentration of wet air at the entrance in the fixed bed.

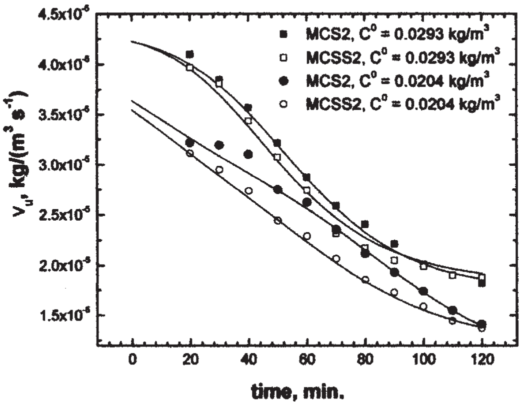


Fig. 6. Neural networks predictions (solid line) and experimental data for drying rate corresponding to MCS2 and MCSS2 at C^0 = 0.0204 kg/m^3 and C^0 = 0.0293 kg/m^3 respectively.

According to the diagram in figure 6, *MCS2* presents slightly higher adsorption characteristics than *MCSS2*.

As it can be noted, all the predicted curves are in very good agreement with the experimental data. The predicted data outside and inside the investigated range of experimental conditions respect the typical behaviour of the investigated process for both types of composite materials.

Conclusions

A neural network modeling for the process of gas drying by adsorption is presented in this paper. The obtained model renders the evolution in time of the adsorption rate, υ_a, drying rate, υ_u, drying degree, η_u, water vapor concentration of wet air at the fixed bed exit, C, and water concentration in the fixed bed, X. Also, two composite adsorption materials were compared and it was emphasized that non-spherical silica gel grains impregnated with *LiBr* presents slightly higher adsorption characteristics than spherical silica gel grains impregnated with *LiBr*.

Data predicted in the training phase were compared with the experimental data on which the training phase was based. The very good agreement between model and experimental data proved that the neural network learned well the behavior of the adsorption parameters. Moreover, the predictions of the neural networks were compared with another set of experimental data that were not employed in the training phase. Therefore, the suggested neural network can be easily used to interpolate and extrapolate data of the adsorption process investigated for different conditions.

Aknowledgment: Financial support for this work was provided by the CNCSIS in the framework of PN-II/IDEI PROGRAM (PN-II-ID-PCE-2007-1, Grant No. 63/01.10.2007, Cod 608).

References

1.ARISTOV, Y, TOKAREV, M.M., CACCIOLA, G., RESTUCCIA, G., React. Kinet. Cat. Lett., 1996, 59, p. 325

2.ARISTOV, Y, RESTUCCIA, G., CACCIOLA, G., PANON, V.N., Appl. Therm. Eng., 2002, 22, p. 191

3.DAWOUD, B., ARISTOV, Y., Int. J. Heat Mass Transfer, 2003, 46, p. 273

4.LIU, Y.F., WANG, R.Z., Sci. China Ser. E., 2003, 46, p. 551

5.ZHANG, X.J., SUMATHY, K., DAI, Y.J., WANG, R.Z., Int. J. Energy Res., 2005, 29, p. 37

6.ZHANG, X.J., LIU, L.M., Energy Conversion and Management, 2007, 48, p. 320

7.PARK, J., SANDEBERG, W.I., Neural Comput., 1991, 3, p. 246

8.WANG, Z., THAM M.T., MORRIS, A.J., Int. J. Control, 1992, 56, p. 655

9.BULSARI, A.B., "Computer-aided chemical engineering, Neural networks for chemical engineers", vol. 6, Elsevier, Amsterdam, 1995.

10.BABU, B.V., RAMAKRISHNA, V, Proceedings of 2nd International Conference of Water Quality Management, February 2003, New Delhi, India. (http://bvbabu.50megs.com/custom.html/#58)

11.HAYKIN, S., "Neural Networks: A Comprehensive Foundation", Prentice Hall, Upper Saddle River, NJ, 1996

12.FLOOD, I., KARTAM, N., "Neural Networks in Civil Engineering. I. Principles and Understanding", J. Computing in Civil Eng. ASCE, 8, 1994, p. 131

13.MORSHED, J., KALUARACHICHI, Advances in Water Resources, 1998, 22, p.145

14.SATISH S., PYDI SETTY, Y., International Communications in Heat and Mass Transfer, 2005, 32, p. 539

15.BASU, S., HENSHAW, P.F., BISWAS, N., KWAN, H.K., Canadian J. of Chem. Eng., 2002, 80, p. 1

16.ZHANG, Z. FRIEDRICH, K., J. Compos. Sci. Tech., 2002, 63, 2029

17.DIACONESCU, R., DUMITRIU, E., EEMJ, 2005, 4, p. 473

18.PETRESCU, S., HOROBA, D.L., GALBEN, I.G., SECULA, M., Rev. Chim. (Bucuresti), **60**, nr. 3, 2009, p. 308

Manuscript received: 11.12.2008