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Neural network and genetic algorithm for modeling and optimization of effective parameters on synthesized ZSM-5 particle size

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A B S T R A C T

The aim of this study is to design a nonlinear model based on neural network for estimation of ZSM-5 particle size. The experimental data were gathered from the literature. The main preparation variables affecting ZSM-5 particle size are SiO_2/Al_2O_3, template/SiO_2, H_2O/SiO_2, and SiO_2/Na_2O ratios, crystallization time, and temperature, which are selected as input variables of the neural model. The results indicate that the designed model can exactly estimate the effects of six input parameters on the ZSM-5 particle size. An optimization paradigm based on genetic algorithm is employed to determine the minimum value of ZSM-5 particle size and the corresponding operating conditions. The optimized gel composition is as follows: $SiO_2/Al_2O_3 = 113.6$, template/$SiO_2 = 0.32$, $H_2O/SiO_2 = 42.10$, SiO_2/Na_2O 73.21 and the optimal temperature and crystallization time are 443 K and 98 h, respectively.

1. Introduction

ZSM-5 zeolite is employed as a typical catalyst in the conversion of methanol to hydrocarbons (methanol to olefin and gasoline) as well as biomass to olefin (BTO) due to its unique acidic and structural properties [1–3]. Terms such as “particle size” and “agglomerate size” are encountered with regards to zeolite size and morphology, particle usually refers to small pieces of matter with known size and geometry, which are visible using SEM and TEM analyses. When the pieces are small, they stick together and form agglomerates. However, very big particles (in micrometer range) do not usually agglomerate and are individually visible. Graeve et al. have performed extensive investigations in this regard [4–7].

ZSM-5 zeolites of particle sizes below 100 nm are considered as potential alternatives for conventional zeolites because of their unique characteristics and advantages [8]. Particle sizes can be decreased by modifying synthesis parameters like the gel composition, the crystallzation temperature or the use of original bifunctional templates (formation of zeolite nanosheets) [9–11].

The development of a model is important in the prediction of the interactions between the input variables and ZSM-5 particle size. Considering the fact that finding an appropriate and reliable model for a system is very difficult or often impossible, an intelligent technique based on the neural network is designed to model ZSM-5 particle size.

Application of a genetic algorithm in particle size analysis by multispectral extinction measurements has been carried out by Xu et al. [12]. In another work, particle size distribution of multimodal polymer dispersions has been optimized by a genetic algorithm [13]. In this study, a genetic algorithm is also employed to find the optimum ZSM-5 particle size and the corresponding operating conditions. This approach is a robust algorithm, which may optimize the nonlinear problems without any knowledge of derivatives of the objective function. In this paper, the optimized value of ZSM-5 particle size and its corresponding optimum operations are presented. The experimental data, used in this research, were gathered using literature reports, and synthesis ZSM-5.

2. Study of the literature data

Reported sizes of ZSM-5 samples were synthesized using a sol–gel medium with the chemical composition of a Al_2O_3: b SiO_2: c template: e Na_2O: f H_2O at different crystallization times and temperatures. The experimental data were gathered from the literature and included six inputs and one response. The data and their references are listed in Table 1 [14–26].

3. Model development based on neural network

ANN has been widely applied in different fields of sciences because of the ability of an artificial neural network (ANN) to represent the nonlinear manner of the process [27,28]. In the

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Table 1
Collected data from literature.

