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# Nonlinear Process Modeling of "Shell" Heavy Oil Fractionator using Neural Network

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**Abstract:** The identification of intrinsic characteristics on distillation column via dynamic modeling has been becoming indispensable in order to fulfill the increasingly stringent product quality and system regulations. Therefore, the aim of the study is to capture the complex dynamics and static interactions of input output using FANN in Shell heavy oil fractionators. With the case study on "Shell" heavy oil fractionator, artificial intelligence is employed to model the 7 operational outputs, where 3 of those are controlled outputs, named as top end point composition, side end point composition and bottoms reflux temperature. The training, testing and validation data for the single layer neural network are generated through the simulation with the presence of disturbances, process gain uncertainties, measurement of noise and step time variations. With Levenberg-Marquardt algorithm and early stopping method oriented network training, parameter iteration method is proposed and applied to iterate over 4 parameters where the representative pairing to generate optimum network prediction accuracy is selected. Based on sum squared error, residual error and correlation coefficient analysis, the network performance on the case of perfect case, high noise-influencing system, Multi Input Multi Output (MIMO) and highly uncertain system is greatly satisfying in terms of prediction accuracy and network robustness. The result shows that the neural network will always customize itself in nonlinear system and shows its ability in understanding the complex system dynamics with great learning efficiency.

**Key words:** Dynamic modeling, neural network, network performance, system nonlinearity, artificial intelligence

## INTRODUCTION

Distillation column or fractionator is generally known to be widely used equipment in industries particularly on petrochemical processing. Its significance for efficient separation process has increasingly been concerned by engineers in looking at the tradeoff between cost effective approach and tightened product specifications. In U.S. the amount of this type of equipment already reaches approximately 40,000 columns and meanwhile consumes around 3% of total U.S. energy usage in the past decade (Osman and Ramasamy, 2010). Hence, the advanced process modeling and control strategy on distillation column is indispensable in creating flexibility in reducing the operating and capital cost, preserving environmental resources, minimizing energy consumption and attaining satisfied production rate and quality. However, distillation column is always well-known with its difficulty on identifying the intrinsically complex system behavior of composition and phase change which affected by local temperature (Jazaveri-Rad, 2004). This is more specifically known as vapor liquid equilibrium and when the physical structure such as number of trays is greater, the computational effort in modeling will also be proportionally substantial. This is due largely to the equilibrium between the formation of vapor and liquid is occur everywhere within this multistage separation system while this process dynamics is not fast and consistent enough to be captured steadily.

Apart from that intricacy of system equilibrium, inherent factors like sluggish process response resulted by gradual temperature and composition change will also contribute to the aforementioned problems. As the distillation column constitutes of 2 heat balance loop, named as reboiler and condenser, the respective heat duty does affect more than one variable, includes temperature, product compositions, vapor and liquid flow rate. This is rather known as control loop interaction in multivariable system since the slight changing of one variable would leave substantial effects to all other control loops (Fernandez De Canete *et al*., 2010). These control loop interactions could substantially result in unpredictable and elusive output patterns that would ultimately induce to high difficulty level of dynamic modeling.

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The objective of this research is to capture the complex dynamics and static interactions of input output complex system with least mean squared error of residual. Artificial neural networks will model the complex, nonlinear or even ill conditioned functional system by referring to the inputs and outputs processing data. This parallel computational model able to learn from experiences and hence no a priori knowledge is required to estimate the possible output trend that must be tailored to the respected input (Marini *et al*., 2006).

Previously, several advanced methods had been resorted on modeling of industrial distillation column, for instance, multivariable nonlinear Model Predictive Control (MPC) on an ill-conditioned distillation column (Waller and Boling, 2005) . In addition, Computer Algebra (CA) program also been used to generate physical property computer code for modeling and simulation of steady state reactive distillation column (Alfradique and Castier, 2005). Meanwhile, dynamic process model for standardized distillation system gained through neural networks based algorithm had also been developed according to specified cases of controller and equipment structures. For example, neural network controller by inverse modeling for distillation plant (Chetouani, 2010) and modeling and control of a packed distillation column by using artificial neural networks (Conradie and Aldrich, 2010). Also, other modeling tools like radial basis function networks also emerges as effective modeling algorithm in estimating nonlinear parameters in expressions (Kennea *et al*., 2006).

