Application of Artificial Neural Network (ANN) in Chemical Engineering: A Review

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ABSTRACT

Many times, we encounter with some system or process where it become complex to determine the correlation between the dependent and independent variables. Chemical engineering has many such examples where we can obtain the output values for predetermined values of input parameters, experimentally. But it is quite complex to develop a mathematical model which can map the behavior and interdependency of process or system parameters. Even sometimes it is not easy to find the solution of such mathematical models. It became time consuming because the complexity increases if the system is nonlinear and requires high level of technical expertise. For such system or process, ANN is getting the attention of the technical world. ANN basically is a computational technique that has the capability to model correlation between the process variables, input and output values. Traditional approaches have some limitation in solving chemical engineering problems, like modeling of highly complex nonlinear systems. Hence for such complexity, artificial neural networks (ANN) is found to solve complicated tasks in a variety of practical applications. In this article several applications of ANN in chemical engineering is discussed.

Keyword: *Artificial Neural Network, Chemical Engineering, Learning Technique, Prediction*

1. INTRODUCTION

Work on the artificial neural networks, has been inspired right from its origin by the recognition that the human brain computes in a completely different manner from the conventional computing machine. The brain is extremely advanced, nonlinear, complex, and parallel computer. It has the potential to organize in structural constituents, known as neurons. So as to perform certain computations e.g. pattern recognition, perception and motor control. Many times faster than the fastest digital computer in the existence today. The idea of artificial neural network has been derived based on the functioning of brain. The definition for neural network can be given as: "A neural network is a massively parallel distributed processor made up of a simple processing units which has a natural propensity for storing experiential knowledge and making it available for use'' [1]. It resembles the brain in two respect.

1. Knowledge is acquired by the network from its environment through a learning process.
2. Interneuron connections strengths, known as synaptic weights, are used to store the acquired knowledge.

1.1 Network Architectures

There are different types of network architectures that have been used for solving complex problems. They are discussed below:

1.1.1 Simple ANN Model

The basic structure of a single processing unit in an ANN as shown in Figure [1], which will be referred to as a node and is analogous to a single neuron in the human brain. A node receives one or more input signals, in which may come from other nodes or from some other source. Each input is weighted according to the value W_j which is called a weight. These weights are similar to the synaptic strength between two connected neurons in the human brain. The weighted signals to the node are summed and the resulting signal is sent to a activation function, which can be any type of mathematical function, but is usually taken to be a simple bounded differentiable function such as the sigmoid. The resulting output of the node, may then be sent to one or more nodes as an input or taken as the output of an ANN model.

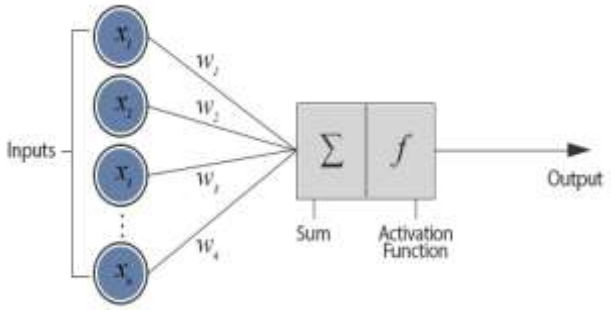

Figure-1: Simple ANN

1.1.2 Feed-Forward Networks

Feed-forward ANN allows signals to travel one way only from input to output. There is no feedback (loops) i.e. the output of any layer does not affect that same layer. Feed-forward ANN tends to be straight forward networks that associate inputs with outputs. They are extensively used in patter recognition. This type of organization is also referred to as bottom-up or top-down.

1.1.3 Feed-Back Networks

Feedback networks can have signals traveling in both directions by introducing loops in the network. Feedback networks are very powerful and can get extremely complicated. Feedback networks are dynamic, their state is changing continuously until they reach an equilibrium point. They remain at the equilibrium point until the input changes and a new equilibrium needs to be found. Feedback architectures are also referred to as interactive or recurrent, although the latter term is often used to denote feedback connections in single-layer organizations.

1.2 Network Properties

The topology of a neural network refers to its framework as well as its interconnection scheme. The framework is often specified by the number of layers and number of nodes per layer. Three types of layer include as shown in Figure [2].

Input layer: The nodes in it are called input units; the activity of the input layer represents the raw information that is fed into the network for processing.

Hidden layer: The nodes in it are called hidden units, which ae not directly observable and hence hidden. They provide nonlinearities for the network.

Output layer: The nodes in it are called output units, which encode possible concepts to be assigned to the instance under consideration.

