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ANN Based modeling of Amine Contactor Column in Natural Gas Sweetening Plant

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Abstract

In this study, Artificial Neural Network is employed to develop a model to predict amine contactor column output variables of Gachsaran natural gas sweetening plant. The developed model is evaluated by process operating data of the natural gas refinery that was simulated by commercial Aspen Hysis simulator and was validated by field data. The simulation results are implemented as inputs and target outputs for ANN model. A set of 4 input and 1 output plant data each consisting of 120 data has been used to train, validate, and test the model. Model development that consists of training, optimization and test was performed using randomly selected 70%, 15%, and 15%of available data respectively. Model estimations are compared with data obtained from simulation based models. Test results showed a good agreement between predicted and observed operating plant data (R^2= 0.9779) that indicated ANN can be a reliable accurate estimation method for amine absorbing column.

Introduction

About 33% of the world's natural gas reserves are discovered in offshore fields and 40 % of the natural gas reserves are sour or acid, containing large quantities of CO_2 and H_2S and other sulfur compounds. To realize its value it has to be brought onshore, to be processed to the required specification and send to distribution networks. Lack of means to bring stranded natural gas to the market leads to increase of remotely located natural gas reserves, flaring and re-injection of associated gas from offshore fields [1-2].

Flaring of associated gas has become an environmental issue with high degree of focus among approving authorities and oil companies. Handling of associated gas for oil developments has become a more critical issue than before. Therefore, this has led the oil and gas industry to seek solutions that can handle the associated gas in an acceptable manner both economically and environmentally. The Iranian offshore oil company (IOOC) is planning for the expansion of the existing onshore Sirri Island complex located in the South East of Sirri Island in the Persian Gulf, Iran. The Sirri Island Gas Gathering and NGL Recovery Project involves expansion of existing reception facilities and the addition of new gas & condensate transmission lines, gas compression and processing facilities, with associated utilities.

There are several treating processes available for H_2S removal from natural gas. Some of these processes use chemical, physical, and hybrid solvents while few others using physical separation by special membranes [3].

Among the addressed methods, alkanolamines for sweetening have been employed widely. The alkanolamine aqueous solutions are capable of absorbing impurities such as hydrogen sulfide and carbon dioxide from natural gas. [4]As the degree of the gas acidity increases, the energy required by the process to achieve sweet gas specifications in terms of H2S and CO2 concentrations will increase.[5] This is particularly true for gas sweetening processes using alkanolamine solvents such as the primary amine: methyl-ethanolamine (MEA), the secondary amines: diethanolamine (DEA) and di-iso-propanolamine (DIPA), and the tertiary amines: triethanolamine (TEA) and methyldiethanolamine (MDEA). Many recent researches have focused on investigating the mixing of different amine solvents [6-9].

In the past few years, mixed amine solvents for the removal of acid gases have received increased attention. [6] Application of mixtures of alkanolamines, a solution of two or more amines in varying concentration, has been shown to produce absorbents with excellent absorption characteristics Reliable accurate models of gas sweetening processes allows one to optimize operating conditions thus minimizing operational costs. This is a necessity due to inherent seasonal variations in feed stream and temperature. Attempts to develop such models include those that are based basic principles and those that are data-based using input/output plant data [10]. Models based on detailed mass and energy balance equations proved to be very complicated and hard to solve especially when coupled with optimization computer routines [11].

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 that should be of interest to you as a chemical engineer [12]. (ANN) represent one of the fastest developing fields of artificial intelligence due to their ability to resemble (to a certain extent) the human problem solving characteristic, which is difficult to simulate using the logical, analytical techniques of expert system and standard software technologies. The wide applicability of ANNs stems from their flexibility and ability to model linear and nonlinear systems without prior knowledge of an empirical model. This gives ANNs

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an advantage over traditional fitting methods for some chemical applications [13].

