ANN MODELING AND SIMULATION OF GAS DRYING BY ADSORPTION ON COMPOSITE MATERIALS

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KEYWORDS

Gas-drying, Gas-solid adsorption, Neural network, Silica gel.

ABSTRACT

An artificial neural network (ANN) modeling 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.

INTRODUCTION

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 (Aristov et al., 1996; Aristov at al., 2002; Dawoud and Aristov, 2003; Liu and Wang, 2003; Zhang et al., 2005; Zhang and Liu, 2007). Comprehensive experimental studies of the physicochemical properties and some application researches of the composite adsorbents have been reported by Aristov et al. (Aristov et al., 1996; Aristov at al., 2002; Dawoud and Aristov, 2003), Liu and Wang (Liu and Wang, 2003) and Zhang et al. (Zhang et al., 2005; Zhang and Liu, 2007). 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 behavior 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 they are able to approximate any continuous non-linear functions (Park and Sandeberg, 1991; Wang et al., 1992), being applied widely in the process modeling and control. Thus, Babu and Ramakrishna (Babu and Ramakrishna, 2003) concluded that the artificial neural networks (ANNs) model gives better results than regression technique for predicting results (output) from adsorption database. 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. Regression equations rendering the evolution in time of the same adsorption parameters were also proposed and analyzed.

OVERVIEW ON ANN

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. 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 (Flood and Kartam, 1994; Satish and Pydi Setty, 2005).

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

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, 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.

Training and testing of the networks were performed by means of the *NeuroSolutions* software,

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors)
ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD)

using the *Marquardt* algorithm and cross validation. In the studied case, the 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

In the experimental investigations was used a laboratory installation (Fig. 1) consisting in an adsorption column, a wetting air column, a fan and devices for measuring and controlling temperature and air flow rate.

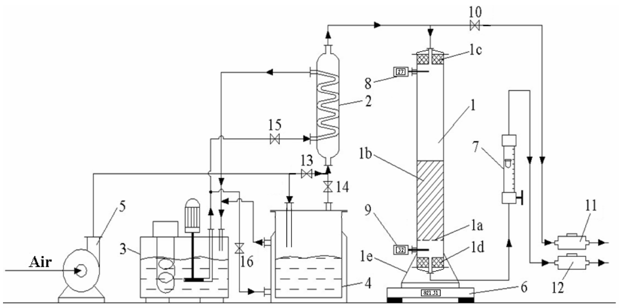


Fig. 1. Experimental installation: 1 – adsorption column, 2 – heat exchanger, 3 – thermostat, 4 – air wetting chamber, 5 – ventilator fan, 6 – digital technical balance, 7 – rotameter, 8, 9 – digital thermometers, 10, 13, 14, 15, 16 – valves, 11, 12 – chambers for measuring air relative humidity at the entrance and relatively exit of the adsorbed column.

The investigations were carried out using two types of composite adsorbent materials obtained from spherical silica gel particles having a diameter of $2.57 \cdot 10^{-3}$ *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 $1.2\ m^3 \cdot h^{-1}$.

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 $2.95 \cdot 10^{-2}$ *m* in diameter.

RESULTS AND DISCUSSIONS

For modeling the adsorption process, the water concentration in the fixed bed, X, water concentration of air at the fixed bed exit, C, adsorption rate, v_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:

$$X = \frac{\Delta m + m_0 \cdot x_0}{m_0 \left(1 - x_0\right)} \qquad (1)$$

where: m_0 – mass of adsorbent bed at $t = 0$, *kg*; Δm – mass of water uptake of the bed, *kg*; x_0 – water mass ratio in adsorbent at $t = 0$;

$$v_a = \rho_v \frac{dX}{dt} \qquad (2)$$

where: ρ_v – apparent density of packing, $kg \cdot m^{-3}$;

$$\eta_u = 1 - \frac{C}{C_0} \qquad (3)$$

where: C_0, C – water vapor concentration in gas phase at the entrance and respectively exit of the adsorbent bed, $kg \cdot m^{-3}$;

$$v_u = \frac{1}{M_v} \frac{dw}{dt} \qquad (4)$$

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

Regression Analysis

Experimental data points corresponding to the above-mentioned variables were collected and processed. Based on the experimental data and using specialized software for curve fitting (Table Curve 2D, 5.01, trial version), a series of statistical equations defining X, C, v_a, η_u, v_u as functions of time were determined. In the selection of these equations, three criteria were followed: the accuracy in modeling the experimental data, the simplicity of the equations and the use of a single equation pattern for all the experimental data sets. Consequently, four order polynomials with different numerical coefficients were considered.

$$y = a + b \cdot t + c \cdot t^2 + d \cdot t^3 + e \cdot t^4 \qquad (5)$$

where y = X, C, v_a, η_u, v_u, and t is the time, min.

