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Technical Note

Neural network analysis of boiling heat transfer enhancement using additives ☆

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Abstract

A model was developed to evaluate and predict boiling heat transfer enhancement using additives. The model is based on the molecular structures of the additives and uses artificial neural network technology. The effects of 30 additives tested by the authors and other researchers on the augmentation of boiling heat transfer were analyzed with the model. The results show that the evaluation of all 30 additives is consistent with the experimental data, which means that the training accuracy of the model is 100%. In addition, the boiling heat transfer enhancement with sodium oleate and 11 other additives was also predicted, with a prediction accuracy of over 90% since the calculated results for 10 of the 11 additives were in agreement with the experimental results.

Keywords: Heat transfer; Neural networks; Boiling enhancement; Additives

1. Introduction

Enhancement of boiling heat transfer with additives has been studied for many years [1,2]. The boiling heat transfer of working fluids, such as water and Freon, can be significantly improved if suitable trace amounts of additives are added into the fluids [3,4]. This technique is specially useful for a mixed working fluid to replace chlorofluorocarbons since such mixed fluids usually have much lower boiling heat transfer coefficients than pure liquids. Therefore, suitable additives are needed to enhance the boiling heat transfer of these working fluids.

More than 40 additives have been tested to date [3,5], though their effects on boiling heat transfer are quite different because of their various molecular structures. Many other substances may also be used as additives, but it is difficult to test all possibilities one by one. Moreover, the effect of a certain additive on the boiling heat transfer cannot be predicted accurately by common mathematical models since the enhancement mechanism for these additives is not well understood. Therefore, a comprehensive evaluation and prediction model is needed for boiling heat transfer enhancement with additives which accounts for their molecular structural characteristics.

Artificial neural networks can effectively analyze strong non-linear problems with stochastic characteristics. Neural networks have been successfully applied to many areas such as electronics, information and control. A comprehensive evaluation model based on the neural network back propagation (BP) technique was used in this study to evaluate and predict the performance of an additive used to enhance boiling heat transfer as a function of its molecular structure.

2. Back propagation model

2.1. Network input and output

The purpose of the model is to evaluate and predict the boiling heat transfer enhancement due to an additive

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Nomenclature

A	output matrix of the first hidden layer
b	bias matrix of the neural network
B	output matrix of the second hidden layer
i	number of samples
j	number of neurons inside the first hidden layer
k	number of neurons inside the second hidden layer
M	molecular weight of the polymer additives
N_c	number of carbon atoms inside the straight carbon chain in the non-polar group
P	input matrix representing the characteristics of the molecular structures of the additives
q	heat flux without additives, W/m^2
q_A	heat flux with additives, W/m^2
R	ratio of the atomic weight for the non-polar group and that for the polar group
T	output of the neural network
W	weight matrix for the network

based on its molecular structure. The evaluation object which is the network output, therefore, was then the enhancement due to the additive. Here, the relative increase in the boiling heat flux at the same temperature difference with the additives was used as the output:

$$T = (q_A - q)/q$$

The network input was the parameters describing the molecular characteristics of the additive. Since all the additives consist of polar and non-polar groups and they can be divided into anionic, cationic or non-ionic types, the following four factors were chosen as the inputs to the network to represent the molecular structures of the additives:

P_1: number of carbon atoms inside the straight carbon chain in the non-polar group or the molecular weight for polymer additives.
P_2: ratio between the atomic weight of the non-polar group and that for the polar group.
P_3: type of additive, anionic, cationic or non-ionic.
P_4: kind of polar group in the additive.

Forty-one additives were selected from the literature as samples for evaluation and prediction. Their molecular structures and their effect on the boiling heat transfer as well as their corresponding network input data are summarized in Table 1.

2.2. Back propagation network structure

A BP neural network with two hidden layers was used in this model. The network structure is shown in Fig. 1. There were four mesh points in the input layer since four factors were used to express the molecular characteristics of each additive. The number of neurons in the first and second hidden layers was assumed to be j and k, respectively. Their final values were determined after the network training. Additionally, S hyperbolic tangent activation function was applied to the first hidden layer with S logarithmic activation function applied to the second hidden layer, with a linear activation function used for the output layer. The detailed calculational process is described later.