In this paper, we will try to apply ANN as a prediction tools to estimate amine contactor column output. The investigated process is carried out in Gachsaran gas sweetening plant. To do so, the process will be simulated by commercial Aspen Hysis simulator and will be validated by field data. The simulation results will be implemented as inputs and target outputs for ANN model.

Experimental

Methods

Acid gas removal unit

In the gas processing industry absorption with chemical solvents has been used commerc-ially for the removal of acid gas impurities from natural gas. Alkanolamines are the most commonly used category of chemical solvents for acid gas capture. In Siri Island NGL project, the Acid Gas Removal unit will treat approximately 143.4 to 143.0 MMSCFD (summer and winter cases) of gas containing approximately 4.12% CO_2 and up to 240 ppm of H_2S. A generic MDEA solution, at 50 wt% strength, is used to sweeten the gas and reduce the CO_2 content to below 2%.

Sour gas is first passed through an Inlet Gas Filter/Coalescer to remove any liquid or particulate contamination, before passing through the Amine Contactor. The Inlet Gas Filter/Coalescer is a vertical vessel comprised of upper and lower chambers, separated by a tube sheet. The Gas first enters the lower chamber, for bulk liquid removal, and then the upper chamber, through the tube sheet and the coalescing filter elements. The flow through the coalescing elements is inside□out. The coalescing filter elements will remove both solids and liquid droplets that are 0.3 microns and larger. Liquid droplets coalesce and grow in size in the elements, descend via gravity, and are collected and removed, at the bottom of the upper chamber. At the same time, the solid particles removed from the gas are swept out of the element by the downward liquid drainage from the elements.

This plant uses the process of chemisorptions to remove H_2S, and other acid gases, such as Carbon Dioxide (CO_2), from the raw gas stream. Chemisorption is a two-step process involving both absorption and chemical reaction. An aqueous amine solution, at a concentration of 50 weight percent, is used to sweeten the raw gas. This solution contains water into which the gases dissolve, and formulated solvent, containing the basic tertiary amine, n-methyl diethanol amine (MDEA), with which the acid gases chemically react. Sour raw gas introduced into the bottom of the tower and is passed, counter current to lean amine solvent, through the Amine Contactor. Gas leaving the topmost tray of the amine contactor should have less than 2 ppm H_2S and less than 2% CO_2 before it proceeds on to the sweet gas cooler.

The amine contactor is a trayed absorption column containing single-pass valve trays. The three topmost trays are water-wash trays used to scrub any entrained amine solution from the exiting gas. The lower trays, promote mass transfer between the aqueous amine solution and the sour gas. The bottom of the tower, directly below the seal pan of the bottommost tray, provides some surge capacity.

Lean amine is fed to top section of the amine contactor, and flows down the column to be collected in the surge section. A lower lean amine feed point will increase the amount of CO_2 in the sales gas stream, and reduce the amount of stripping energy required. Amine in the surge section is rich and must be regenerated before it is reused.

Demineralized water is fed to the topmost tray, Tray #1, and blends into the amine solution flowing down the column. This sweet gas passes through the sweet gas cooler (11-A-101), where the temperature is reduced to 55^{o}C.

This will condense water from the gas stream prior to entering the molecular sieve dehydration unit and reduce the load on the dehydration system. If the stream is cooled too much some of the hydrocarbons will start to condense and reduce the product recovery. If the temperature is too warm the water loading on the molecular sieve dehydration unit will be increased and water breakthrough could possibly occur.

The 2-phase stream from the sweet gas cooler is separated in the sweet gas scrubber (11-D-101), to remove the free liquid from the gas stream. The gas flows upward through a wire mesh mist eliminator where liquid droplets greater than 10 microns are removed and flows to the Sweet Gas Filter/Coalescer. The liquid is level controlled and flows to the closed drain tank.