Besides that, distillation column with different system was modeled by researchers using artificial neural networks, for instance, binary system of methanol-water separation modeling by multilayer feedforward neural networks (Yu and Yu, 2003). There are 2 hidden layers being applied while the modified backpropagation algorithm is used for networks training purpose. Steady state inverse modeling for neural networks controller generation was conducted by Zhang *et al*. (2007) on methanol-water binary system. The training data was obtained from the system dynamic simulation on both laboratory scale column and real industrial distillation column. In view of modeling on this heavy oil fractionator system using neural networks, the universal scientific studies are not sufficient to provide the detailed information on the generalized networks performance in terms of consistent accuracy, robustness and limitations or susceptibility (Nascimento *et al*., 2000).

The neuro simulation technique targets the establishment of a power symbiosis between hard computing and soft computing protocols (Ayala *et al*., 2007). In neuro simulation, hard computing techniques are couple with soft computing techniques for the development of powerful expert systems. Numerical models provide a precise and formal expertise at a significant computational expense that can be taught to a soft computing tool, once trained, can exploit and apply the learned expertise through much less intense computational work (Silva *et al*., 2000).

## NEURAL NETWORK ARCHITECTURE AND MODELING

Artificial intelligence works on the characteristic to mimic human thinking behaviors and learn from previous experiences or examples in order to make decisions or conclusions more precisely when resolving the problems. Meanwhile, neural networks exhibit satisfying compromise among high speed computation, robustness, adaptability and good filtering capability towards excessive noise and incomplete processing information (Ahmad and Zhang, 2006). Analogous with biological neural systems, neural networks are designated to comprise of a number of highly interconnected nodes or specifically named as information processing elements as illustrated in Fig. 1 (Ahmad *et al*., 2009). These nodes determine the specific characteristics of architectures but more importantly, it accomplish the model computation through high-speed signal transmission using digital computers. By capturing the neuron architecture and information processing in human brain, neural networks is developed with the combination of a number of closely interconnected nodes which responsible in information distribution and processing(Al-Alawi *et al*., 2008). The neural networks can be applied in varied forms with different in unique architecture and reason for usage. In fact, the neuron interaction in human brain is relatively complicated and invisible but this microscopic processing will later be exhibited as an identifiable or “macroscopic” behavior. This is because the output signal generated from the input stimulus will be transformed into some kind of corrective actions, for instance, opening or closing of

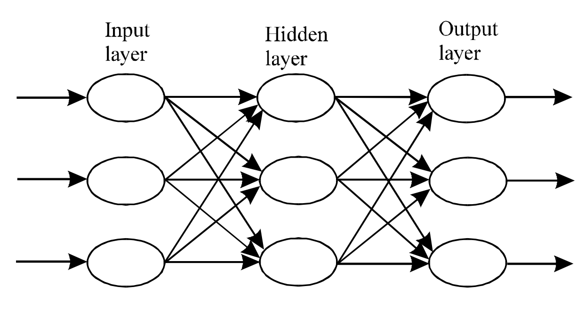


Fig. 1: General structure of neural networks

control valve. Artificial neural network is a physical cellular system, which can acquire, store and utilize experiential knowledge (Li and Liu, 2006).

The major procedures in conducting this modeling research are classified as input-output data generation, computational program creation and network performance optimization (Sharkey *et al*., 2000). For the actual analytical case, the system simulation is performed using Simulink, MATLAB which takes measurable or immeasurable factors into accounts for the sake of generating the adequately nonlinear yet approximate to industrial-based operating data. Concisely, there are 5 inputs components, comprising 3 manipulated inputs and 2 disturbance variables. For those 2 disturbances, one of it is measured disturbance while the other is unmeasured disturbance.

In particular, the scaled data will be distributed normally with the characteristic of zero mean and standard deviation (Silva *et al*., 2000). This step is especially imperative for the sake of handling order of magnitude differences among input variables where the network will tend to introduce the weight incommensurately to the input. As a result, the network will not be effective again since the magnitude of the variables is deviated significantly. Equally important, the data scaling is also prerequisite by virtue of the not self-regulating characteristic of activation function that is being applied on hidden layer. Explicitly, the limit of hyperbolic tangent sigmoid transfer function is ranged from lower constraint of-1 to upper value of 1. Consequently, the input variables which are larger than value of 5, for instance, 10 and 100, will ultimately be transformed as identical value of 1. The network will not be able to distinguish the differences between those two values and so the network prediction accuracy will be degraded (Baughman and Liu, 1995).

