Neural Network for Overall Porosity Prediction of Hollow Fiber Membrane

MOHAMMAD ABBASGHOLIPOUR GHADIM, MUSA BIN MAILAH, INTAN ZAURAH, A. F. ISMAIL, M. REZAEI DASHTARZHANDI, MAHDI ABBASGHOLIPOUR

Abstract: This study aims to introduce an attractive and convenient method of calculating the overall porosity of Hollow Fiber Membrane (HFM). Artificial Neural Network (ANN) was used to estimate the overall porosity of HFMs. Overall porosity is predicted as a function of effective surface porosity of fabricated HFMs which depends on polymer solution composition, dope extrusion flow rate and bore fluid flow rate. The artificial neural network (ANN) converted the qualitative information based on quantitative results from the outer surface analyzed through a Field Emission Scanning Electron Microscopy (FESEM) images. A neural network with one hidden layer with three neurons was created to map the relationship between input and output. An image processing computer program was developed to measure the HFM surface porosity using the FESEM images. Obtained data by image processing program was used as input data for designed ANN. The calculated overall porosity of the HFM was compared with the achieved value from the mathematical model. It was found that there was no significant difference between the results of both methods, thereby confirming the applicability of ANN for assessing the membrane porosity.This work presents a novel approach and provides a useful framework to evaluate the overall porosity of HFM considering different dope compositions and spinning conditions.

Key-Words: Hollow fiber membrane, Image processing, Artificial neural network, Overall porosity

I. Introduction

Nowadays, based on membrane configuration, HFMs are the most favored membrane geometry in its separation applications, such as spiral wound and tubular. HFMsfibers have much larger surface area per unit volume of the membrane modulein compared with flat sheet membranes, and higher productivity is the main key in HFM technology. They are self-supporting mechanicallyand have good flexibility in operation. However, during membrane formation, the preparation of the hollow fibers often requires more controlling parameters than those of flat sheet membranes (i.e. structure and dimensions of the spinneret, viscosity and possibility of the spinning dope, nature of the internal and external coagulants, flow rate of the bore fluid, dope extrusion rate, air gap length, take-up speed, etc.).

A porosity prediction of the porous HFMs seems crucial before applying the membranes in real application. It helps membranologists to detect an optimum solution composition and spinning condition based on the requirements of a specific membrane application in a minimum time.The prediction involves the examination of the surface and cross-section characteristics of the membranes. The overall porosity of the HFM can be obtained by several methods including molecular weight cut-off (MWCF) method [1], pressure of bubbles approach [2], mercury intrusion method [3], liquid–liquid or liquid-gas displacement approach [4].Control membrane structure (porosity and pore size) is one of the important goals in membrane technology and thus membrane performance [5]. According to [6], spinning process of a HFM with a specific performance is not an easy task and the effect on hollow fiber membrane morphology and permeation properties reported in the literature often provides conflicting observations

Recently, digital image processing (DIP) as a strong tool was also applied to determine the porosity of the membrane. The method uses FESEM images to detect the surface pores and then predict the overall porosity of membrane. However, since the membrane surface pores are not exactly cylindrical and straight, the predicted porosity may not be accurate. Therefore, an approach is proposed by training artificial neural network (ANN) which is expected able to predict the overall porosity of the HFMs better without considering the shape of the pores. Recently ANNs implementations in digital image analyzing applications have increased rapidly. In the reference [7] author reported that the designed and trained ANN is able to establish the non-linear relationship among the intensity of input images as well as their compression ratio for finding the optimized ratio.

The ANN offers the advantage of being easy to use and reduces the computing time of the membrane process simulation [8]. In the ANNs error between observation data and estimated data is the most important issue for evaluation the designed and trained network [9]. Architecture of the ANN has been investigated by many researchers. Three ANN architecture including online, batch and resilient backpropagation algorithms were used to intrusion detection. They reported batch and online algorithms are more quick in compared with resilient however has best performance [10]. A type of ANN based on Radial Basis Function (RBF) was also employed for modeling the membrane process as described in [11]. However, the implementation of the ANN methods in this area of research is relatively in its infancy stage and still under development. Besides, the works did not consider aspects of determining the porosity of membrane which is regarded as a crucial factor to measure the mass transfer rate in porous membranes. Therefore, this work attempts to predict the membrane porosity using ANN and image processing techniques. The RBF network with three layers (input, hidden and output) using *Levenberg-Marquardt*(LM) algorithm was used to predict the overall porosity of the fabricated HFMs. The model was trained by the obtained porosity of membranes differing in dope compositions and spinning conditions.

