Microporous and Mesoporous Materials 208 (2015) 50–54

Contents lists available at ScienceDirect

Microporous and Mesoporous Materials

journal homepage: www.elsevier.com/locate/micromeso

Prediction of gas storage capacities in metal organic frameworks using artificial neural network

Zeynep Yıldız*, Harun Uzun

Ondokuz Mayıs University, Engineering Faculty, Department of Chemical Engineering, Kurupelit, 55139 Samsun, Turkey

ARTICLE INFO

Article history:
Received 17 April 2014
Received in revised form
14 January 2015
Accepted 23 January 2015
Available online 29 January 2015

Keywords:
Adsorption
Artificial neural network
Gas storage
MOFs

ABSTRACT

In this study, artificial neural network was developed to forecast adsorption capacity of hydrogen gas in metal organic frameworks. Surface area, adsorption enthalpy, temperature and pressure were selected as input parameters. Hydrogen storage capacities of MOFs were computed using these four parameters. An artificial neural network was used to model the adsorption process. The prediction results were remarkably agreed with the experimental data.

1. Introduction

The design and synthesis of coordination polymers with unusual structures and properties are gaining increasing interest, not only for their intriguing molecular topologies, but also for their potential applications as functional materials [1–3]. The construction of molecular architecture depends on the combination of several factors, like the coordination geometry of metal salt and ligand [1–7]. Metal organic frameworks (MOFs) have been identified as a new group of porous materials with excellent potential in gas storage and gas separation applications because of their wide range of pore sizes, chemical functionalities, good thermal and mechanical properties [8–10]. MOFs, also known as coordination polymers. A variety of physical and chemical properties of MOFs make them attractive in a wide range of applications such as gas storage, gas separation, drug delivery, sensing, and catalysis [11].

Artificial neural network (ANN) uses interconnected mathematical neurons to create a structure that models complicated systems [12]. In the network, all neurons are connected to each other. The input signal passes through the neuron and the output is calculated by weight and bias associated with connections. A substantial kind of ANN for anticipation, optimization and classification is established in different fields including computer science economics, chemistry and chemical engineering and water resources engineering [13–15].

2. Materials and methods

2.1. Adsorbents

Metal Organic Frameworks (MOFs) have been used as adsorbent in this work. We studied thirteen different metal organic frameworks (MOFs) which are expected to high surface areas. The synthesis of MOFs followed that described in the literature. The composites were prepared as those described in details in Refs. [20–24]. According to references, the temperature is at 77 K. Brunauer–Emmett–Teller surface area range is 10–2847 $m^2\ g^{-1}$. The adsorption enthalpy (ΔH_{ads}) is between 6.1 and 10.5 kJ mol^{-1}. Moreover, The pressure is generally at 1.2 bar.

2.2. Artificial neural network modeling

The modeling of nonlinear systems is difficult and success has been restricted to restrictive classes of nonlinear systems. The major application of artificial neural network (ANN) is that they tender the potential of a generic approach to the modeling of nonlinear systems [16,17].

The modeling of adsorption processes because of possessing nonlinear nature and multiple inputs and outputs is not easy. ANN

* Corresponding author.
E-mail addresses: zeynepyildiz.omu@gmail.com (Z. Yıldız), harunuzun.omu@gmail.com (H. Uzun).