Also, a few parameters have been noticed to be influential and effective in improving the overall network performance which are known as number of hidden neurons, system dynamic order, random weight and also bias forwarded to hidden and output layer. Equally important, there is constantly 1 neuron in output layer while for input layer, the number of neurons is varied according to the dynamic order where first order implies 2 neurons and so forth. These 3 parameters will firstly be iterated for each output variable and the final parameter values will subsequently be applied for modeling to attain the most satisfied result.

Explicitly, the number of hidden of neurons is the amount of neurons in intermediate layer in performing information processing by 2 major algorithms of summation and activation (Adeloye and Munari, 2006; Ahmad and Zhang, 2006). From the MATLAB command for network training algorithm, the particular expressions for weights and bias are shown as follows:

$$w1 = p1 * (rand\,(nn, 4) - p2); \tag{1}$$

$$w2 = p1 * (rand\,(1, nn) - p2); \tag{2}$$

$$b1 = p1 * (rand\,(nn, 1) - p2); \tag{3}$$

$$b2 = p1 * (rand\,(1, 1) - p2); \tag{4}$$

where, p1 (parameter 1) and p2 (parameter 2) are constant, "nn" represents number of hidden neurons and * represent multiply.

## CASE STUDY

This research was carried out at School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia from December 2009 till July 2010. The detailed process descriptions and fundamental mechanistic models of this research are virtually procured from the literature authored by Maciejowski (2002). From Fig. 2, the product streams are divided into 3 parts which are from top, side and bottom of the fractionator. Next to this, there are 3 circulating loops (or reflux) located at the top, middle (known as intermediate reflux) and bottom of fractionator. The heat is originated from the gaseous feed stream while the reflux loops that act like heat exchanger will be responsible in removing certain amount of heat from the

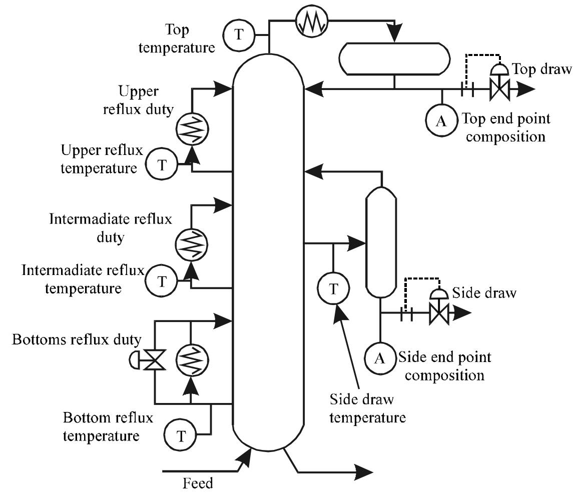


Fig. 2: Schematic diagram of "Shell" heavy oil fractionator (Maciejowski, 2002)

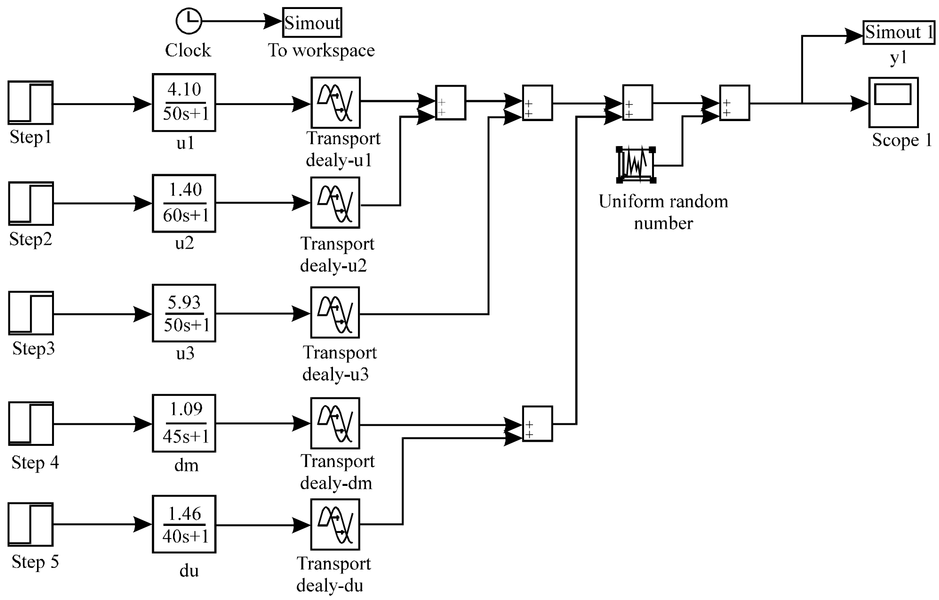


Fig. 3: Block diagram for combination of FOPTD system for real case simulation on generating top end point composition (y1) with the manipulation of top draw flow rate (u1)