This simple type of network is interesting because the hidden units are free to construct their own representations of the inputs. The weights between the input and hidden units determine when each hidden unit is active.

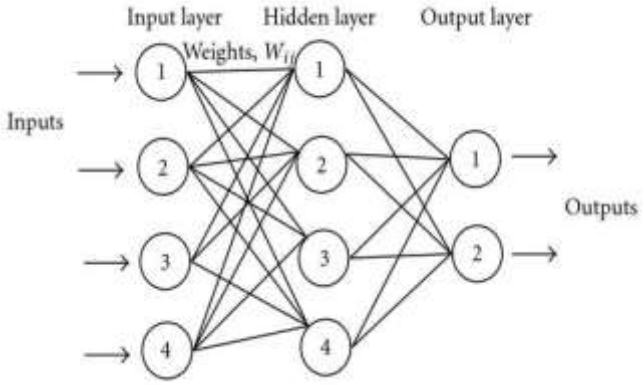

Figure -2: Artificial Neural Network with one hidden layer

1.3 Transfer Function

The behavior of an ANN depends on both the weights and the input-output transfer function that is specified for the units. This function typically falls into one of three categories:

• Linear
• Sigmoid
• Threshold

For *linear units*, the output activity is proportional to the total weighted output.

For *sigmoid units*, the output varies continuously but not linearly as the input changes. Sigmoid units bear a greater resemblance to real neurons than do linear or threshold units, but all three must be considered rough approximations.

For *threshold units*, the output are set at one of two levels, depending on whether the total input is greater than or less than some threshold value.

To make a neural network that performs some specific task, we must choose how the units are connected to one another and we must set the weights on the connections appropriately. The connections determine whether it is possible for one unit to influence another. The weights specify the strength of the influence.

1.4 The Back-Propagation Algorithm

In order to train a neural network to perform some task, we must adjust the weights of each unit in such a way that the error between the desired output and the actual output is reduced. This process requires that the neural network compute the error derivative of the weights (EW). In other words, it must calculate how the error changes as each weight is increased or decreased slightly. The back propagation algorithm is the most widely used method for determining the EW.

2. ANN IN CHEMICAL ENGINEERING

Artificial neural network is been used many field for predicting the output. Traditional approaches of solving chemical engineering problems frequently have their limitations, as for example in the modeling of highly complex and nonlinear systems. Artificial neural networks (ANN) have proved to be able to solve complex tasks in a number of practical applications. Here are several applications of ANN in chemical engineering.

Juan [2] proposed an adaptive neural network control algorithm for a class of a two continuous stirred tank reactors with unknown functions. The neural networks are used to approximate the unknown functions. The reactor modelling has nonlinearity property and unknown function appear in each subsystem. This property results in the difficulties in the design. By designing a new back stepping method, the difficulties are avoided. The Lyapunov stability analysis proved that all the signals are bounded and the system output converges to a small neighborhood of zero.

Valente et al. [3] used electrocoagulation to reduce the chemical oxygen demand of dairy industry effluent. The effects of operating parameters were evaluated, including the electric current density, initial effluent pH, electrolysis time and distance between electrodes. The characteristics of the effluent, namely, the solids content and its fractions, turbidity and chemical oxygen demand, were also considered. An artificial neural network was constructed to model chemical oxygen demand after electrocoagulation; it was trained and validated, yielding a correlation coefficient of 0.96 between predicted and experimental values. Input variables were ranked by their relative importance for the prediction of chemical oxygen demand after treatment by electrocoagulation. Among effluent the total dissolved solids concentration had the greatest relative importance, followed by the chemical oxygen demand. It can be concluded that an artificial neural network can predict chemical oxygen demand after treatment by electrocoagulation. In practice, operating parameters may be adjusted to obtain a greater reduction of chemical oxygen demand and to allow automation of the handling process.

Humberto et al. [4] studied, the automatic startup of a nuclear reactor subjected to period scram constraint is considered. To achieve this operation in a minimum time avoiding the difficulties associated with the application on-line of maximum principle or dynamic programming, first the optimal trajectory is calculated off-line. Next, the nuclear plant considered as a black box is identified by a differential neural network. The structure provided by this neural identifier is fed back to follow the optimal trajectory. The modeling error is compensated by the usage of the power derivative. Thus, the asymptotic stability of the tracking error can be guaranteed.