II. EXPERIMENTAL

Since the HFM fabrication and characterization are difficult and time consuming and also many interrelating key factors have effect on structure and performance of HFM [12]. Only 56 samples were used for training and experimentation.

a. Membrane preparation

Commercial *Polysulfone* (PSf) polymer pellets (1700) were purchased from Arkema Inc., PA, USA. *1-Methyl-2pyrrolidone* (NMP) and *Polyvinylpyrrolidone K90* (PVP) were used as solvent and non-solvent additives in the polymer solution, respectively. The materials were dried in a vacuum oven for 48hours at 60±2 ^{o}Ċ to remove the moisture content. PVP with content of 2.5 wt% of polymer was added in the solvent (NMP) for 1 hour under vigorous stirring. PSf polymer indifferent concentration (12%- 22%) was then gradually added to the mixture in order to produce five different bathes of dope formulations then mixed thoroughly under a constant mechanical stirring at 58 ^{o}Ċ. To form a homogenous solution, at least 28 h was needed. Finally, the formulated dope solutions were degassed before spinning to remove whole micro-bubbles that might exist. The prepared solutions were loaded into storage tank and pressured nitrogen of 1 bar forced the polymer solution to flow into the spinneret plant.

Water was utilized as the bore fluid liquid and loaded into the spinneret via the syringe pump. The HFMs were fabricated at ambient temperature of about 22-25 ^{o}Ċ. Polymer concentration, dope extrusion and bore fluid flow rates were assumed as variables in our analysis. Water was used as the external coagulant bath and the temperature was kept constant during spinning.

Table 1 summarizes the spinning conditions for HFM fabrication. Dope extrusion flow rate, bore fluid flow rate and composition of solution were assumed as variables during the spinning process, other spinning parameters were kept constant. The nascent fibers were not drawn (no extension) as the take-up velocity of the hollow fiber was nearly the same as the falling velocity in the coagulation bath. A detailed description for hollow fiber spinning was given elsewhere [13], [14]. The as-spun membranes were stored in water bath at room temperature for at least 72 h to remove the residual solvent and then stored in a 10 wt% Ethanol solution for at least 20 min. The membranes were then dried naturally in air at ambient condition before used for making test module.

Table 1 HFM spinning conditions

Parameter	Value
Dope extrusion rate (mL/min)	2-4.7
Bore flow rate (mL/min)	0.7-1.6
Bore composition (wt%)	Distilled water
External coagulant	Tap water
Air gap distance (cm)	0
Collection drum speed (m/min)	2.8
Spinneret OD/ID (mm)	1.1/0.55
Spinning dope temperature (◦C)	25
External coagulant temperature (◦C)	25
Bore fluid temperature(◦C)	25

The detailed HFM fabrication via wet spinning method is described elsewhere [15]. The fabricated HFMs were immersed in water for 72 hours to remove the rest of NMP and PVP inside the spun HFMs. Table 2 lists specific detailed of the spinning procedure.

Table 2 HFM composition and spinning conditions

Composition			Parameter		
PSf (gr)	PVP (gr)	NMP (gr)	DER (cm^3/ min)	BFR (cm3/ min)	D_s (rpm)
12.00	1.67	86.33	2.00	0.66	0.7
12.00	1.67	86.33	2.50	0.83	0.9
12.00	1.67	86.33	3.00	1	1.1
12.00	1.67	86.33	3.50	1.16	1.3
12.00	1.67	86.33	4.00	1.33	1.5
12.00	1.67	86.33	4.50	1.5	1.7
12.00	1.67	86.33	5.00	1.66	1.9
12.00	1.67	86.33	5.50	1.83	2.1
12.00	1.67	86.33	6.00	2	2.3

DER: Dope extrusion rate; BFR: Bore fluid flow rate; D_S: speed of collecting drum

The composition of polymer was varied according to 14, 16, 18, 20 and 22 wt% with the same values for other variables in the next experiments.

b. Overall porosity

The porosity of the membrane has been defined as the ratio of the pores volume to the total volume of the membrane [16, 17]. The basic porosity equation of the HFM can be calculated using the following expression.

$$\varepsilon_m = \frac{\Delta m}{\rho x \Delta V} \tag{1}$$

Hence, the overall porosity of a membrane can be obtained as follows:

$$\varepsilon_m = \frac{\rho_w(w_1 - w_2)}{\rho_p(w_1 - w_2) + \rho_w(w_2)} \qquad (2)$$