2.3. Range division and quantification

The complex structures of the additives were expressed quantitatively so they could be input to the network. The inputs P_1, P_2 and P_4 were divided into five subgroups while P_3 was divided into three subgroups. In addition, the increased boiling heat transfer heat flux due to the additive was not a fixed number, but varied over a certain range. Hence, the network output was also divided into subgroups. The divisions and their corresponding quantified values are summarized in Table 2.

For each additive in Table 1, the subgroups and corresponding values for its input were determined from Table 2 according to its molecular structure. The network output was then a result of the training as explained later. The boiling heat transfer enhancement relative to its output value was then found from Table 2.

2.4. Training of the back propagation neural network

Matlab was used to define the BP neural network. The calculational process included two parts, network training and network simulation. Three Matlab functions were used in the calculation:

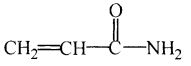
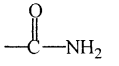
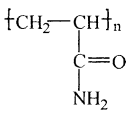
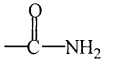
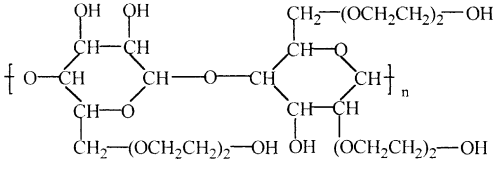
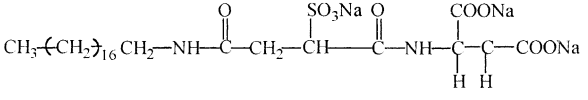
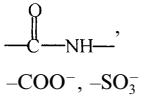
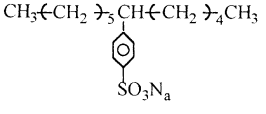
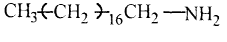
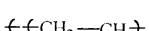
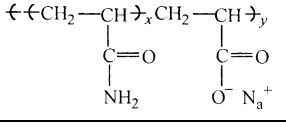
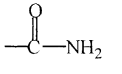
(1) Network initialization, initff:

$$[w_1, b_1, w_2, b_2, w_3, b_3] = \text{initff}(p, j, \text{'tansig'}, k, \text{'logsig'}, t, \text{'purelin'})$$

where the parameters are

w_i calculated initial weight matrix for the ith layer
b_i calculated initial bias vector for the ith layer

Table 1
Structural characteristics of additives and their boiling heat transfer enhancement

No	Additive name	Structural formula	P_1	P_2	P_3	P_4	T		Reference
							Experiment	Calculation	
1	Acrylamide		2	0.61	Non-ion		<0	⩽0	[6]
2	Polyacrylamide		1000th	0.61	Non-ion		1 ∼ 1.4	1 ∼ 3	[6]
3	Polyacrylamide		2000th				0.5 ∼ 0.8	0.5 ∼ 1	
4	Hydroxyethyl cellulose L		70th	1.21	Non-ion	–OH, –O–	0.5 ∼ 1	0.5 ∼ 1	[6]
5	Hydroxyethyl cellulose M		100th	1			0.5 ∼ 1		
6	Hydroxyethyl cellulose H		200th				1 ∼ 1.6	1 ∼ 3	
7	Aerosol		18	1.2	Anion	 –COO^-, –SO_3^-	2.5	1 ∼ 3	[7]
8	Ethanol	CH_3–CH_2–OH	2	1.7	Non-ion	–OH	<0	⩽0	[8]
9	Sodium lauryl benzene sulfonate		12	3.06	Anion	–SO_3^-	0.5	0 ∼ 0.5	[9]
10	Octadecylamine		18	15.8	Non-ion	–NH_2–	2.5	1 ∼ 3	[10,11]
11	Polyoxyethylene		2000th	1.75	Non-ion	–O–	1	0.5 ∼ 1	[12]
12	Separan		2500th	0.61	Anion	–COO^-, 	0.5	05 ∼ 1	[12]

Note: Additives 13–41 are listed in Liu [3] and Wu et al. [4].