Froio et al. [5] proposed artificial neural networks (ANNs) for the evaluation of the heat load to the cryoplant. First, two simplified thermal-hydraulic models for an ITER Toroidal Field (TF) magnet and for the ITER Central Solenoid (CS) are developed, based on ANNs, and a detailed analysis of the chosen networks' topology and parameters is presented and discussed. The ANNs are then inserted into the 4C model of the ITER TF and CS cooling circuits, which also includes active controls to achieve a smoothing of the variation of the heat load to the cryoplant. The training of the ANNs is achieved using the results of full 4C simulations (including detailed models of the magnets) for conventional sigmoid-like waveforms of the drivers and the predictive capabilities of the ANN-based models in the case of actual ITER operating scenarios are demonstrated by comparison with the results of full 4C runs, both with and without active smoothing, in terms of both accuracy and computational time. Exploiting the low computational effort requested by the ANN-based models, a demonstrative optimization study has been finally carried out, with the aim of choosing among different smoothing strategies for the standard ITER plasma operation.

Chang et al. [6] provided the simulated verification and validation of the hybrid neural-network rate-function (HNNRF) approach for modeling batch reactor systems. In chemical reactor processes, some measurements may not be easily obtainable, and the designed neural-network rate-function (NNRF) model in our previous work did not propose a method to include the state variables for the suggested dynamic model. To overcome this difficulty, the approximated mechanistic equations characterizing these immeasurable state variables could be incorporated into the NNRF model to form the hybrid neural-network rate-function model. The sequential pseudo-uniform design (SPUD) is used to locate the sufficient but limited experiments to provide the HNNRF model with rich information. In this research, the HNNRF modeling capability over a large operating region was evaluated employing a simulated polymerization reactor system. In addition to the comparative benefit of short time expenditure for building the model, the performance of the identified HNNRF model is quite acceptable in the face of noisy measurements and the identified model could be applied to determine the optimal recipe or the operating conditions of the reactor systems.

Dirion et al. [7] developed a neural controller to regulate the temperature in a semi-batch pilot-plant reactor. The experimental unit employs a monofluid heating-cooling system to raise the reactor to the operating temperature, and then remove the heat generated by an exothermic reaction. Preliminary experiments form the neural-network learning database. These involve regulation of the reactor by either an advanced control algorithm or by operator (manual control). The results suggest that such neural controllers can provide excellent set point-tracking and disturbance rejection.

Giwa et al. [8] in their work, a new configuration of an electrically-enhanced membrane bioreactor has been introduced to treat medium strength wastewater. The integrated setup enhanced the reduction of wastewater contaminant concentrations. The investigated components in this study were chemical oxygen demand (COD), orthophosphates (PO_4^{3-}-P) and ammonium (NH_4^+-N). The percentages of COD, PO_4^{3-}-P, and NH_4^+-N removal obtained were 98, 99, and 98%, respectively. Variation in environmental compositions such as mixed liquor dissolved oxygen (DO), volatile suspended solids (MLVSS), pH, and electrical conductivity influenced the effluent concentration of wastewater components. Artificial neural networks (ANNs) based ensemble model was used to model the experimental findings of COD, PO_4^{3-}-P and NH_4^+-N removal given the initial mixed liquor compositions. Comparison between the model results and experimental data set gave high correlation coefficients for COD($r = 0.9942$ PO_4^{3-}-P ($r = 0.9998$) and NH_4^+-N ($r = 0.9955$).

Molga and Cherbanski [9] has done a detailed investigations have been carried out to check the ability of multilayer neural networks to model the simultaneous mass transfer and chemical reaction in the liquid-liquid reacting system. In this approach the intrinsic reaction kinetics and diffusive mass transfer are represented by a black-box and only the input-output signals are analyzed. The data for training of the net have been taken from the experiments performed in a RC1 Mettler Toledo reaction calorimeter. The hydrolysis of propionic anhydrite catalyzed with sulphuric acid has been chosen as a testing reaction. The hybrid, first-principle-neural-network model has been defined to describe batch and semi batch stirred tank reactors operating at different conditions. Good accuracy and flexibility of the proposed approach have been obtained for a properly defined experimental programme supplying data for learning.

Yang [10] studied three different approaches for modelling a semi-batch polymerization reactor using artificial neural networks (ANN). Based on the characteristics of the semi-batch reactor a multi-stage strategy is recommended. It divides the whole reaction process into two periods, semi-batch and batch, and further divides the

semi-batch part into two sub-periods that are before and after the maximum temperature is reached. Different ANN architectures are used to model the three parts separately. The results demonstrate that the multi-stage approach proposed can be used to estimate difficult-to-measure polymer variables with acceptable accuracy for semi-batch processes. Concentrations of the monomer and the initiator in the reactor are estimated from reactor temperature, feed temperature and the concentration of the initiator in the feed.