Where, w_1 and w_2 are the weights of the wet and the dry membrane, respectively while ρ_w and ρ_p are density of the water and polymer solution, respectively. Based on the mentioned equation, the porosity ε_m can be described as a non-dimensional parameter and in most literature, it is written as a percentage concentrate (%).

c. Field emission scanning electron microscopy (FESEM)

The membranes were put on holders and coated by sputtering platinum. A *Zeiss Supra 35VP* FESEM, from Carl Zeiss, Inc., (MN, USA) was used to observe the outer surface of the fabricated membranes. The FESEM images were used as the feed of the ANN to get an accurate overall porosity.

d. Image processing

Generally, the grey images from the outer surface of a porous membrane obtained from FESEM are between zero and 255 pixels in which, the pixels with low and high luminance were assumed as pore areas and background, respectively.

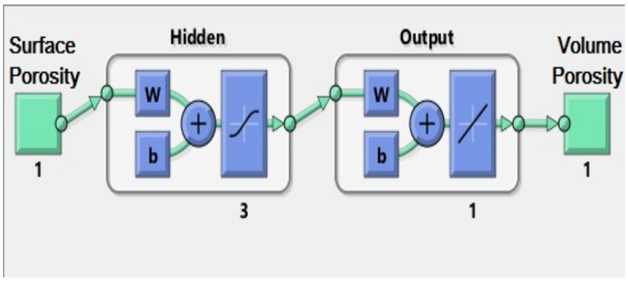
In the first step, the FESEM images were resized into 1000×1000 square pixels in order for them to be transferred to the computer for analysis. For filtration, specific function was used to eliminate the noises from the colour images. Then, an algorithm was used to increase the intensity of the images and edges. Before classification, the images were adjusted as red, green and blue (RGB) images to detect of the pore boundaries clearly. The surface porosity of the fabricated membranes was calculated using the following equation:

$$\varepsilon = \frac{\int_0^h (A_p) z dz}{(A_t)} \qquad (3)$$

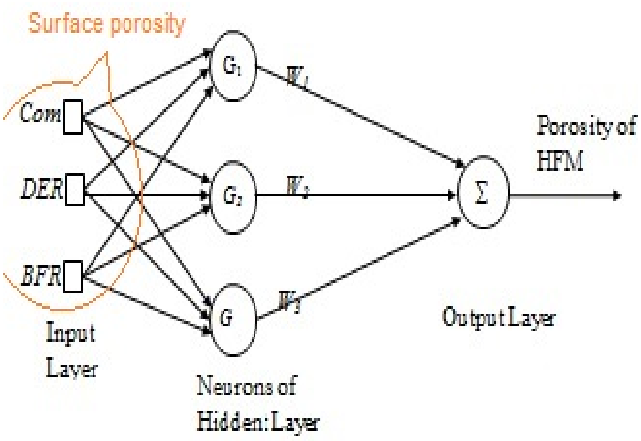
Where At is the total area of image, Ap is the area porosity at distance z and h is the height of image.

e. Application of neural network

The objective of a neural network is to compute the porosity values by some internal calculations on FESEM images of membranes in different dope composition, DER and BFR rates. Neurons (or cells) are processing elements that carry out simple computations from a vector of composition, DER and BFR rates. A neuron performs a non-linear transformation of the weighted sum of the incoming neuron inputs to produce the output of the neuron. Poggio and Girosi [18] in similar with the results of Antsaklis [19] revealed that the RBF network amongst all the feed-forward networks has the highest ability to predict the approximation properties of the membranes. In this work, the RBF network was used to predict the porosity of the membranes using image processing. The model was trained, taking into account the obtained porosity of membranes differing in dope compositions and spinning conditions. For the data composition, 70% is assumed as the training data, 15% as testing data and the rest is assumed as validation data. The essential building block of neural network applied in this study is shown in Fig. 1.



(a)



(b)

Fig. 1 (a) Schematic view of the function fitting neural network (b) Neural network with one hidden layer with G and W are the functions in hidden layer and weights, respectively

III. Results and Discussion

The results obtained from the study are presented, analyzed and discussed in the following sections.

A. FESEM and image analyses (pre-processing)

Figure 1 shows FESEM surface micrographs of fabricated membranes in different compositions and spinning conditions. As can be seen, the membranes of lower polymer concentration possess larger surface pore size and higher porosity as depicted in Figure 2 (f) compared to that of higher concentration as shown in Figure 2 (a).