Table 1: Relationships between Inputs and outputs in the form of transfer function

| Variables | $u_1$ | $u_2$ | $u_3$ |
|---|---|---|---|
| $y_1$ | $4.05\, e^{-27s} \frac{1}{50s+1}$ | $1.77\, e^{-28s} \frac{1}{60s+1}$ | $5.88\, e^{-27s} \frac{1}{50s+1}$ |
| $y_2$ | $5.39\, e^{-18s} \frac{1}{50s+1}$ | $5.72\, e^{-14s} \frac{1}{60s+1}$ | $6.90\, e^{-15s} \frac{1}{40s+1}$ |
| $y_3$ | $3.66\, e^{-2s} \frac{1}{9s+1}$ | $1.65\, e^{-20s} \frac{1}{30s+1}$ | $5.53\, e^{-2s} \frac{1}{40s+1}$ |
| $y_4$ | $5.92\, e^{-11s} \frac{1}{12s+1}$ | $2.54\, e^{-12s} \frac{1}{27s+1}$ | $8.10\, e^{-2s} \frac{1}{20s+1}$ |
| $y_5$ | $4.13\, e^{-5s} \frac{1}{8s+1}$ | $2.38\, e^{-7s} \frac{1}{19s+1}$ | $2.38\, e^{-7s} \frac{1}{19s+1}$ |
| $y_6$ | $4.06\, e^{-8s} \frac{1}{13s+1}$ | $4.18\, e^{-4s} \frac{1}{33s+1}$ | $6.53\, e^{-1s} \frac{1}{9s+1}$ |
| $y_7$ | $4.38\, e^{-20s} \frac{1}{33s+1}$ | $4.42\, e^{-22s} \frac{1}{44s+1}$ | $7.20 \frac{1}{19s+1}$ |

u1, u2, u3 are controlled input, y1, y2, y3, y4, y5, y6, y7 are controlled output

fractionator as a mean of heat recovery. This heat will subsequently be used for the other processes purposes like steam generation. Besides that, the heat removed from circulating loop is corresponding to the term "heat duty" where the small heat duty implies the small heat removed and large amount of heat being recirculated back into the fractionator. Nonetheless, there is a significant difference among those 3 circulating loops where the intermediate reflux loop is considered to be measured disturbance (ready for feed forward control) while upper reflux loop is unmeasured disturbance. The controlled loop at the bottom reflux loop is thereby known to be manipulated variable. In addition, the top and side product flow with the control valves are also known to be the manipulated variables. Thoroughly, from those 5 inputs, 3 of those are manipulated variables while the rest 2 are disturbances. The block diagram for combination of first order plus time delay system for real case simulation on generating top end point composition (y1) with the manipulation of top draw flow rate (u1) are shown in Fig. 3. From Fig. 3, the additional block in Simulink™ is used to sum the previous block together in other to connect to the next block.

The transfer function form the control inputs (manipulated variables) to all the outputs are shown in Table 1. Note that all the time constants and time delays are expressed in minutes. The transfer functions from the two disturbance inputs to the outputs are shown in Table 2. These tables show the nominal transfer functions. The gain in each transfer function is uncertain, the uncertainties associated with each input being

Table 2: Transfer functions from disturbances to outputs

| Variables | $d_m$ | $d_u$ |
|---|---|---|
| $y_1$ | $1.20\ e^{-27s}\ \frac{1}{45s+1}$ | $1.44\ e^{-27s}\ \frac{1}{40s+1}$ |
| $y_2$ | $1.52\ e^{-15s}\ \frac{1}{25s+1}$ | $1.83\ e^{-15s}\ \frac{1}{20s+1}$ |
| $y_3$ | $1.16\ \frac{1}{11s+1}$ | $1.27\ \frac{1}{6s+1}$ |
| $y_4$ | $1.73\ \frac{1}{5s+1}$ | $1.79\ \frac{1}{19s+1}$ |
| $y_5$ | $1.31\ \frac{1}{2s+1}$ | $1.26\ \frac{1}{22s+1}$ |
| $y_6$ | $1.19\ \frac{1}{19s+1}$ | $1.17\ \frac{1}{24s+1}$ |
| $y_7$ | $1.14\ \frac{1}{27s+1}$ | $1.26\ \frac{1}{32s+1}$ |