Li and Li [11] showed that the intensified continuous reactor was designed to replace conventional batch reactor for three-phase catalytic slurry hydrogenation. The control of intensified continuous reactor imposes difficulties due to complex three-phase reaction kinetics, inherent process nonlinearities and stringent temperature limitation. In this work, two nonlinear model predictive control (NMPC) algorithms based on neural networks are proposed and implemented for the intensified continuous reactor. One is the NMPC with nonlinear optimization that is solved by sequential quadratic programming (SQP). The other is the NMPC with local linearization that is applied at each sample instant, a linear model with parameter varying is obtained and the optimization in NMPC can be written as a quadratic programming (QP) problem like linear MPC. Simulations results show that the NMPC with local linearization presents satisfactory performance.

Messai [12] studied a detailed method for fault detection of an in-core three wires Resistance Temperature Detectors (RTD) sensor is introduced. The method is mainly based on the dependence of the fuel rod temperature profile on control rods elevation and coolant flow rate in a given nuclear reactor. For the implementation, an artificial neural network (ANN) technique has been developed to model the dynamic behavior of the considered temperature sensor. In order to have more refined model estimation, ANN has been combined with additional noise reduction algorithms. The effective de-noising work was done via the discrete wavelet transform (DWT) to remove various kinds of artefacts such as inherent measurement noise. The principle of the adopted fault detection task is based on the calculation of the difference between the ANN model estimated temperature and the online being measured temperature and then compare the deviation with a certain detection threshold to decide the sensor fault. The efficiency of the method is evaluated first on a simulated case and then on the on-line measurements obtained from a real plant. Results confirm the capacity of the developed ANN-based model to estimate a fuel rod temperature with a reasonable accuracy.

Mazrou [13] finds a new methodology of a suitable artificial neural network architecture which improves its performances capabilities in predicting two significant parameters in safety assessment i.e. the multiplication factor k_{eff} and the fuel powers peaks $P_{\max}$ of the benchmark 10MW IAEALEU core research reactor. The performances under consideration were the improvement of network predictions during the validation process and the speed up of computational time during the training phase. Consequently, the speed up of several popular algorithms has been assessed during the training process. The comprehensive neural system was subsequently trained on different transfer functions, number of hidden neurons, levels of error and size of generalization corpus. Thus, using a personal computer with data created from preceding work, the final results obtained for the treated benchmark were improved in both network generalization phase and much more in computational time during the training process in comparison to the results obtained previously.

Hernandez et al. [14] proposed a neural networks state observer to estimate biomass, substrate and methane in a continuous anaerobic reactor is introduced in this paper. The observer is designed from a recurrent high order neural network with a hyperbolic tangent as activation function and an extended Kalman filter as learning algorithm. The observer structure is validated via simulations and using experimental data obtained from an anaerobic continuous stirred tank at lab scale. This prototype is used to treat real slaughterhouse wastewater and it is operated in continuous mode. The obtained results show that the proposed observer is able to reproduce adequately the biomethane production and the substrate (related to chemical oxygen demand) in the methanogenesis stage; besides, methanogenic bacteria are also well estimated but some modifications are required in order to reach better results.

Basile et al. [15] presents a theoretical approach via artificial neural networks model for studying the water gas shift reaction in hydrogen selective membrane reactors, based on an experimental campaign useful for training the aforementioned model. In particular, parameters such as the reaction pressure, reaction temperature, gas hourly space velocity (GHSV), sweep gas flow rate, H_2O/CO feed molar ratio and feed have been considered from both a modeling and an experimental point of view in order to analyze their influence on the water gas shift performance (in terms of CO conversion, hydrogen recovery, hydrogen permeate purity) in two membrane reactors, allocating dense Pd-Ag membranes, having different active membrane surface areas. As best experimental results, by using a

Cu-Zn based catalyst and co-current configuration of sweep gas, CO conversion around 100% and H2 recovery of about 70% were reached. Meanwhile, the artificial neural networks model has been validated by using part of the experimental tests as training values and, then, it was used for optimizing the system to achieve as much as possible high hydrogen recovery. The model predicted the experimental performance of the water gas shift membrane reactors with an error on CO conversion lower than 0.5% and around 10% for the H2 recovery over the experimental tests not used during the model training.

3. CONCLUSION

The computing world has a lot to gain from neural networks. Their ability to learn from the previous example makes them very flexible and powerful. Furthermore there is no need to devise an algorithm in order to perform a specific task. ANN is also suited for real time systems because of their response and computational times are due to their parallel architecture. By using ANN, the computation time requirement is decreases and it become easy to predict the final results. From above discussion we can say that ANN can be used in chemical engineering field instead of other rigorous techniques.

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