Rich amine is collected, at the bottom of the amine contactor, and flashed down to near 6 Bara. The flashed gases and amine enter the Flash Tank (11-D-102), to allow the release of absorbed hydrocarbon gases and the separation of absorbed hydrocarbon liquids. The vapour is back pressure controlled and flows to the acid gas incinerator (19-X-101).

The rich amine flows through a particle filter (11-F-102 A/B) to remove solid impurities before a slip-stream flows through an activated carbon filter (11-F-103) to remove residual hydrocarbons in the rich amine. Before being fed to the top tray of the amine regenerator, the stream is preheated in the rich/lean heat exchanger (11-E-101).

The amine sweetening process involves an acid-base reaction between acid gases and amine. In order to reverse this chemical reaction, pressures are decreased and temperatures are increased, thus liberating the acid gases (H2S and CO_2) and regenerating the amine solution. Regeneration is accomplished using the Amine Regenerator (11-C-102), Amine reboiler (11-E-102), and associated reflux equipment.

The amine regenerator is a trayed distillation tower equipped with valve trays. Rich amine enters the tower, flows down through the trays, and is collected in the surge section of the tower, before flowing to the Amine Reboiler. Reflux is returned to the tower, on the topmost tray, Tray #1. Hot vapours, from the reboiler, enter the tower's surge section and flow upward, counter current to the amine, and exit the tower, overhead. During normal operation, the liquid level, in the surge section of the tower, is determined by the weir height in the reboiler and the liquid and vapour hydraulics.
The Amine Reboiler is a horizontal kettle reboiler designed to provide the duty required to drive the stripping in the Amine Regenerator. Amine is fed into the shell side and LP steam flows through the tubes. The shell is divided into two compartments by a weir. In the inlet compartment, heat is transferred from the steam to boil the incoming amine. The boiled vapour is routed back to the surge section of the Amine Regenerator and will travel up through the tower's trays. Lean amine, in equilibrium with the boiled vapour, will overflow the weir, into the reboiler's downstream compartment.

This lean amine will be cooled by the Lean/Rich Amine Heat Exchanger (11-E-101) and sent to the Lean Amine Surge Tank (11-T-101).Temperature control is achieved by changing the flow rate of the heat transfer medium. Pressure, in the Amine Reboiler, is controlled by increasing or decreasing the back pressure on the regeneration system. The amine regeneration reflux circuit consists of: the amine reflux condenser (11-A-102), the amine reflux accumulator (11-D-103), and the amine reflux pumps (11-P-103A/B).

The amine reflux condenser is a forced-draft air cooler used to cool the amine regenerator overhead vapours. This cooler is

equipped with variable pitch fan blades and automatic louvers on the air outlet and for temperature control. The cooled acid gases and condensed water enter the amine reflux accumulator. The water/acid-gas mixture temperature must be controlled near its set point.

If the mixture is over-cooled, the cold water will quench the amine regenerator and increase reboiler duty. If the mixture leaving the amine reflux condenser is too hot, the acid gas fed to the Acid Gas Incinerator will have more water. More water in the acid gas will increase the water make-up requirements of the amine system and increase the fuel gas requirements of the acid gas incinerator.

The amine reflux accumulator is a vertical separator. During normal operation, the liquid is pumped back to the amine regenerator as reflux. The vapour is back pressure controlled and flows to the acid gas incinerator. Figure 1 shows PFD diagram of the sweetening unit.

The aim of this workis to prepare an estimation model in order to predict the effect of feed gas flow rate, amine flow rate, feed gas and feed gas composition (H_2S%) on amine absorber column outputs. Therefore, process validation and optimization have been done by comparing simulation rsults and field data. After the model validation, lots of simulations have been performed to investigate the addresed parameters effect on absorber column.

ANN Model

The ANNs have the potential of enhancing our knowledge of prediction issues. Artificial neural networks can be adopted in a variety of applications like prediction and optimization and prediction. Performing non-linear, multidimensional interpolations between input and output parameters makes it possible to identify non-linear relationships that exist between input and output.