Dm is measured disturbance, du is unmeasured disturbance

Table 3: Extent of gain uncertainty in each transfer functions

| Variables | $u_1$ | $u_2$ | $u_3$ | $d_m$ | $d_u$ |
|---|---|---|---|---|---|
| $y_1$ | $4.05\pm2.11\delta_1$ | $1.77\pm0.39\delta_2$ | $5.88\pm0.59\delta_3$ | $1.20\pm0.12\delta_4$ | $1.44\pm0.16\delta_5$ |
| $y_2$ | $5.39\pm3.29\delta_1$ | $5.72\pm0.57\delta_2$ | $6.90\pm0.89\delta_3$ | $1.52\pm0.13\delta_4$ | $1.83\pm0.13\delta_5$ |
| $y_3$ | $3.66\pm2.29\delta_1$ | $1.65\pm0.35\delta_2$ | $5.53\pm0.67\delta_3$ | $1.16\pm0.08\delta_4$ | $1.27\pm0.08\delta_5$ |
| $y_4$ | $5.92\pm2.34\delta_1$ | $2.54\pm0.24\delta_2$ | $8.10\pm0.32\delta_3$ | $1.73\pm0.02\delta_4$ | $1.79\pm0.04\delta_5$ |
| $y_5$ | $4.13\pm1.71\delta_1$ | $2.38\pm0.93\delta_2$ | $6.23\pm0.30\delta_3$ | $1.31\pm0.03\delta_4$ | $1.26\pm0.02\delta_5$ |
| $y_6$ | $4.06\pm2.39\delta_1$ | $4.18\pm0.35\delta_2$ | $6.53\pm0.72\delta_3$ | $1.19\pm0.08\delta_4$ | $1.17\pm0.01\delta_5$ |
| $y_7$ | $4.38\pm3.11\delta_1$ | $4.42\pm0.73\delta_2$ | $7.20\pm1.33\delta_3$ | $1.14\pm0.18\delta_4$ | $1.26\pm0.18\delta_5$ |

$|\delta_j|\leq 1$ for each j, $\delta_j$ is process gain

correlated with each other. Table 3 specifies the uncertainty in each gain. The nominal model is obtained when $\delta j = 0$ for each j; but it is assumed that each $\delta j$ can vary in the range $-1 \leq \delta \leq$.

## RESULTS AND DISCUSSION

The network prediction accuracy and robustness are assessed though mathematical error analysis to which sum-squared error, residual error and coefficient correlation between the predicted and actual data is computed. Random noise, disturbances and gain uncertainties have been associated to the generated data to create system complexity and similarity to real industrial data. There are 7 operational outputs being simulated and studied with the manipulation of one or multiple input but only the most imperative component of top end point composition is taken as the subject of discussion in this session.

**Perfect case and high noise-influencing system modeling:** The perfect case is defined as the system being simulated under the condition where disturbances and others uncertainty is absent. Under this circumstance, the output curve will be a smoothly proportional curve with the steady state value resulted directly from the step change and process gain. Instead, high noise-influencing system is associated by the large and unpredicted noise measurement with the introduction of disturbances and gain uncertainties at the same time so that the system will be increasingly nonlinear to be predicted. Virtually, the function of noise is to generate nonlinear response curve instead behaves as real noise since the magnitude of noise will generally not be so significant.

**Perfect case with the absence of process disturbances and gain uncertainties:** The system being considered here is single-input single-output (SISO) system with only top draw flow rate manipulated for output top end point composition. The network dynamics from first to third order is simulated where only the pairing which results in least training and testing sum squared error is selected as the final model. In the absence of disturbance, measurement noise and gain uncertainties, the simulated output response is appearing in smooth curve up to a steady state value as it is named as perfect case.

In here, the analysis on the network performance is conducted for the sake of investigating the network ability in handling perfect response albeit it will not exist in real case. Furthermore, the utmost limit of the network is identified so that the network capability can be clarified in view of the comparison for the actual network performance in the rest cases. From Table 4, the pairing with its simulated result for all of 3 network dynamic orders are shown while third order dynamics is ultimately

Table 4: Summary on neural network parameter values for top end point composition (y1) with the manipulation of top draw flow rate (u1) in perfect case

| Component | System dynamic order First | Second | Third |
|---|---|---|---|
| No. of hidden neuron | 2.0 | 10.0 | 9.0 |
| Parameter 1 | 0.1 | 0.4 | 0.4 |
| Parameter 2 | 0.1 | 0.3 | 0.4 |
| Residual error | 11.5828 | 5.6787 | 4.6223 |
| Correlation coefficient | 0.9533 | 0.9902 | 0.9930 |
| Validation SSE | 9.8225 | 1.9913 | 1.3133 |

