ARTIFICIAL NEURAL NETWORKS FOR ESTIMATION OF HEAT TRANSFER PARAMETERS IN A TRICKLE BED RERACTOR USING RADIAL BASIS FUNCTIONAL NETWORKS

B.V.Babu* and Sangeetha Shekar
Chemical Engineering Group, FD-1
Birla Institute of Technology and Science
PILANI – 333 031 (Rajasthan) India

ABSTRACT

The effective heat transfer parameters in a trickle bed reactor (gas-liquid co-current downflow through packed bed reactors), k_{er}, the effective radial thermal conductivity of the bed, and h_w, the effective wall-to-bed heat transfer coefficient are estimated for air-water system over a wide range of flow rates of air (0.01-0.898 kg/m^{2}s) and water (3.16-71.05 kg/m^{2}s) covering trickle, pulse, and dispersed bubble flow regimes in a 50 mm I.D. column employing ceramic spheres (2 mm), glass spheres (4.05 and 6.75 mm) and ceramic raschig rings (4 and 6.75 mm) as the packing materials. Radial temperature profile method is used for the estimation of k_{er} and h_w using the experimentally measured radial temperature profile in conjunction with the solution of the two-dimensional pseudo-homogeneous two-parameter model. Radial Basis Functional Networks (RBFN) of Artificial Neural Networks (ANN) are also applied for modeling the effective heat transfer parameters in the trickle bed reactor. The RBFN designed to suit the present system has 7 inputs (four temperatures at four radial positions in the bed, liquid and gas rates, and the ratio of column to particle diameter) and 3 outputs (k_{er}, h_w, and the flow regime). The network predictions are found to be in a very good agreement with the experimentally observed values of k_{er}, h_w, and the flow regime

Key Words: Trickle Bed Reactor (TBR), Artificial Neural Networks (ANN), Radial Basis Functional Network (RBFN), Radial Temperature Profile Method (RTP), Heat transfer characteristics

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*Corresponding Author.
E-mail: bvbabu@bits-pilani.ac.in

Introduction:

One of the most widely used multiphase reactors is the gas-liquid co-current downflow packed bed reactor, which is often called trickle bed reactor (TBR). It is commonly used either for the transfer of momentum, heat and mass using inert packing or to carry out chemical reactions with catalytic pellets (Shah, 1979; Rao & Drinkenburg, 1985; Hugo de Lasa, 1986; Babu, 1993; Lamine et al., 1996; Babu & Sastry, 1998)). The reactors can also be used for the absorption followed by homogeneous catalytic chemical reaction in the liquid phase, using inert packing which produces large gas-liquid interfacial area and mixing between the phases. Due to their wide applications it becomes very important to understand and to be able to predict in detail what will the values of the effective heat transfer parameters h_w and k_{er} and how they vary with the change in other variables. Any attempt to empirically correlate the data using the physical modeling has its own limitations such as inapplicability for wide range of operating conditions.

Application of Artificial Neural Networks (ANN) in various chemical engineering fields is catching up, and the Radial Basis Functional Networks (RBFN) are proving to be a very powerful tool in most of the applications of Neural Networks (Behera et al., 1995). It is the latest technique in Neural Networks by which a surface in multi-dimensional space that provides the best fit for the data can be found. It is better than all the conventional methods of Neural Networks because it does not require linearity in the functions (Behera, 1997). RBFN learns quickly, i.e., the data points need to be passed fewer times but a larger number of data need to be passed in one go. Usually online and offline learning techniques vary significantly but when it comes to applications of RBFN in systems of present nature, any technique is expected to give good results (Niranjan & Fallside, 1990).

Radial Basis Functional Networks:

Both Radial Basis Functional Networks (RBFN) and the Multilayer Layer Network (MLN) of ANN are examples of non-linear layered feedforward networks and both of them are universal approximators. However, they differ from each other in many important aspects (Mezard & Nadal, 1989). The linear characteristic of the output layer of the RBFN means that such a network is more closely related to Rosenblatt's perceptron than the MLN perceptron. However, the RBFN differs from MLN in that it is capable of implementing arbitrary non-linear transformations of the input space.

In this approach, learning is equivalent to finding a surface in a multidimensional space that provides a best fit to the training data. This is generally known as the curve fitting approximation problem in contrast to back propagation algorithm, which is a stochastic approximation. This classification and functional approximation paradigm is known as Radial Basis Functional Network (RBFN). These RBFNs find a wide range of applications and are most effective in load forecasting, weather forecasting, modeling, pattern recognition, and image compression and many more.