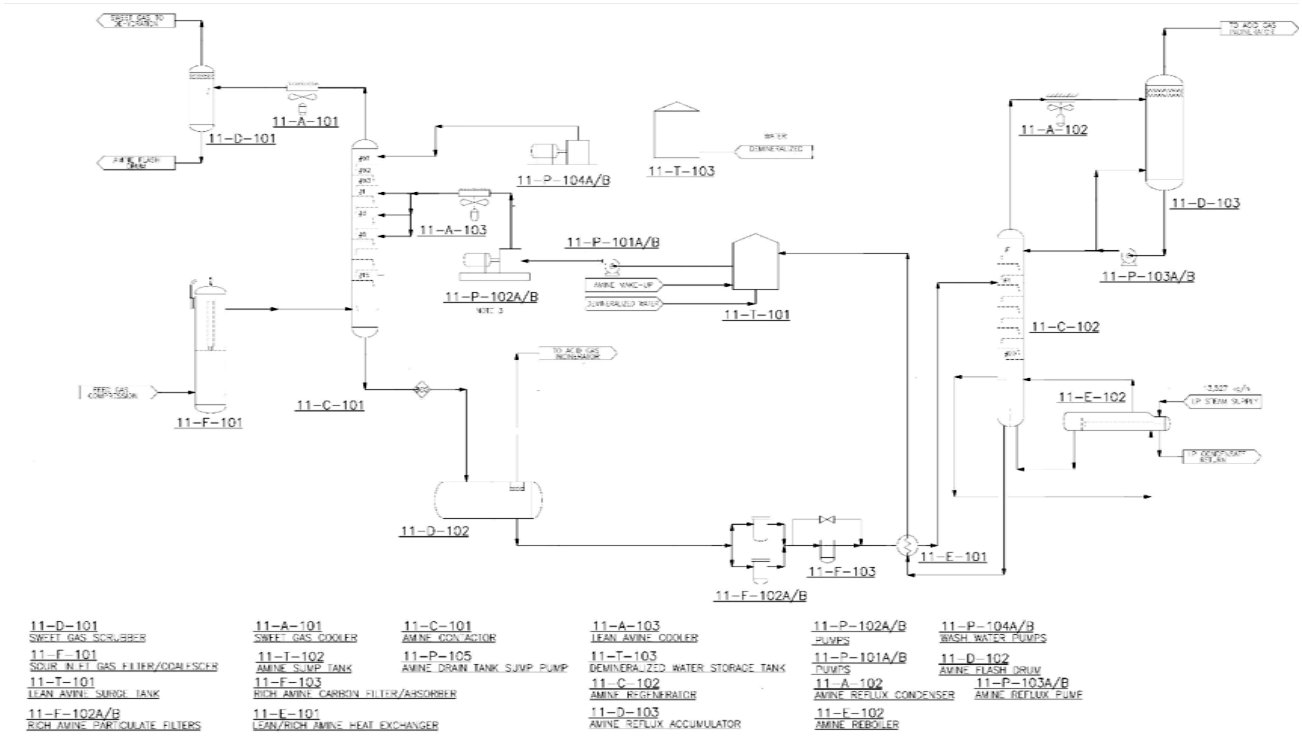

Figure 1: PFD of the Amine Sweetening Unit

Simulation and Optimization

Simulation is done using amine package with Kent Eisenberg's thermodynamic Model for aqueous amine solutions and non ideal vapor phase model. The input gas composition for base model can be found in table 1.