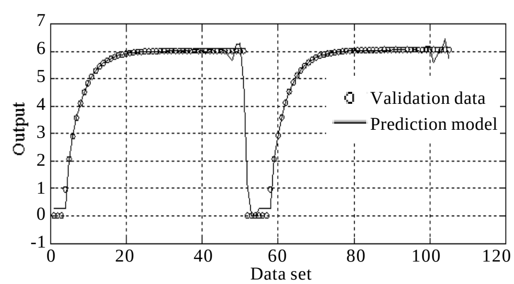


Fig. 4: Neural network validation performance for top end point composition (y1) with manipulation of top draw flow rate (u1) in perfect case

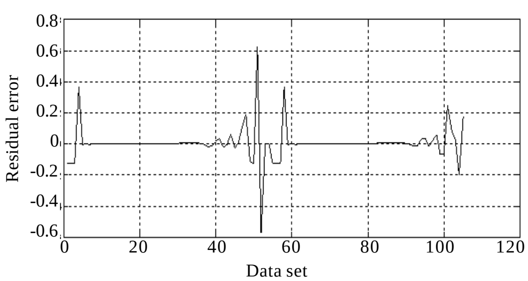


Fig. 5: Residual between actual and predicted validation data for top end point composition (y1) with manipulation of top draw flow rate (u1) in perfect case

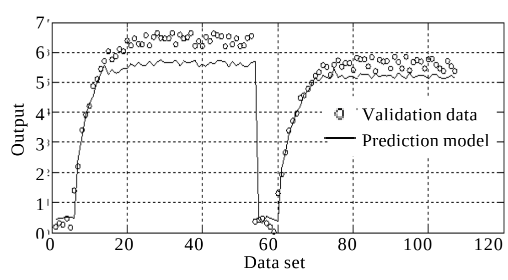


Fig. 6: Neural network validation performance for top end point composition (y1) with manipulation of top draw flow rate (u1) and measurement noise of 0.5

chosen as the neural network model because of the minimum training and testing sum squared error.

As illustrated from Fig. 4, the neural network prediction model along the delay, immediate response and steady state part closely links the actual validation data. In addition, this third order dynamics network has inflicted in slight oscillation at the end of the steady state portion while the other part has been accurately predicted by the network with the associated error near to zero. From the mathematical error analysis, the validation residual error and sum squared error has been greatly reduced to unusually low values and denoted as 4.6223 and 1.3133, respectively. When the overall system error is considered as displayed in Fig. 5, the residual error on system transition is less than 0.6 while the error on system lag is lower than 0.4 and hence the network is stated to be able to capture the system transition well in view of the insignificant deviation.

**Nonlinear system with the introduction of elevated measurement noise:** The analysis is conducted on the top end point composition based on the manipulation of solely to draw flow rate but with elevated measurement noise, which is 0.5 and 1.0 instead of 0.1 as being applied previously. The network validation performance is shown in Fig. 6 with the validation data which in nonlinear trend at steady state part is not accurately captured by the network. Owing to the influence of increased measurement noise in causing high nonlinearity of the response, the associated error inflicted from network prediction is found to be relatively great with its mathematical values tabulated in Table 5. The degree of oscillation particularly at steady state portion is appreciable while the generalized neural network model in first order dynamics and 11 hidden neurons still unable to predict the changing trend and delay of the nonlinear dynamics with the obvious deviation of around 1.0 unit. The network performance on the second step change is slightly improved closer proximity between data and model.

Basically, the comparison is also made on the case with measurement noise of 0.1 which is tabulated in Table 5, to study the effect of dynamic nonlinearity to the ability of network prediction. From the Table 5, the residual error and validation sum squared error from measurement noise of 0.1 to 0.5 has been increased at least 400% while the correlation coefficient is only decreased from 0.9653 to 0.9424. From Fig. 7, the effect of random noise that causes nonlinearity is truly significant in view of the great increment in prediction associated error. In addition, the major error contributor still falls on the system transition error which accounts for approximately 3.0 while the

