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RESEARCH PAPER

Modelling and optimization of the pore structure of carbon aerogels using an artificial neural network

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Abstract: An intelligent simulation method for predicting and optimizing the pore structure of carbon aerogels is proposed by using an artificial neural network (ANN) algorithm. The ANN model has been optimized based on an improved genetic algorithm from six typical training algorithms. The volumes and diameters of pores in the simulated samples are predicted by the optimized ANN model, which shows correlation coefficients R^2 of 0.992 and 0.981 and root-mean-square prediction errors (RMSPE) of 0.077 and 0.054 between the predicted and experimental values for the volumes and diameters of pores, respectively. The proposed model is expected to have practical applications in the pore structure control of carbon aerogels.

Key Words: Carbon aerogels; Pore structure; Neural network; Training algorithms; Modelling

1 Introduction

Carbon aerogels have high ratios of surface or interface atoms owing to their particles in nanometer scale that form them [1]. Compared with conventional granular materials, carbon aerogels have a series of excellent physical and chemical properties such as low densities, high electrical conductivity, high special surface area, biocompatibility, and anticorrosion by acid and base [2,3]. It is considered as a promising material for various electrochemical applications, catalyst supports, adsorbents, and chromatography packings [4-6].

In this study, a new type of carbon aerogels was prepared by sol-gel polymerization method using phenol, melamine and formaldehyde as raw materials. Pore structure of carbon aerogels is essential to carbon aerogels because it will directly affect their performance. However, it is difficult to control practically pore structure parameters of carbon aerogels due to the constraints of time and cost.

In recent years, interest using artificial neural networks (ANNs) as a tool in material technology has increased. ANNs have been successfully used in several types of material applications like analysis, classifications, predictions or control and others [7,8].

ANNs are mathematical models that have the capabilities to relate input to output parameters. They can learn from examples by iteration without requiring a prior knowledge of the relationships between process parameters and properties of materials [9].

The neural network is determined by the architecture, training algorithms and learning rule. The most often used ANN for material applications is a fully connected and supervised network with a back propagation learning rule. The neural network architecture is designed by means of a trial-and-error process with a human intervention. Although there are some studies carried out on the automatic design of architectures [10], how to design an appropriate architecture systematically and autonomously remains a challenging problem. The genetic algorithm (GA) is quite effective in solving optimization problems owing to its inherent property of implicit parallelism [11]. In this paper, we have established an optimal structure of ANN by GA. Plumb et al [12] have shown that a proper selection of the training function has a significant effect on the predictive ability of a network. Therefore, one of the aims of this paper is to obtain an optimized ANN to control and predict the pore structure for carbon aerogels through selecting training algorithms. To do this, six training algorithms have been evaluated.

Performances of ANN have been optimized by varying the numbers of neurons in the hidden layer, optimizing the architecture of neural network and selecting a proper training algorithm. Then, the numerical simulation results from the optimal controlling and predicting model are compared with experimental ones. The purpose of this paper is to investigate the behaviors of pore structure for carbon aerogels and

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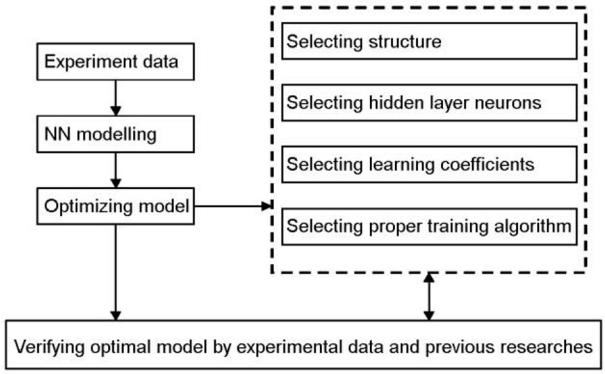

Fig. 1 Flowchart of this study.

establish controlling and predicting model using the neural network method. The flowchart of this study is shown in Fig. 1.