Table 1: Feed Gas Composition for base model

Feed	Mole Fraction %	Feed	Mole Fraction %
MDEA	0	CH_4S	0.00040894
Methane	71.2449	COS	9.53E-05
Ethane	11.5462	P-C6*	0.30987
Propane	7.23941	P-C7*	0.14999
Isobutane	1.224	P-C8*	0.0638791
n-Butane	2.1139	P-C9*	0.015633
Isopentane	0.56633	P-C10*	0.0034371
n-Pentane	0.55066	P-C11*	0.00073686
Hexane	0.017739	P-C12*	0.00011709
Water	0.22848	P-C13*	5.81E-05
Nitrogen	0.58282	P-C14*	5.93E-06
Carbon Dioxide	4.1173	P-C15*	6.56E-07
Hydrogen Sulfide	0.024006	P-C16*	9.50E-08

Generally, neural networks consist of neuron layers which perform calculations. A neuron layer includes the combination of the weights, the multiplication and summing operation, the bias b, the transfer function f, a net input vector ξ and an output vector a. The inputs vector is not involved in a layer. Each neuron in a particular layer is connected with all neurons in the next layer. The connection between neurons is characterized by the weight coefficients. The weight coefficient reflects the degree of importance of the given connection in the neural network. The output value of the i^{th} neuron is determined by equations (1) and (2). It holds that:

$$\xi_i = b_i + \sum_{j=1}^{R} W_{i,j} * X_j \quad (1)$$

$$a_i = f(\xi_i) \quad (2)$$

Where the first index indicates the particular neuron destination for the weight and the second index indicates the source of the

signal fed to the neuron. ξ is the net input to the transform function. f is called transfer function takes the input and produce output according to the expression like:

$$f(\xi_i) = \frac{1}{1+\exp(-\xi_i)} \quad (3)$$

A three-layer network with 6 input elements, two hidden layer with three neurons and an output layer were shown in figure 2. Superscripts indicate the source (l) connection and the destination (k) connection of layer weight matrices and input weight matrices.

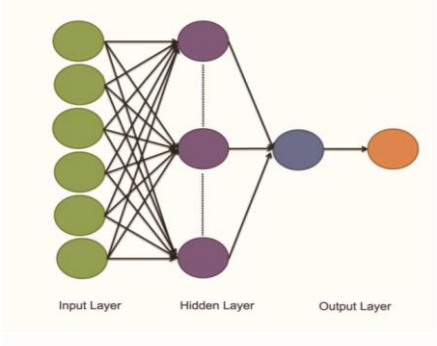

Figure 2: Architecture of the ANN with two hidden layer and one output layer

The first step to develop the neural network is to decide which training algorithm to use. The back-propagation network which is a powerful multilayer, feed-forward neural networks was employed in the present study because of allowing to network to adopt. This generalization property of back-propagation network makes them enable to train a network on a typical set of input/output pairs and obtain good results without training the network on all possible input/output pairs. Feed-forward networks often have one or more hidden layers of sigmoid neurons followed by an output layer of linear neurons. Multiple layers of neurons with nonlinear transfer functions allow the network to learn nonlinear and linear relationships between input and output vectors.

There are generally four steps in the training process:

1. Assemble the training data
2. Create the network object
3. Train the network
4. Simulate the network response to new inputs

Figure 3 shows require stages in constructing a proper network.

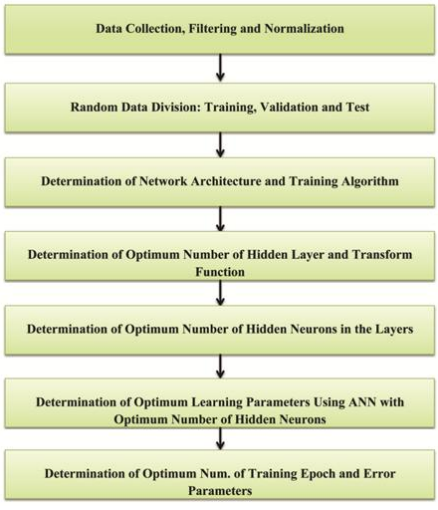

Figure 3: Chart designed for ANN model

Results and Discussion

Model Validation

In order to prepare sufficient and optimized data sets for ANN prediction model, the simulation model results for base feed gas composistion is compared with actual field data. As the figure 4 shows, the similated results are in a good agreement with field data.