No.	Time (h)	Temperature (K)	Template type[a]	Stoichiometric ratios range				Average size (nm)	Ref.
				Si/Al	Template/SiO_2	SiO_2/Na_2O	H_2O/SiO_2		
1	48	363	1	40–60	0.15–0.25	200–300	16.2–22.2	35–87	[14]
2	26	433	1	25	0.12	50	60	120	[15]
3	16–48	423–190	–	20–30	–	5.56	40	1750–4000	[16]
4	12–120	438	1	25	0.36	312.5	12–19.8	15–60	[17]
5	24	453	2	30–62	0.08–0.15	7.5–15.6	22.5–36.6	1000–9000	[18]
6	9–220	424–463	–	12.5–33.5	–	7.14–14.28	15–29	1500–6000	[19]
7	52	373	2	25–246	0.03–0.05	6.67–14.49	30–55	650–2640	[20]
8	45	503	1	20	0.043	17.85	13.87	50	[21]
9	12–72	413–428	1;2	30	0.36	50	40	54–146	[22]
10	160	373	2	25–77	0.05	10	40	3500–5000	[23]
11	12–55	453–503	1	20–25	0–0.215	7.5–8.33	9.5–25	15–79	[24]
12	24	453	–	25	–	7.14–10	25	15–21	[25]
13	60–72	373–463	1	41.5	0.2	250	19.2	150–2000	[26]

[a] (1): tetrapropylammonium hydroxid; (2) tetrapropylammonium bromide.

neural network, there are layers of a number of interconnected neurons. There are many types of neural network architectures, in which feed forward neural network has been frequently applied in process modeling. This network consists of an input layer, hidden layer(s), and an output layer. The number of the neurons in the input layer and output layer is equal to the number of input and output measured variables of the model, respectively, whereas, the number of hidden layers and their neurons is selected through an iterative method so that the acceptable threshold of the network training error is fulfilled. The mean squared error (MSE) is defined as the error of the training neural network.

$$\mathrm{MSE} = \frac{1}{N}\sum_{k=1}^{N}(E_k - y_k)^2 \quad (1)$$

where, N is the number of the training, y_k and E_k are the output values from kth neuron of the output layer and kth is the output value of the experimental data, respectively.

4. Genetic algorithm optimization

Genetic algorithm is capable of searching over a wide range bases on stochastic process. In this algorithm, an initial population of adjustable variables is randomly generated, represented as chromosomes and the fitness function of each chromosome is then obtained in the population. In order to better access fitness value, the new population during the three operations (i.e. selection, cross over and mutation) replaces the current one [29]. In this work, obtaining maximum generation is selected as the termination criterion.

5. Results and discussion

In this paper, 85 sets of experimental data are presented 75% of which are selected for training and the remainders are used for the testing neural network. Since the effects of SiO_2/Al_2O_3, template/SiO_2, H_2O/SiO_2, SiO_2/Na_2O ratio parameters, time and temperature on the particle size of ZSM-5 are investigated, the network used for modeling system should have 6 input and 1 output layers. The appropriate number of hidden neurons is selected 8 by trial and error in the proposed neural network model. Fig. 1 shows a schematic diagram of the designed neural network model.

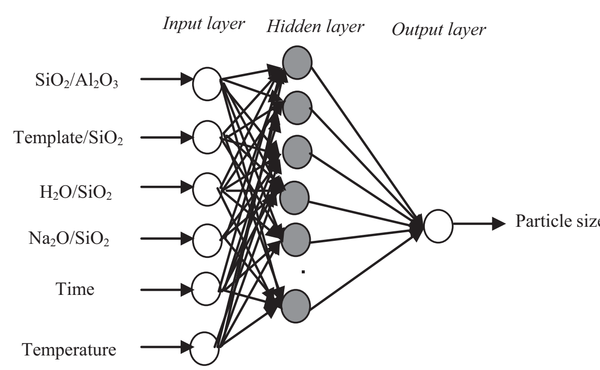

Fig. 1. Architecture of the proposed neural network model.