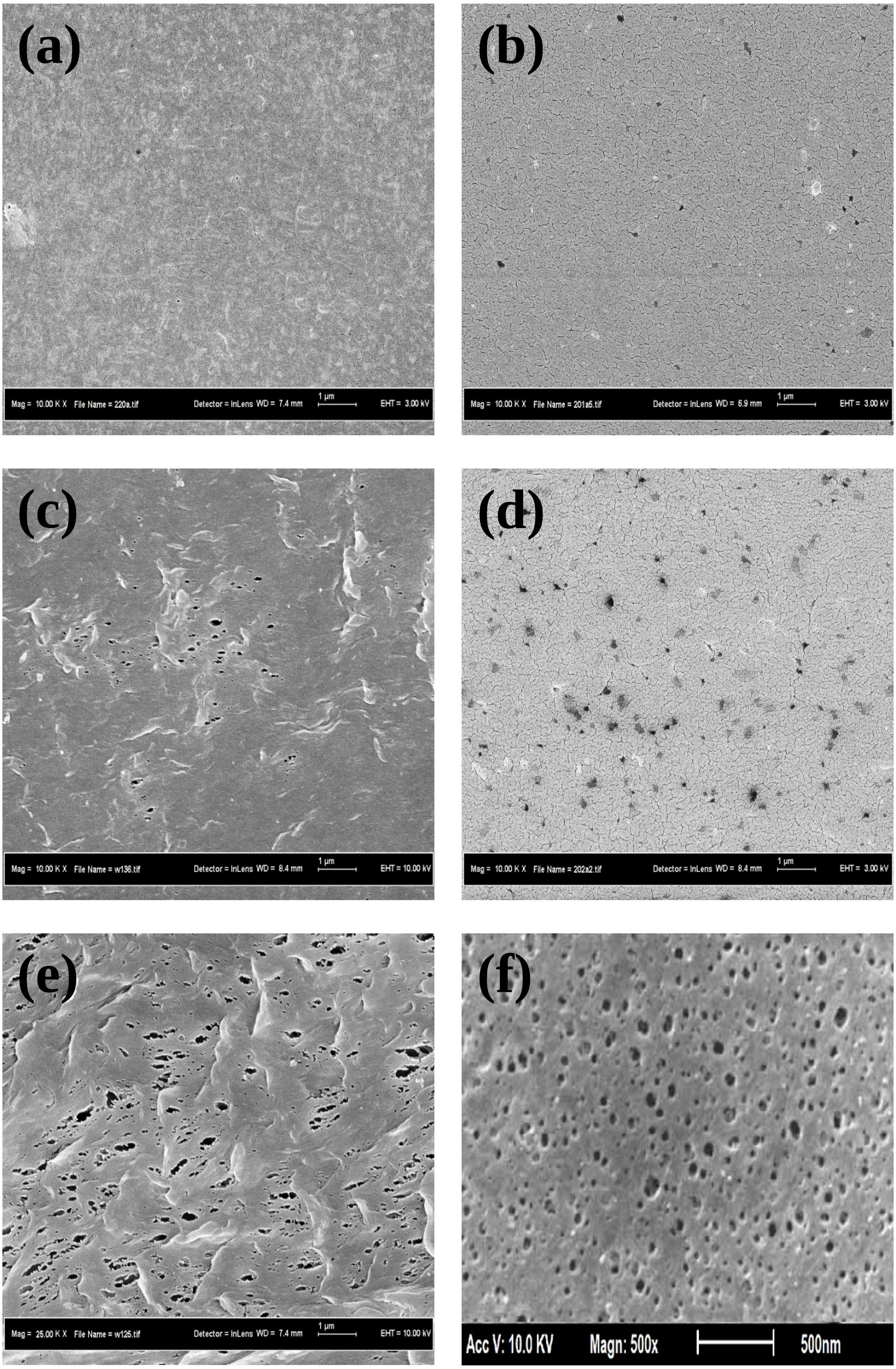


Fig. 2. FESEM image of the outer surface of the PSF HFMs: (a) HFM: PSf22 wt%; (b) HFM: PSf20wt%; (c) HFM: PSf18 wt%; (d) HFM: PSf16 wt%; (e) HFM: PSf14 wt%; (f) HFM: PSf 12wt%

The FESEM images that qualitatively give the porosity of the membrane surface were adjusted to achieve the best threshold incorporating the triangle algorithm. For detecting the objectives (pores), FESEM images were converted to binary images and also triangle algorithm was utilized to extract the final real pores from Figures 1

(a) and (b). (some pores were assumed as 'failed' pores and hence were conveniently eliminated for the analysis). An example of the real extracted pores by surface image analysis from FESEM images is shown in Figure 3.