Table 5: Summary on neural network parameter values for top end point composition (y1) with the manipulation of top draw flow rate (u1) in elevated measurement noise

| | Measurement noise | | |
|---|---|---|---|
| Component | 0.1 | 0.5 | 1.0 |
| No. of hidden neuron | 5.0 | 11 | 9.0 |
| Parameter 1 | 0.4 | 0.5 | 0.2 |
| Parameter 2 | 0.2 | 0.4 | 0.3 |
| Dynamic order | Second | First | Second |
| Residual error | 8.7129 | 34.4599 | 36.3546 |
| Correlation coefficient | 0.9653 | 0.9424 | 0.9214 |
| Validation SSE | 5.2260 | 23.4533 | 26.7449 |

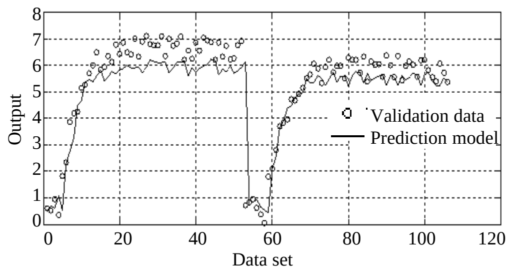


Fig. 7: Neural network validation performance for top end point composition (y1) with manipulation of top draw flow rate (u1) and measurement noise of 1.0

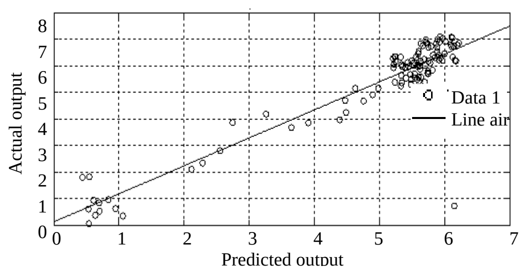


Fig. 8: Proportionality between actual and predicted validation data for top end point composition (y1) with manipulation of top draw flow rate (u1) and measurement noise of 1.0

accumulation of slight error on other portion ends up with the final sum squared error of 24.4533.

From Table 5, the system that associated with measurement noise of 1.0, the prediction error is noticed to be expectedly greater where the validation sum squared error and total residual error are computed as 26.7449 and 36.3546, respectively. Hence, it can be stated that the network prediction performance in this case is the worst among all of other cases. But, according to the error increment from measurement noise of 0.5 to 1.0, it is also perceived that the increased error is not as significant as from measurement noise of 0.1 to 0.5.

In here, a conclusion could be made where the neural network would tend to customize in highly nonlinear system where the prediction error would not exponentially increase with the magnitude of random noise. With increasingly high random noise, the network prediction error will be gradually increased instead of rapidly changed since the neural network start to depict its ability in handling complex and nonlinear system dynamics. When the linearity between validation and predicted data is analyzed as shown in Fig. 8, the generated correlation coefficient is decreased to 0.9214 where the data point is deviated within acceptable distance from the generalized straight line.

## MULTIPLE-INPUT SINGLE-OUTPUT (MISO) DYNAMIC MODELING

For previous analysis, the network output simulation is performed with only 1 manipulated variable being altered in step change basis. In order to further assess the network performance, there are 3 manipulated variables introduced simultaneously with it known to the network during the training and testing phase instead of being veiled. In addition, the network is examined in 2 stringent conditions where the step time is fixed and varied.

**Step change simulation on constant step time amongst manipulated variables:** On this case, the step changes for 3 manipulated variables are introduced simultaneously at the same and constant step time of 1. As for comparison with the previous case of top end point composition, this analysis is aimed to investigate the ability of the network in handling multiple input systems. In this juncture, each mentioned input is actually linked to different process function with gain uncertainties, which directly increase the sophistication of the system. In addition, there are only 3 controllable outputs are being modeled, namely top end point composition, side end point composition and bottoms reflux temperature, by virtue of its significance in this distillation system. The network will be simulated from first to third dynamic order whilst the optimum condition will be chosen to form the network model. From Table 6, first order dynamic with 4 hidden neurons is selected by virtue of its capability in inducing lowest training and testing sum squared error if compared with second and third order dynamics.