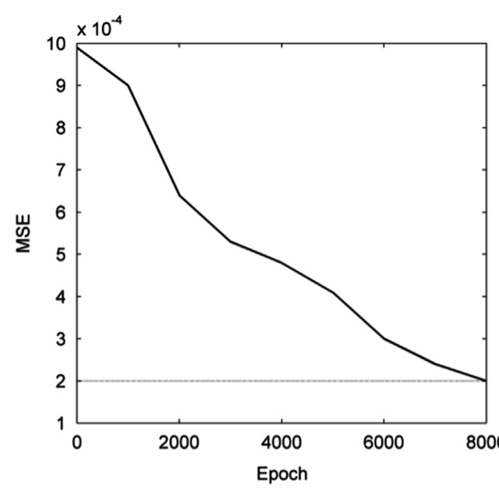

Fig. 2. Error performance of the proposed neural model versus epochs.

For each neuron of the proposed neural network, a "tan-sigmoid" transfer function is applied, formulated as:

$$Tansig(x) = \frac{1}{1+e^{-2x}} - 1 \quad (2)$$

Back propagation with descent gradient is used as the training algorithm and the learning and momentum rates are chosen 0.03

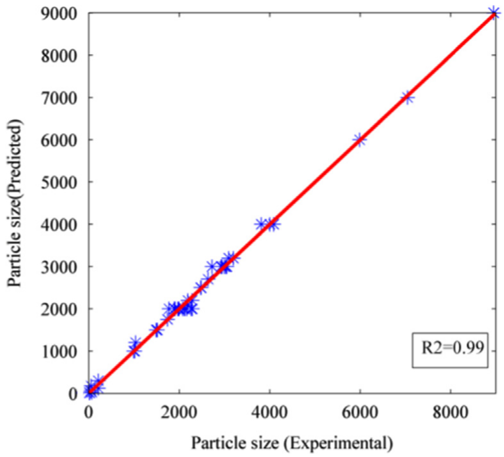

Fig. 3. Comparison of the predicted model and the experiment data.

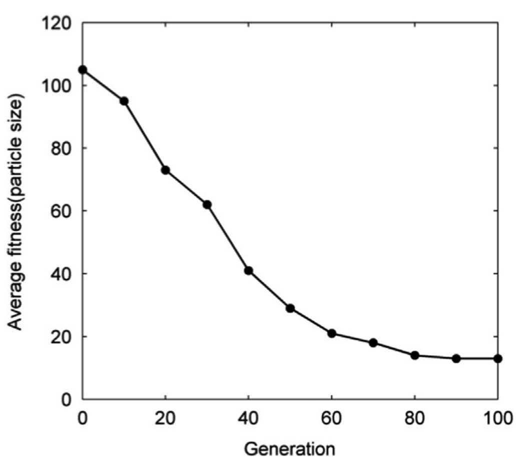

Fig. 4. Average fitness of GA optimization versus generation.

and 0.9, respectively. The error trend of the proposed neural network model is shown in Fig. 2.

ZSM-5 size particle predicted from the designed model versus the corresponding value from experimental data is in shown Fig. 3. From the regression analysis, the correlation coefficient (R^2) obtained is 0.99, which indicates an accurate prediction for ZSM-5 size particle. The optimum ZSM-5 particle size is obtained through GA based on the proposed neural network model. The fitness curve of GA for ZSM-5 particle size is shown in Fig. 4. The minimum ZSM-5 particle size under the optimized operating conditions and optimized gel composition is as follows: time = 98 h, temperature = 443 K, $SiO_2/Al_2O_3 = 113.6$, template/$SiO_2 = 0.32$, $H_2O/SiO_2 = 42.10$ and $SiO_2/Na_2O = 73.21$. The designed model and optimization are performed in MATLAB software.

6. Conclusions

In this work, the modeling of synthesized ZSM-5 particle size is designed based on a neural network. The neural network is used to predict the ZSM-5 particle size, based on collected data from the literature using six input variables (SiO_2/Al_2O_3, template/SiO_2, H_2O/SiO_2, SiO_2/Na_2O ratio parameters, crystallization time, and temperature of crystallization). The presented model is suitable for prediction of the synthesized ZSM-5 particle size process with R^2 of 0.99. The minimum value of the ZSM-5 particle size obtained is 13 nm through genetic algorithm.

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