2 Experimental

2.1 Preparation and experimental design

In the present experiments, the total reactant concentration is 20%, and the molar ratio of phenol and m-cresol is 1:2. The catalyst concentration is 100 mmol/L. We investigate the effect of the reactant concentration, the molar ratio of phenol and m-cresol in the solution, etc on pore structure of carbon aerogels. The reactants are mixed in propyl alcohol to form transparent solutions. The solutions are poured into sealed glass ampoules (8 cm×2 cm, internal diameter, each filled with 20 mL solution) and heated at 90 °C for 48 h in a water bath. Then, the black organic gels are moved into a pressure vessel and supercritically dried at 270 °C and 8 MPa. Finally, with a heating rate of 5 °C/min, the carbon aerogels are formed by pyrolysis of the organic aerogels in a horizontal tube furnace at 800 °C for 3 hours under nitrogen protection. As a comparison, phenol-furfural (m-C/P=0) and m-cresol-furfural (m-C/P=∞) are polymerized in 1-propanol under the same conditions [13].

Samples are named MP/RC/CC in accordance with preparation conditions, in which MP is melamine/phenol molar ratio, RC is the concentration of the reactants and CC is the catalyst concentration. Under certain conditions (solvent exchange, supercritical drying and pyrolysis), the influences of different reaction temperatures, reaction times, various melamine/phenol molar ratios (M/P) on pore structure of carbon aerogels are studied.

2.2 Analysis and characterization

Main analysis and characterization methods of this paper are as follows:

Laser particle size analyzer. Particle size distribution and average particle size were measured by a laser particle size analyzer.

Nitrogen adsorption. Adsorption and desorption isotherms of nitrogen were measured at 77 K using a commercial adsorption apparatus (ASAP2020M, Micromeritics). Samples were degassed at 200 °C under vacuum for 12 h. The BET surface areas (S_{BET}) were analyzed by the Brunauer-Emmett-Teller (BET) method from the adsorption isotherm of nitrogen at p/p_0 from 0.05 to 0.2. Micropore volumes (V_{mic}), micropore surface areas (S_{mic}), and external surface areas (S_{ext}) were obtained by the *t*-plot method using an adsorption branch of the isotherms. Mesopore size distributions, mesopore volumes (V_{mes}) and average pore diameters (D_p) were obtained with the BJH (Barrett-Johner-Halendar) model using the desorption branch of the isotherms.

3 ANN description

An ANN concept, which is from artificial intelligence family, has been developed to model nonlinear processes in many areas. An ANN is a parallel-distributed information processing system. It stores the samples with distributed coding, thus forming a trainable nonlinear system. The main idea of the neural network resembles the functions of human brains. It is self-adaptive to the environment so as to respond different inputs rationally [14].

An overview of neural network algorithms was provided by McCulloch and Pitt[15]. A neuron as a unit with process of stimulus and reaction is generalized in this system. A set of training data for learning is performed with weight (connection strength), transfer function and biases. In this study, a back-propagation (BP) algorithm is used for the neural network, which is simple from the viewpoint of structure and easy analysis with mathematics. The back propagation neural network scheme, which has a great learning ability in training and mapping the relations between inputs and outputs, is the most commonly used network models [16,17]. The basic structure of BP neural network is shown in Fig. 2.

The neuron shown in Fig. 2 can be classified into three types, input, output and hidden neurons. Input neurons are the ones that receive input signal from external sources. Output neurons are those that send the signals to external sources. Neurons, which have inputs and outputs, are called hidden neurons. There are one or several nodal points in the output layer, which generate output data.

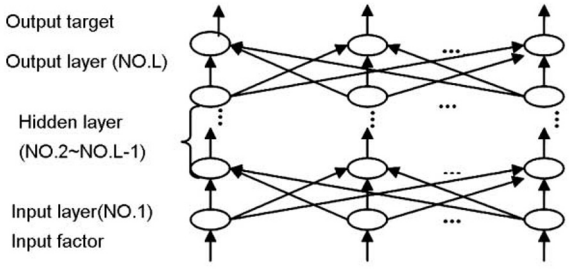

Fig. 2 Basic structure of BPNN.