Fig. 3. Real pore extracted by data analyzing result

The overall porosity of the membrane has been defined as the ratio of the pores volume to the total volume of the membrane which the obtained results are assumed as experimental data. Table 3 summarizes the obtained overall porosity from equation 2 for some samples.

Table 3. Obtained overall porosity of hollow fiber membranes from mathematical equation

PSf(gr)	Wet Weight	Dry Weight	Deference Weight	Porosity
12.00	0.358	0.0746	0.2834	0.806589
12.00	0.4566	0.1018	0.3548	0.792789
12.00	0.4832	0.1074	0.3758	0.793438
12.00	0.49	0.1114	0.3786	0.78862
12.00	0.5806	0.1335	0.4471	0.786164
12.00	0.6066	0.1416	0.465	0.782842
12.00	0.6179	0.1432	0.4747	0.784438
12.00	0.5624	0.135	0.4274	0.776558
12.00	0.6467	0.1517	0.495	0.781756
14.00	0.4365	0.1038	0.3327	0.778691
14.00	0.4526	0.1072	0.3454	0.779591
14.00	0.4997	0.1257	0.374	0.765601
14.00	0.5263	0.135	0.3913	0.760874
14.00	0.5123	0.1353	0.377	0.753623
14.00	0.5513	0.1475	0.4038	0.750329
14.00	0.5616	0.1502	0.4114	0.750424
14.00	0.6162	0.1621	0.4541	0.754615
14.00	0.6985	0.1891	0.5094	0.747294

As it can be seen, the overall porosity of HFMs is increased with decreasing the polymer composition and also is reduced with increasing the dope extrusion flow rate.

B. Neural network

The surface porosity of the HFMs was obtained by an image processing package (IPP). Afterward, the obtained data were used as the input layer data in the designed ANN configuration. Since the HFM fabrication and characterization are typically difficult and time consuming, only 57 samples were used for designing the ANN. Determining the number of hidden layers, number of neurons in the hidden layer, type of transfer function, type of network function, and type of training algorithms are legitimate questions with no precise answers because they are case sensitive. Therefore, we need to study every one of them for building the optimal neural network model for our problem.

In general, fewer numbers of neurons with less hidden layers is better to reduce the effect of memorization. Determining the optimal number of neurons in the hidden layer requires trial and error technique. Determining the type of transfer function is similar to determining the number of neurons in the sense that it requires trial and error analysis. Similarly, the optimal type of network function is *newff* since it has high correlation coefficient values and lower error values. Using the same technique of trial and error, the optimal type of training algorithm is *Levenberg-Marquardt* since it has high correlation coefficient values and lower error values. Figure 4 shows the obtained results from the designed ANN with RBF scheme.