Table 1 presents the numerical values of the coefficients in equation (5) of the adsorption parameters corresponding to 0.6 m^3/h and 60 %RH.

Table 1. Some values of the coefficients in eq. (5).

Nr. Crt.	Dep. Var.	Mat.	Coefficients				
			a	b	c	d	e
1	X	MCSS2	4.8E-03	1.7E-03	-2.2E-06	-4.2E-08	1.9E-10
2	C		1.2E-03	-9.8E-06	3.7E-06	-3.8E-08	1.1E-10
3	v_a		2.2E-02	2.2E-04	-9.8E-06	9.9E-08	-3.4E-10
4	η_u		9.6E-01	3.4E-04	-1.3E-04	1.3E-06	-4.0E-09
5	v_u		4.6E-05	1.7E-08	-6.3E-09	6.5E-11	-2.0E-13
6	X	MCS2	5.0E-03	1.7E-03	5.0E-06	-1.2E-07	4.5E-10
7	C		2.6E-03	-2.1E-04	7.4E-06	-6.3E-08	1.8E-10
8	v_a		2.0E-02	2.5E-04	-7.4E-06	5.4E-08	-1.2E-10
9	η_u		9.1E-01	7.3E-03	-2.6E-04	2.2E-06	-6.2E-09
10	v_u		4.2E-05	4.8E-07	-1.6E-08	1.4E-10	-4.3E-13

The obtained equations allow the determination of the adsorption dependent variables (X, C, v_a, η_u, v_u) at any moment in the time range investigated experimentally.

Table 2. Statistical parameters of the suggested equations.

Nr. Crt.	Statistical parameters			
	R^2 Coef Det	Fit Std Err	F computed	F-distribution, (α=0.05)
1	0.99998	2.3765E-04	115589.45	4.75
2	0.99897	1.5746E-04	1689.92	4.96
3	0.99679	3.5095E-04	544.09	4.96
4	0.99897	5.4744E-03	1689.92	4.96
5	0.99968	1.4063E-07	4719.49	5.12
6	0.99632	5.1310E-05	474.01	4.75
7	0.99998	2.5968E-04	124886.05	4.96
8	0.99947	1.9873E-07	2848.64	4.96
9	0.99949	4.6569E-03	3405.93	4.96
10	0.99881	2.5826E-04	1471.41	5.12

As can be seen in Table 2, the values of the determination coefficient of equations are near unity, while standard error and maximum absolute error have very low values, which show four-order polynomial functions fit very well the experimental data. Moreover, F-computed >> F-distribution for α = 0.05, which underlines that all the suggested equations are adequate.

Regression equations allow the determination of the adsorption parameters at any moment in the experimental time range. Working with these equations is not difficult, but the numerical coefficients for different conditions of the adsorption process are necessary. Compared to these empirical models, the neural network modeling presents the advantage of supplying rapidly and easily the parameter values.

Artificial Neural Network

The 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, v_a, η_u and v_u were considered as the output values. Thus, 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 3) indicate that the neural models describe well the adsorption process.

In Fig. 2 is presented an example 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 behavior of the studied process.

Table 3. Statistical characterization for training phase.

Variable	*R*	*MSE*	*MAE*
X (kg/kg)	0.99679	2.6574E-05	4.06677E-03
C (kg/m^3)	0.99707	2.0000E-07	3.3460 E-04
v_a (kg/m^{3}s^{-1})	0.98820	2.0085E-08	1.1103 E-04
η_u	0.99829	3.2270E-13	3.9882E-07
v_u(kg/m^{3}s^{-1})	0.99901	1.1403E-04	7.6367E-03

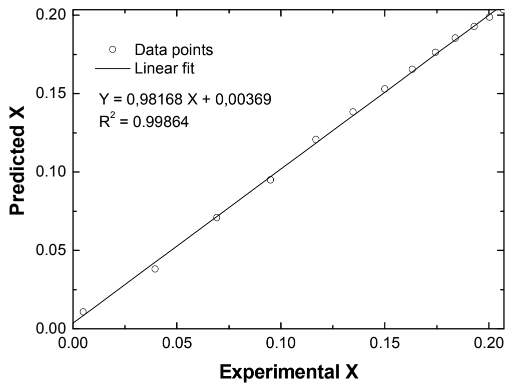


Fig. 2. ANN predictions versus experimental values for water concentration of *MCS2* at $C^0 = 0.02876\ kg/m^3$ and $M_v = 1.2\ m^3/h$.