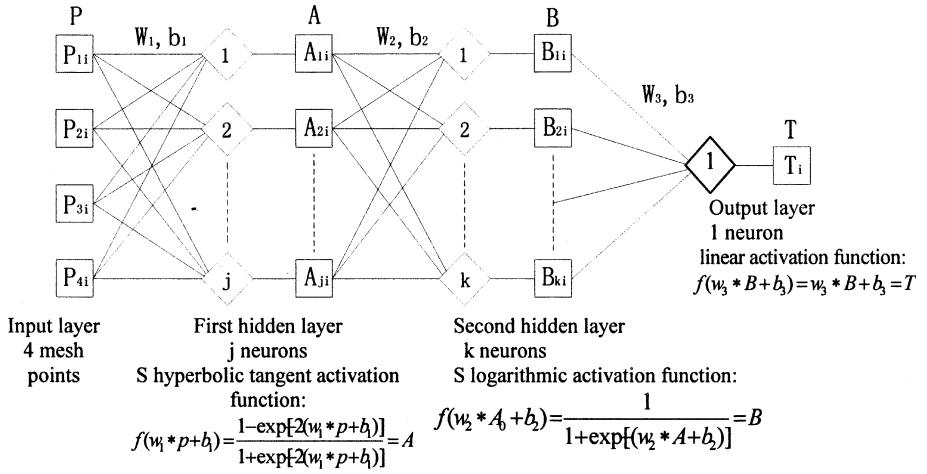


Fig. 1. BP neural network structure.

p matrix of input vectors
j, k number of neurons in the first and second layers
t matrix of output vectors

'tansig': hyperbolic tangent activation function

$$f(w_1 \times p + b_1) = \frac{1 - \exp[-2(w_1 \times p + b_1)]}{1 + \exp[-2(w_1 \times p + b_1)]}$$

'logsig': logarithmic activation function

$$f(w_2 \times A_0 + b_2) = \frac{1}{1 + \exp[-(w_2 \times A + b_2)]}$$

'purelin': linear activation function

$$f(w_3 \times B + b_3) = w_3 \times B + b_3$$

(2) Network training, trainbp:

$$[w_1, b_1, w_2, b_2, w_3, b_3, \text{epoche}, \text{error}] = \text{trainbp}(w_1, b_1, \text{'tansig'}, w_2, b_2, \text{'logsig'}, w_3, b_3, \text{'purelin'}, p, t, \text{TP})$$

where the parameters represent w_i on the left hand side: new calculated weight matrix for the ith layer, w_i on the right hand side: initial weight matrix for the ith layer, b_i on the left hand side: new calculated bias vector for the ith layer, b_i on the right hand side: initial bias vector for the ith layer, epoche: number of epochs in the training period, error: training errors.

TP, training parameters, which include TP(1): epochs between display updates, 3000 in this calculation; TP(2): maximum number of training epochs, 30 000 in this calculation; TP(3): sum-squared error goal, 0.001 in this calculation; TP(4): learning rate, 0.01 in this calculation.

(3) Network simulation, simuff:

$$t_1 = \text{simuff}(p, w_1, b_1, \text{'tansig'}, w_2, b_2, \text{'logsig'}, w_3, b_3, \text{'purelin'})$$

here t_1 is the calculated matrix of target vectors.

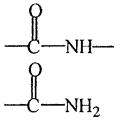
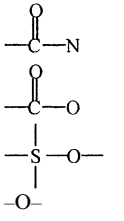
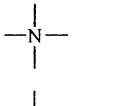
The first 30 additives in Table 1 were used as the training samples with the remaining 11 additives used as the prediction samples. The training and prediction calculations were carried out with the number of neurons in the first and second hidden layers, j and k, varied from 1 to 14. The optimum numbers of neurons in the first and second hidden layers were found to be 6 and 3, which minimized the error between the experimental and calculational results.