RBFN consists of three different layers – an input layer, a hidden layer, and an output layer. However, the hidden layer is multidimensional and is functionally different from the hidden layer of a multilayer perceptron. The hidden units provide a set of functions that constitute an arbitrary basis for the input patterns when they are expanded into the hidden-units space. The hidden units are known as radial counters and are represented by the vectors C_1, C_2... C_n. The transformation from the input space to the hidden unit space is non-linear whereas the transformation from the hidden-unit space to the output space is linear. Thus RBFN produce a linear combination of non-linear basis functions. The dimension of input matches with the dimension of each radial center, i.e., each center for a 'p' input network is 'p x 1'.

The Radial basis function in the hidden layer produces a significant non-zero response only when the input falls within a small localized region of the input space. Each hidden unit, known as radial center has its own 'receptive fields' in the input space, i.e., each center is representative of one or some of the input patterns. This is called 'local representation of inputs' and the network is also known as 'localized receptive field network'. The given problem is solved once the input space is matched with these receptive fields (Behera, 1997). The inputs are clustered around the centers and the output is linear.

$$y = \sum_{i=1}^{h} \phi_i w_i \qquad (1)$$

Thus we obtain a 'smooth fit' to the desired function. The hidden units in RBFN usually have Gaussian activation functions as

$$\varphi_i = \phi(\| x - c_i \|) \qquad (2)$$

where $\| x - c_i \|$ is the Euclidean norm function.

Gradient Descent Learning Algorithm:

One of the most natural approaches to update c_i and w_i is supervised training by error correction learning. This is easily implemented by using a gradient descent procedure. The update rule for center learning are given below:

$$c_{ij}(t+1) = c_{ij}(t) - \eta_1 \frac{\partial E(t)}{\partial c_{ij}(t)} \qquad (3)$$

The output being linear, we can assume that $w_{ij} = y^d$; however, this is not optimal when overlaps between the radial centers are taken into account. This can be optimized by the rule

$$w_i(t+1) = w_i(t) - \eta_2 \frac{\partial E(t)}{\partial w_i(t)} \qquad (4)$$

The cost function is $E = \frac{1}{2}\sum (y^d - y)^2$ (5)

And the actual response is calculated as

$$y = \sum_{i=1}^{h} \varphi_i w_i \quad (6)$$

The activation function is taken to be

$$\varphi_i = e^{-z_i^2 / 2\sigma^2} \quad (7)$$

where, $z_i = \| x_i - c_i \|$ (8)

and σ is the bandwidth (i.e. width of the center).

Differentiating Eq. (5) & Eq (8) w.r.t c_{ij}, and Eq. (7) w.r.t. z, we get,

$$\frac{\partial E}{\partial c_{ij}} = \frac{\partial E}{\partial y} x \frac{\partial y}{\partial \varphi_i} x \frac{\partial \varphi_i}{\partial c_{ij}} = -(y^d - y) w_i \frac{\partial \varphi_i}{\partial z_i} \frac{\partial z_i}{\partial c_{ij}} \quad (9)$$

$$\frac{\partial \varphi_i}{\partial z} = \frac{z_i}{\sigma^2} \varphi_i \quad (10)$$

$$\frac{\partial z_i}{\partial c_{ij}} = \frac{\partial}{\partial c_{ij}} \left(\sum_j (x_{ij} - c_{ij})^2 \right)^{1/2} \quad (11)$$

Simplifying the above, we obtain the update rule for center learning:

$$c_{ij}(t+1) = c_{ij}(t) + 2\eta_1 w_i (y^d - y) \frac{\varphi_i}{\sigma^2} (\sum_j (x_{ij} - c_{ij})^2)^{1/2} (x_{ij} - c_{ij}) \quad (12)$$

and the update rule for the linear weights is:

$$w_i(t+1) = w_i(t) + \eta_2 (y^d - y) e^{-(\| x_i - c_i \|)^2 / 2\sigma^2} \quad (13)$$

The gradient descent vector $\partial E / \partial c_{ij}$ exhibits a clustering effect. Note that in this method (RBFN), there is no back-propagation of error unlike the supervised learning in MLN.

Experimental Set-up:

The schematic diagram of the experimental set-up is shown in Fig. 1. The detailed description of the set-up, experimental procedure, data collection and reduction are reported elsewhere (Babu, 1993; Babu & Rao, 1994; Babu & Sastry, 1998). Experiments were carried out to obtain the heat transfer parameters k_{er} and h_w for co-current downflow of air and water through packed beds over a wide range of flow rates of air (0.01-0.898 kg/m^{2}s) and water (3.16-71.05 kg/m^{2}s) covering trickle, pulse, and dispersed bubble flow regimes in a 50 mm I.D. column employing ceramic spheres (2 mm), glass spheres (4.05 and 6.75 mm) and ceramic raschig rings (4 and 6.75 mm) as the packing materials. Radial temperature profile method is used for the estimation of k_{er} and h_w using the experimentally measured radial temperature profile in conjunction with the solution of the two-dimensional pseudo-homogeneous two-parameter model (Tsang et al., 1976). On the whole, 240 experimental data points were obtained covering the wide range of experimental conditions as mentioned above.