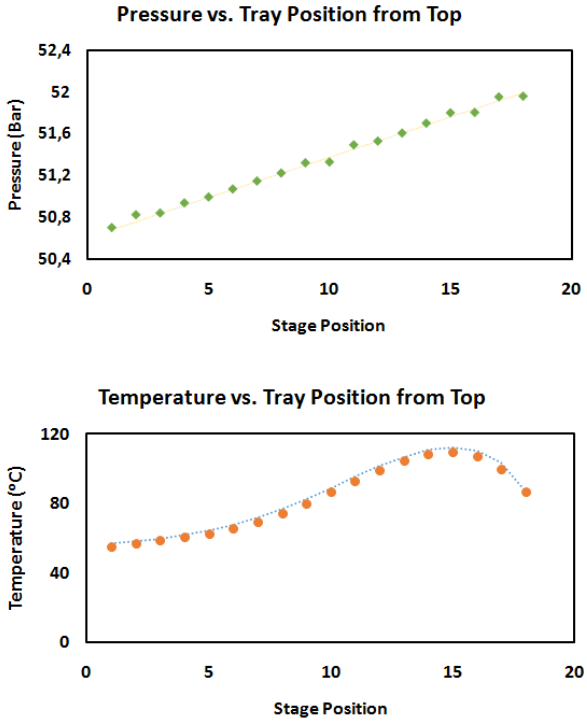

Figure 4: Comparison Between Field Data and Simulation Results

ANN Results

In this paper, extensive simulation runs were carried out to generate sufficient output parameters to train artificial neural network (ANN) prediction model. The generated data divided into training, validation and test subsets. One fourth of the data for the validation set, one fourth in the test set and one half of the training set were taken. To achieve acceptable predictions, several neural network architectures were tried, and a three-layer network, with tan-sigmoid transfer function in the hidden layers and a linear transfer function in the output layer was found to give better results than other architectures. Optimization procedure was used to determine the optimum number of neurons in the hidden layer. After normalizing data, the optimization process showed that network with 30 neuron numbers exhibits the best performance presenting acceptable R^2 values in the range of 1 to 40 neurons. Levenberg-Marquardt function of training was employed to combine the speed advantage of the Gauss–Newton algorithm and the stability of the steepest descent method. To avoid running into local optima instead of global optima, the network weights and biases reinitialized and the network retrained several times to provide the best solution. To reinitialize, the variable learning rate technique was employed to avoid local minima which allow the learning rate to change during the training process. An adaptive learning rate tries to keep the learning step size as large as possible whilst keeping learning stable. An adaptive learning rate needs some modifications in the training process. First, the initial network output and error are calculated. At each epoch new weights and biases are calculated using the current learning rate. New outputs and errors are then calculated.

Figure 5 gives a comparison study of the predictions of this neural network with those of the simulation results for sweet gas H_2S content. Although only a few sets in the input patterns were considered, it can be concluded that an ANN is able to predict the sweet gas H_2S content. This is mainly attributed to the ability of neural networks to find nonlinear functional patterns effectively.