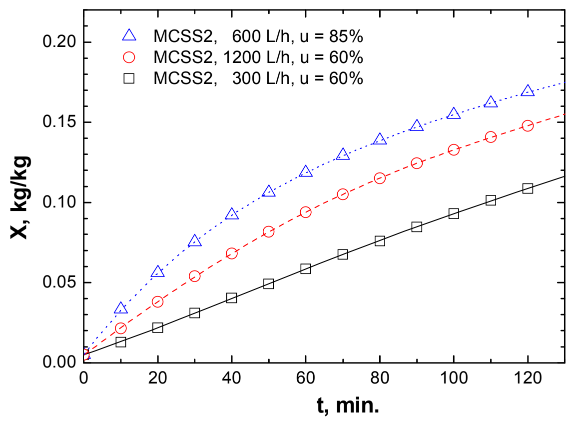
The purpose of direct neural modeling lies in the obtaining the network (group of formula) describing the dependences between the experimental data defining the investigated process. The elaborated neural model was then applied for several sets of experimental data in order to generate the necessary 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)* received inputs unemployed in the training process and generated output values. Several of the achieved results corresponding to MCSS2, 0.6 m^3/h and 60 %RH are presented in Table 4.

Table 4. Statistical characterization for validation phase of MLP (4:8:1).

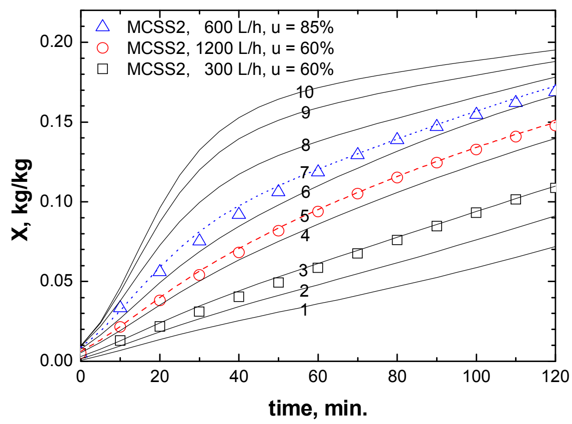
Nr. Crt.	Dep. Var.	*t (min.)*	y_{exp}	y_{RNA}	*Rel. error (%)*
1	X	10	2.144E-02	2.350E-02	9.61
2	C	30	3.421E-02	3.098E-03	9.42
3	v_a	50	2.026E-03	1.991E-03	1.72
4	η_u	60	6.407E-01	6.386E-01	0.32
5	v_u	50	2.514E-05	2.447E-05	2.67

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 4), 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 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 Figs. 3-5.

In Fig. 3 are shown the regression equations and neural network predictions for water concentration in MCSS2 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.



(a)

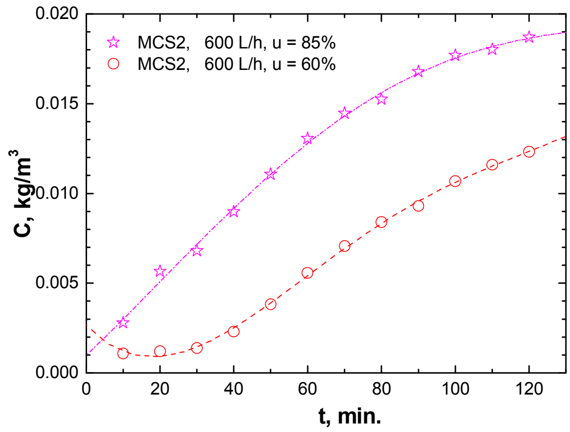


(b)

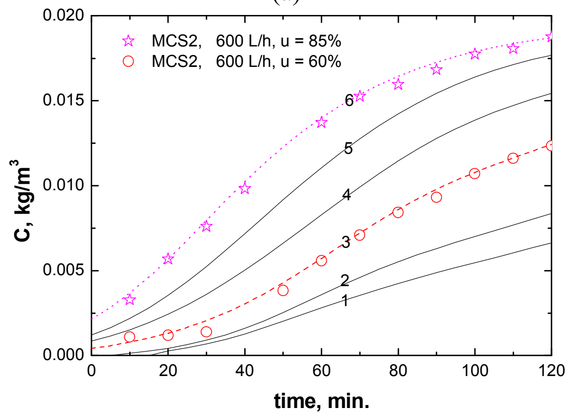
Fig. 3 Regression equations (a) respectively ANN predictions (b) (lines) and experimental data (□ - $M_v = 0,3\ m^3/h$, ○ - $M_v = 0,6\ m^3/h$, △- $M_v = 1,2\ m^3/h$) for water concentration in *MCSS2*. In (b) $C^0 = 0.0204\ kg/m^3$ and: 1- $M_v = 0.1\ m^3/h$; 2 - $M_v = 0.2\ m^3/h$; 3 - $M_v = 0.3\ m^3/h$,; 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 - $M_v = 2\ m^3/h$.