Results and Discussion:

The RBFN designed to suit the present system has 7 inputs (i.e.) T_1, T_2, T_3, T_4, L, G, D_t/d_p and the 3 outputs k_{er}, h_w, and the flow regime, where

k_{er} = effective radial thermal conductivity of the bed, W/mK

h_w = effective wall-to-bed heat transfer coefficient, W/m^2K

L = superficial mass velocity of liquid, kg/m^2s

G = superficial mass velocity of gas, kg/m^2s

D_t/d_p = ratio of reactor diameter to particle diameter, m

T_1, T_2, T_3, T_4 = temperature at various radial positions (r/R = 0, 0.4, 0.8, 1.0) of the bed, ^oC

A set of 120 experimental data points were sent to the RBFN and the network was trained. The above data points were split into eight parts and eight different networks were used to identify input patterns corresponding to those regions. Two procedures were used for training the neural network.

(1) In this method the center nodes were assigned random numbers at start. Then the data points were passed to the network and only those values of the center were updated whose radial distance from the input data was least at every stage the learning rate, α, is decremented by a constant step value. The above procedure was carried out until α almost nearly becomes zero after which center updating will not occur. In the next phase the weights connecting the radial activation center's layer and the output layer were randomly assigned some small random numbers. The training data set was passed through the network and the values of the output nodes were calculated. This output obtained was compared with the desired output values and the error was used to update the weights. The number of times this data set to be sent to the neural network depends on the accuracy desired. Here the learning rate η was gradually increased in very small steps.

(2) First as many center nodes are there that many data points were extracted from the data file and assigned to the center nodes. Next a set of data points were passed to the neural network and the initial estimation of the weights connecting the radial centers larger and the output layer was done. With this phase 1 of training was over. In phase 2 the rest of the data points are now passed to the neural network and the centers and weights were updated using the gradient descent technique until a satisfactory rms error was achieved. These updated weights and contents were now tested with fresh data and the results are compared.

The root mean square error (rms error) as a function of number of epochs (the number of times the RBFN was trained with the experimental data) for two typical sets of data (training set NN-1 & NN-2) is shown in Figs. 2 & 3 respectively. As can be seen from these figures, the rms error is 0.1 for the training set NN-1 and it is 0.12 for the training set NN-2 for 10,000 epochs which is quite good.

After training the network (RBFN) with the 120 data points, the final successful weights of the entire network (mapping) for different sets were stored. Then, these mapped weights were used to predict the outputs (k_{er}, h_w, and the flow regime) for the untrained data from the original data (120 data points from the total 240 experimental data points). And the typical comparison of the experimental and the RBFN predicted values of k_{er} and h_w, for the networks 1,2, and 3 is shown, in Table-1 and Table-2 respectively. It may be noted that the prediction of the flow regime (Trickle, Pulse, and Dispersed bubble flow regimes) is exactly same as the experimental values. As can be seen from the Table-1 and Table-2, the predictions of RBFNs are quite satisfactory.

Conclusions:

The Radial Basis Functional Networks (RBFN) of Artificial Neural Networks (ANN) were found to give satisfactory results in predicting the effective heat transfer parameters such as k_{er} & h_w and the flow regime of a trickle bed reactor.

Table-1. Comparison of experimental and the network (RBFN) predicted values of k_{er} for the Network sets 1,2, and 3.

Network-1		Network-2		Network-3	
k_{er} exptl. (W/mK)	k_{er} pred. (W/mK)	k_{er} exptl. (W/mK)	k_{er} pred. (W/mK)	k_{er} exptl. (W/mK)	K_{er} pred. (W/mK)
17.739981	18.013695	20.849949	19.404438	14.909960	14.391531
19.789965	23.546707	19.629978	22.532982	20.819988	21.186939
27.729963	30.621702	27.700003	26.608980	27.889948	29.145155
53.509945	53.565670	49.659962	48.861111	52.379971	51.895100
65.890015	66.635056	73.810005	74.238792	62.130035	64.370682

Table-2. Comparison of experimental and the network (RBFN) predicted values of h_w for the Network sets 1,2, and 3.

Network-1		Network-2		Network-3	
h_w exptl. (W/m^2K)	h_w pred. (W/m^2K)	h_w exptl. (W/m^2K)	h_w pred. (W/m^2K)	h_w exptl. (W/m^2K)	h_w pred. (W/m^2K)
893.00000	991.59008	1173.81054	1418.51086	1941.12695	2143.04003
1822.80188	1782.50805	2385.37377	2113.22631	2732.95361	2511.34765
2295.38354	2412.46167	2521.53198	2739.05981	2631.80664	2686.95459
2807.85742	2942.70556	2940.06445	3009.19995	3187.38476	3245.80761
3642.95703	3678.68725	3237.37719	3267.99365	3759.00000	3816.81030

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