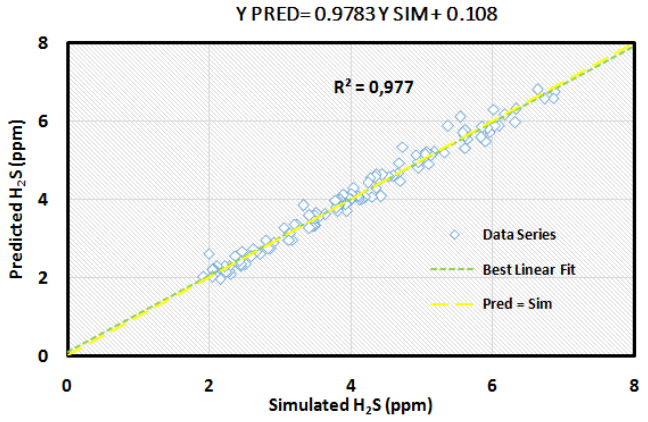

Figure 5: Comparison of Simulated and Predicted values of H_2S in sweet gas

To overcome over fitting issue in the network and improve generalization, the early stopping method has been used. In this technique three subsets must be considered from the available data. The subsets are training set, validation set and test set. Updating the network weights and biases has been performed by using the training set. The error on the validation set is monitored during the training process. The validation error will normally decrease over the first step of training, like the training set error. However, when the network begins over fitting the data, the error on the validation set will generally start to increase. When the validation error increases for a specified number of iterations, the training is stopped, and the weights and biases at the minimum of the validation error are returned. The test set error is not used during the training, but it is used to compare different models. Figure 6 shows data sets error. The result here is reasonable, since the test set error and the validation set error have similar characteristics, and any significant over fitting does not occurred.

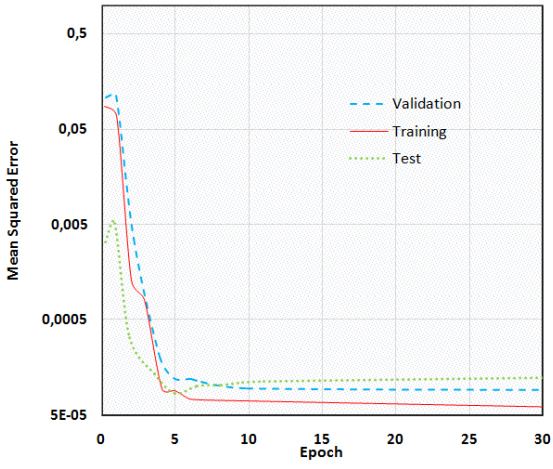

Figure 6: Training, Validation and Test Errors.

To perform some analysis of the network response, the entire data set was put through the network (training, validation and test) and a linear regression between the network outputs and the corresponding targets were performed. The network outputs are plotted versus the targets as square in the figure 5. The best linear fit is indicated by a dashed line. The perfect fit (output equal to the targets) is represented by the solid line. The output seemed to follow the target reasonably well and scattered in a straight line with an acceptable coefficient of determination (almost 0.9779). As the figures show, it can be concluded that ANN model is able to predict the Amine Contactor Output well which is due to the network capability to capture the nonlinear functional patterns effectively. Figure 7 shows the residual plot. In a valid regression analysis, the residuals should be randomly distributed around zero, i.e. the scatter plot of the residuals should be disordered with no trend.

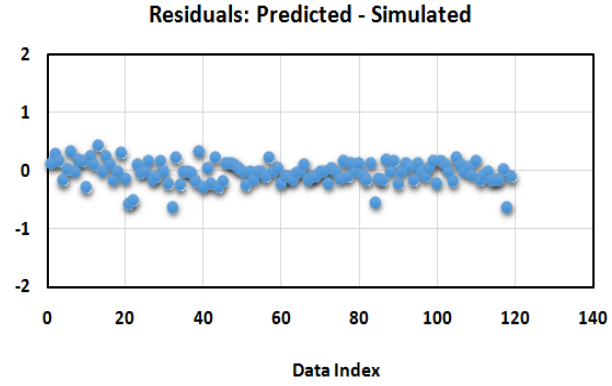

Figure 7: Residual plot

Conclusions

This study demonstrates the applicability of ANN to prepare accurate prediction model of the operational variables of an industrial natural gas sweetening plant which includes absorptioncolumn and amine regenerator column. Beside thegeneral advantages that are cited for ANN as an input/output modeling tool, the predicted data in this study showed good performance of artificial neuralnetworks in terms of accuracy. The cofficient of determination calculated for amine contactor column outputshowed a high accuracy of 97% that is of greatimportance if the predicted data are to be used for monitoring and/or control purposes.

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