In addition to the suitable numbers of neurons in the first and second hidden layers, the corresponding weights and biases for the networks were also obtained as:

$$w_1 = \begin{bmatrix} 0.52 & 1.68 & -0.79 & 0.82 \\ 4.51 & 1.56 & 0.73 & -2.73 \\ -1.47 & 0.15 & 0.86 & 3.17 \\ -1.54 & 2.19 & -2.60 & 3.11 \\ -0.25 & 0.38 & -0.70 & 2.13 \\ 2.29 & -0.08 & 0.77 & 0.07 \end{bmatrix}$$

$$b_1 = \begin{bmatrix} 1.42 \\ -0.19 \\ -2.34 \\ 0.20 \\ 1.47 \\ -2.36 \end{bmatrix}$$

Table 2
Subgroups and quantification of network input and output

Sub-group	T		P_1		P_2		P_3		P_4	
	Value range	Mapping range	Value range	Value	Value range	Value	Type	Value	Type	Value
1	$Y \leqslant 0$	[0, 0.2)	$0 < N_c \leqslant 10$	0	$0 < R \leqslant 1$	0	Anion	0	$-COO^-$ $-SO_4^-$	0
2	$0 < Y \leqslant 0.5$	[0.2, 0.4)	$10 < N_c$	0.25	$1 < R \leqslant 1.5$	0.25	Cation	0.5	$-NH_2$ 	0.25
3	$0.5 < Y \leqslant 1$	[0.4, 0.6)	$0 < M \leqslant 5 \times 10^4$, $2.5 \times 10^6 < M$	0.5	$1.5 < R \leqslant 2$	0.5	Non-ion	1		0.5
4	$1 < Y \leqslant 3$	[0.6, 0.8)	$5 \times 10^4 < M \leqslant 1 \times 10^5$, $1.5 \times 10^6 < M \leqslant 2.5 \times 10^6$	0.75	$2 < R \leqslant 3$	0.75	–		$-SO_3^-$	0.75
5	$3 < Y$	[0.8, 1]	$1 \times 10^5 < M \leqslant 1.5 \times 10^6$	1	$3 < R$	1	–		 –OH –COOH	1

$$w_2 = \begin{bmatrix} 0.08 & -1.82 & 2.12 & -1.13 & -0.64 & 0.62 \\ -0.36 & -1.64 & -2.42 & -2.59 & 0.86 & -3.08 \\ -2.12 & 3.62 & -1.08 & 3.14 & -1.59 & 1.65 \end{bmatrix}$$

$$b_2 = \begin{bmatrix} 2.57 \\ 2.92 \\ 1.18 \end{bmatrix}$$

$$w_3 = [0.63 \quad 1.62 \quad 1.39]$$

$$b_3 = -2.05$$

The predicted results then used these weights and biases as described by Li [13].

3. Results and discussion

The predicted heat transfer enhancements of the first 30 additives in Table 1 are compared with experimental data in Table 1. The results show that the predicted enhancements for all 30 additives are in agreement with the experimental results, which proves that the model is reliable because its training accuracy is 100%, as shown in Fig. 2. In addition, the boiling heat transfer enhancement using sodium oleate and 11 other additives was predicted with this model. The results in Fig. 3 show that the predictions for 10 of the additives are consistent with the experimental data. Thus the BP neural network model can be used to predict the effectiveness of an additive for boiling enhancement since the prediction accuracy of the model is over 90%.

Analysis of all the materials listed in Table 1 shows that: (1) The function of an additive mainly depends on input factors P_4 and P_1, which represent the kind of polar group in the additive and the number of carbon atoms in the non-polar group or the polymer molecular weight. (2) There was usually no obvious effect on the boiling heat transfer for additives with less than 10 carbon atoms in their non-polar group, or whose molecular weights were very small or very large (smaller than 50×10^4 or greater than 2.5×10^6). (3) The additives having the best effect on the boiling heat transfer included the polar groups $-COO^-$, $-SO_4^-$, $-NH_2$ or –CO–NH–. (4) Additives with more than 10 carbon atoms or with suitable molecular weights ($10^5 < M \leqslant 1.5 \times 10^6$) and with one of these polar groups will substantially enhance the boiling heat transfer rate.