As can be seen, water concentration in adsorbents increases in time, while increasing of air flow rate accelerates the adsorption process.

In Fig. 4 are described the variations in time of water vapor concentration of wet air at the exit from the fixed bed at several values of air moisture.



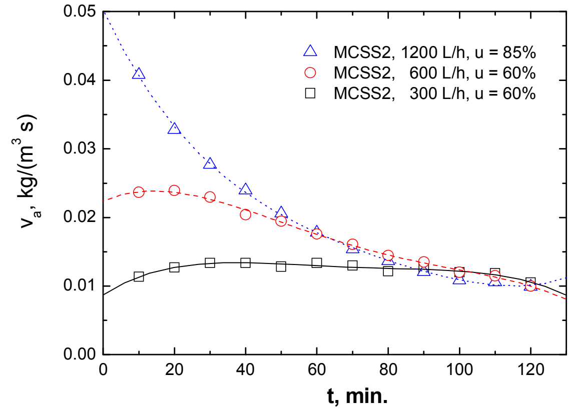
(a)



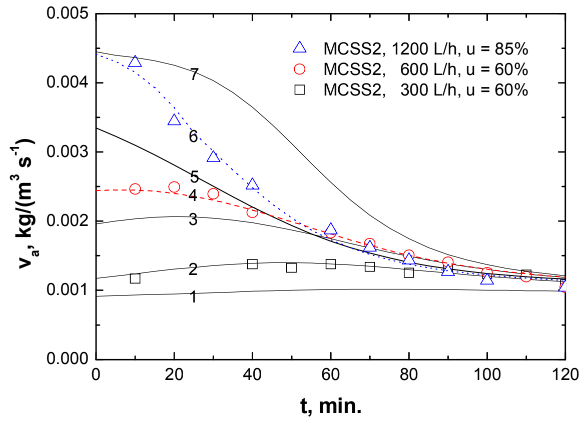
(b)

Fig. 4. Regression equations (a) respectively ANN predictions (b) (lines) and experimental data (○ - $C^0 = 0.02876\ kg/m^3$, ☆ - $C^0 = 0.04145\ kg/m^3$) for water vapor concentration of wet air at the exit from the fixed bed of *MCS2*, at $M_v = 0.6\ m^3/h$. In (b) 1 - $C^0 = 0.021\ kg/m^3$; 2 - $C^0 = 0.024\ kg/m^3$; 3 - $C^0 = 0.02876\ kg/m^3$; 4 - $C^0 = 0.0323\ kg/m^3$; 5 - $C^0 = 0.037\ kg/m^3$ şi 6 - $C^0 = 0.04145\ kg/m^3$.

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.



(a)



(b)

Fig. 5. Regression equations (a) respectively ANN predictions (b) (lines) and experimental data (□ - M_v = *0,3 m³/h*, ○ - M_v = *0,6 m³/h*, △- M_v = *1,2 m³/h*) for adsorption rate corresponding to *MCSS2*, at C^0 = *0.02876 kg/m³*. In (b): 1- $M_v = 0.1$ *m³/h* ; 2 - $M_v = 0.3$ *m³/* ; 3 - $M_v = 0.5$ *m³/h* ; 4 - $M_v = 0.6$ *m³/h*, 5 - $M_v = 0.9$ *m³/h* ; 6 - $M_v = 1.2$ *m³/h*; 7 - $M_v = 1.4$ *m³/h*..

In Fig. 5 are depicted the time dependences of adsorption rate for MCSS2 composite material 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.

As it can be noted, 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 behavior of the investigated process.

Though the results of the empirical polynomial equations seem to be better than those of the neural models, one should have in mind that each equation is based on its own set of numerical coefficients, while the neural network weights are available for the entire experimental range. It can be concluded that the experimental data are well modeled by both empirical polynomial equations and neural networks. However, the empirical equations are difficult in handling, while the neural models are easy to built, have simple topologies and short training times.

CONCLUSIONS

This work presents two types of empirical models for gas drying by adsorption, namely, artificial neural networks and regression equations. These models render the evolution in time of the ratio of water to adsorbent material, X, water vapour concentration of wet air at the exit from the fixed bed, C, adsorption rate, v_a, drying degree, η_u, and drying rate, v_u.

Regression equations represented by forth-order polynomials were proposed to model the considered adsorption parameters. These equations were validated by the determination coefficients, and their adequacy was tested by using Fischer test. However, the fact that the numerical coefficients have to be changed for each set of experimental conditions represents a major drawback. In addition, for any new operating conditions outside the investigated domain, the numerical values of the coefficient are no longer valid.

The artificial neural network models were validated by two methods. 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.

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