http://dx.doi.org/10.1016/j.micromeso.2015.01.037
1387-1811/

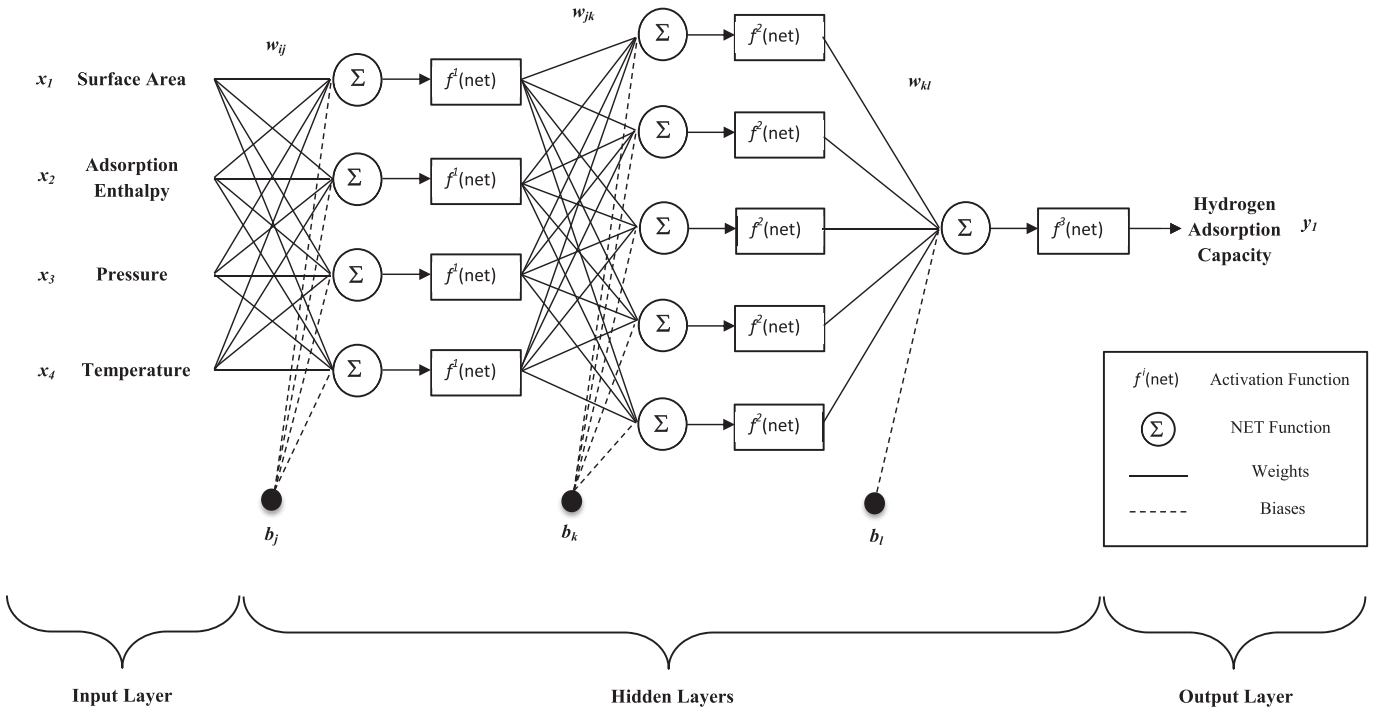

Fig. 1. Multi layers artificial neural network architecture.

has been successfully utilized for prediction adsorption processes of different sorbates from aqueous solution with various adsorbents [18,19].

Four inputs has been made to apply an Artificial Neural Network (ANN) model to predict the gas storage capacities of MOFs using different parameters such as temperature, adsorption enthalpy, surface area, pressure.

There are different neural network architectures. The basic architectures include multilayered feed-forward networks that are trained using back-propagation training algorithms. A variation in the architecture of such a network can be due to a variation of the number of layers, the number of neurons in each layer, the transfer function of neurons in each layer [18].

An artificial neural networks structure contains layers, inputs, weights, outputs, NET function and activation function (Fig. 1). Information of input layer plays important roles in the construction system. Important of this information is obtained using weights. NET function is the inputs of weights total.

Net inputs come to cell and they are converted to outputs using activation function and transferred to other cells. The mechanism is shown in Equation (1).

$$y = f_3\left[\sum_{k=1}^{l}\left(f_2\left[\sum_{j=1}^{k}\left(f_1\left[\sum_{i=1}^{j}x_i w_{ij} + b_j\right]\right)w_{jk} + b_k\right]\right)w_{kl} + b_l\right] \quad (1)$$

3. Results and discussion

3.1. Metal organic frameworks datas

In Table 1, Porosity data and H_2 storage properties for porous metal-organic frameworks are described. SA_{BET}, ΔH_{ads} are the Brunauer–Emmett–Teller surface area, the adsorption enthalpy, respectively. Nine different metal organic frameworks data were used for training. Four metal organic frameworks

Table 1
Data of metal organic frameworks used in artificial neural network.

	Metal organic frameworks[a]	SA_{BET} [$m^2\ g^{-1}$]	ΔH_{ads} [kJ mol^{-1}]	P [bar]	Temperature [K]	H_2 uptake [wt%]	Ref.
Calibrating data	$Cu_6O(tzi)_3(NO_3)$	2847	9.5	1	77.0	2.4	[20]
	Co_3 $[(Mn_4Cl)_3(btt)_8]2\cdot1.7CoCl_2$	2096	10.5	1.2	77.0	2.12	[21]
	Fe_3 $[(Mn_4Cl)_3(btt)_8]_2\cdot FeCl_2$	2033	10.2	1.2	77.0	2.21	[21]
	Zn_3 $[(Zn_{0.7}Mn_{3.3}Cl)_3(btt)_8]_2\cdot2ZnCl_2$	1927	9.6	1.2	77.0	2.10	[21]
	$Li_{3.2}Mn_{1.4}$ $[(MnCl)_3(btt)_8]_2\cdot0.4LiCl$	1904	8.9	1.2	77.0	2.06	[21]
	$Li^+@Zn_2(ndc)_2(diPyNI)$	756	6.1	1	77.0	1.63	[22]
	$Mn_2(bdt)Cl_2$	530	8.8	1.2	77.0	0.82	[23]
	$Mn_3(bdt)_3$	290	8.4	1.2	77.0	0.97	[23]
	$Mg_3(ndc)_3$	10	9.5	1.2	77.0	0.46	[24]
Testing data	$Ni_{2.75}Mn_{0.25}$ $[(Mn_4Cl)_3(btt)_8]_2$	2110	9.1	1.2	77.0	2.29	[21]
	Mn_3 $[(Mn_4Cl)_3(btt)_8]_2\cdot0.75CuPF_6$	1911	9.9	1.2	77.0	2.00	[21]
	Cu_3 $[(Cu_{2.9}Mn_{1.1}Cl)_3(btt)_8]_2\cdot2CuCl_2$	1695	8.5	1.2	77.0	2.02	[21]
	$Zn_3(bdt)_3$	640	8.7	1.2	77.0	1.46	[23]

[a] Abbreviations: tzi = 5-tetrazolylisophthalate; btt = 1.3.5-benzenetristetrazolate; ndc = 2.6-naphthalenedicarboxylate; diPyNI = N,N′-di-(4-pyridyl)-1.4.5.8-naphthalenetetracarboxydiimide; bdt = 1.4-benzeneditetrazolate.