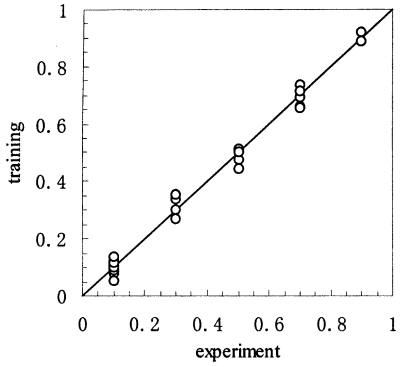


Fig. 2. Experimental and training mapping ranges for the boiling heat flux enhancement with additives.

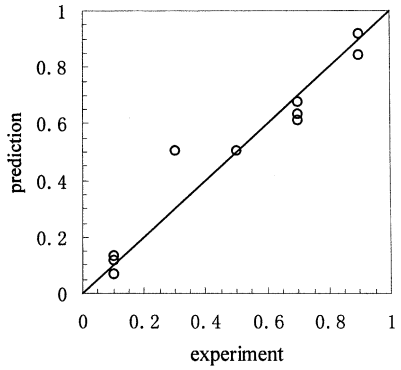


Fig. 3. Experimental and predicted mapping ranges for boiling heat flux enhancement with additives.

4. Conclusions

A BP neural network model was developed to evaluate the boiling heat transfer enhancement due to additives. The model is based on the molecular structures of the additives. The model training accuracy was 100% and its prediction accuracy was over 90%, so the model is reliable. The effect of each additive on the boiling heat transfer enhancement can be predicted by the model. Therefore, the model can be used to select proper additives for working fluids. Analysis of the data also showed that the molecular weights of the additives and their polar groups had the greatest effect on the enhancement.

References

[1] M. Jakob, W. Linke, Effect of surfactants on boiling heat transfer, Phys. Z. 36 (2) (1935) 267–272.
[2] W.T. Wu, Y.M. Yang, J.R. Maa, Pool boiling incipience and vapor bubble growth dynamics in surfactant solutions, Int. J. Heat Mass Transfer 42 (13) (1999) 2483–2488.
[3] T.Q. Liu, Enhancement of boiling heat transfer with additives, Ph.D. Thesis, Dalian University of Technology, Dalian, China, 1988.
[4] W.T. Wu, Y.M. Yang, J.R. Maa, Enhancement of nucleate boiling heat transfer and depression of surface tension by surfactant additives, ASME J. Heat Transfer 117 (2) (1995) 526–529.

[5] Y.L. Tzan, Y.M. Yang, Experimental study of surfactant effects on pool boiling heat transfer, ASME J. Heat Transfer 112 (1) (1990) 207–212.
[6] P. Kotchaphakdee, M.C. Williams, Boiling enhancement with polymer additive, Int. J. Heat Mass Transfer 13 (5) (1970) 835–848.
[7] J.E. Jontz, The effect of dynamic surface tension on nucleate boiling coefficients, AIChE J. 6 (1) (1960) 34–38.
[8] R.A.W. Shock, Nucleate boiling in binary mixtures, Int. J. Heat Mass Transfer 20 (6) (1977) 701–709.
[9] Y.M. Yang, J.R. Maa, Pool boiling of dilute surfactant solutions, ASME J. Heat Transfer 105 (1) (1983) 190–192.
[10] G.Z. Filippov, Steam–liquid media heat mass transfer and hydrodynamics with surface-active substance additives, in: U. Grigull (Ed.), Proceedings of the Seventh Heat Transfer Conference, Hemisphere Publishing Corporation, Washington, 1982, pp. 443–447.
[11] G.A. Saltanov, A.N. Kukushkin, Surfactant influence on heat transfer at boiling and condensation, in: C.L. Tien (Ed.), Proceedings of the Eighth Heat Transfer Conference, Hemisphere Publishing Corporation, Washington, 1986, pp. 2245–2250.
[12] A.T. Papaioannon, The effect of polymer additives on nucleate boiling, in: U. Grigull (Ed.), Proceedings of the Seventh Heat Transfer Conference, Hemisphere Publishing Corporation, Washington, 1982, pp. 67–72.
[13] X.Q. Li, Formation process of mixed fouling of microbe and $CaCO_3$ in water systems, Masters Thesis, Dalian University of Technology, Dalian, China, 2001.