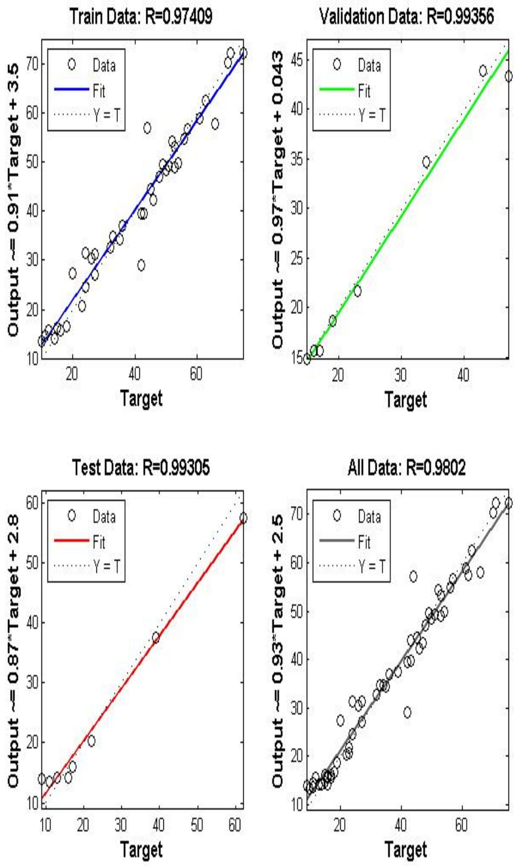
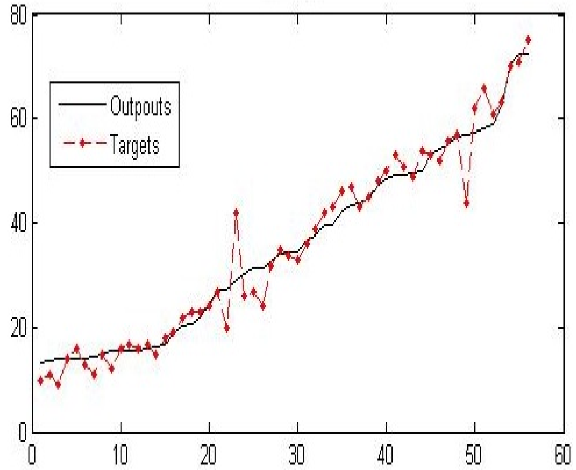
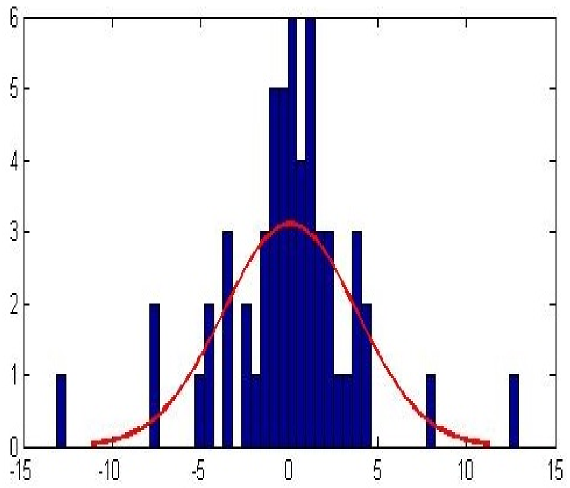


Fig. 4. Results obtained from training, testing and validation of designed neural network



(a)



(b)

Fig. 5. Best performances for the RBF network for (a) predicted overall porosity from surface porosity (R = 0.984), (b) histogram with fitting line (Mean = 0.048 and root mean square error = 2.73)

Figure 5 illustrates the best performances of trained network. The corresponding generalization performance of the network shows some small but unrealistic oscillations as can be seen in Figure5 (a). These fluctuations are due to the noise content of the training data which can be alleviated if the learning algorithm is equipped with some proper noise filtering facility. Based on Figure 5(b), the mean value is near zero and the root mean square error (RMSE) merit function is a small value. The results suggest that in order to achieve a higher computational speed, a neural network simulator can be used to replace the earlier models in the process of calculating the membrane porosity. The experimental data and the results of the trained neural network for the overall porosity are shown in Figure 6.

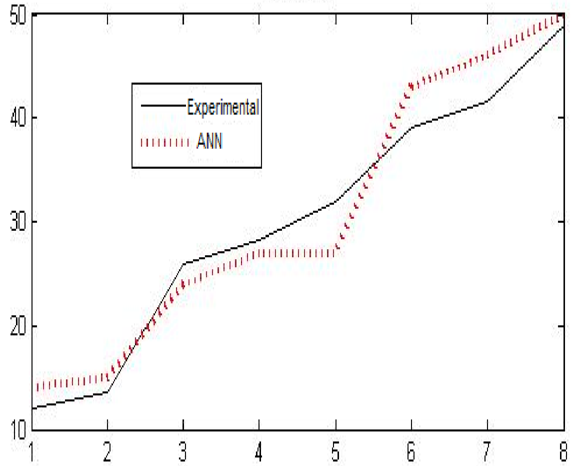


Fig. 6. Porosity prediction of HFM based on the experimental results and the data from trained ANN

As can be seen in Figure 5, the output from ANN is in good agreement with the experimental counterpart, thereby implying that it is capable to predict the overall porosity of HFMs effectively.

IV. Conclusion

An image processing package was developed to measure the membrane surface porosity supplying the FESEM images as the input feed with the PSf HFMs were spun in various dope compositions and spinning conditions. ANN method was utilized and were applied to predict the membrane overall porosity. The results obtained by trained neural network were compared with those acquired through the mathematical model (weight equation). The results were in good agreement and hence confirming the applicability of the approach for computing the overall porosity of HFM.

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