As noticed from similar Table, the third order dynamic system, which able to result in lower validation error may not necessarily well trained, as it is not applied as the model in this case. From the Fig. 9, the network seems capable in capturing the system delay well but the problem arisen on the steady state portion where the deviation is obvious. The discrepancy on the second

Table 6: Summary on neural network parameter values for top end point composition (y1) in multiple input system with constant step time

| Component | First order | Second order | Third order |
|---|---|---|---|
| No. of hidden neuron | 4.0 | 3.0 | 2.0 |
| Parameter 1 | 0.3 | 0.2 | 0.3 |
| Parameter 2 | 0.1 | 0.1 | 0.1 |
| Residual Error | 20.2480 | 27.8946 | 15.0118 |
| Correlation coefficient | 0.9514 | 0.9088 | 0.9517 |
| Validation SSE | 11.5029 | 20.6646 | 9.0918 |

Table 7: Summary on neural network parameter values for multiple input systems with constant step time

| Component | y1 | y2 | y7 |
|---|---|---|---|
| No. of hidden neuron | 4.0 | 3.0 | 3.0 |
| Parameter 1 | 0.3 | 0.3 | 0.3 |
| Parameter 2 | 0.1 | 0.4 | 0.3 |
| Dynamic order | First | Third | Third |
| Residual error | 20.2480 | 9.5644 | 14.0662 |
| Correlation coefficient | 0.9514 | 0.9515 | 0.9489 |
| Validation SSE | 11.5029 | 6.5825 | 9.3581 |

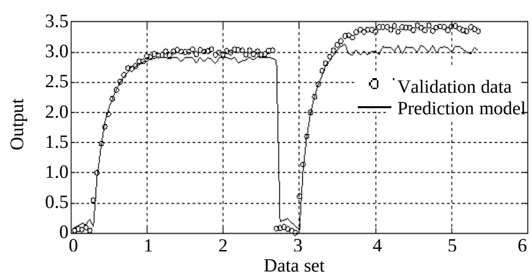


Fig. 9: Neural network validation performance for top end point composition (y1) in multiple input system with constant step time

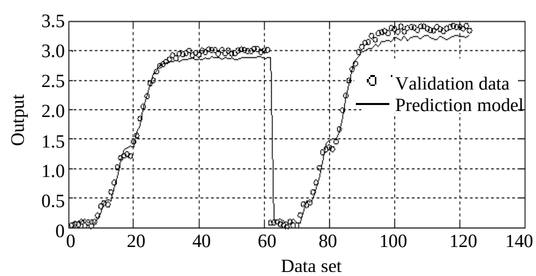


Fig. 10: Neural network validation performance for top end point composition (y1) in multiple input system with varied step time

step change is somewhat significant as this degraded accuracy would directly influence the whole process control performance and effectiveness.

The ability of the network in capturing the MISO system for side end point composition is analyzed and the network performance is found to be satisfying with the close matching between the data and model. The network is noticed to be able to handle multiple input systems properly as the computational effort is increased with the complexity of the system. In particular, this network is trained in third order dynamics with 3 neurons embedded in hidden layer while the performance is superior to the previous case.

With the tabulated result in Table 7 the network performance is noted to be satisfying with the moderate validation sum squared error generated albeit the case for top draw flow rate depicts slightly higher error. For these 3 cases, the parameter 1 is at constant value of 0.3 whilst the number of hidden neurons is not found to be as high as more than 10. Virtually, the relationship between these parameters and network performance is still elusive to be interpreted while for this moment, iteration among these parameters would serve to be a simple yet direct approach in procuring the optimum model.

**Step change simulation on varied step time amongst manipulated variables:** After the network is proven to be capable in handling multiple input systems with 3 input variables being manipulated simultaneously, the analysis is advanced with the step time for manipulated changed. In here, the step time for u1, u2 and u3 have been varied to 10, 50 and 100 respectively instead of at time of 1 as previously. Consequently, the difficulty for the network to apprehend and predict the system dynamics will be elevated as the effect of step change of different manipulated variable may create confusion to the network. As illustrated in Fig. 10, the effect of the manipulated variables with different step time is depicted along the immediate response curve where the stage-liked curve is formed.

Nonetheless, the network still able to predict the extent to which the dynamics will be disturbed by the manipulated variables. This prominent performance is not persisting on the steady state part where the slight deviation still can be perceived obviously. However, the computed result is fairly satisfying where the validation sum squared error accounts for 7.9774 while the total residual error is 14.1813. In addition, the linearity between actual validation data and prediction model is high where the correlation coefficient amounts to 0.9759 while this figure implies great capability of the network in handling this MISO system.

For the second controlled output of side end point composition (y2), the changing trend of the curve along the immediate response is even more remarked because the manipulation is performed abruptly in appreciable magnitude of step change. In this case, the network performance is good since the close fitting between the data and the model is attained with only small deviation is observed. Mathematically, this second order dynamics network with 4 hidden neurons is associated with 5.9661 as validation sum squared error.

Table 8: Summary on neural network parameter values for multiple-input single-output (MISO) systems with varied step time

| Component | y1 | y2 | y7 |
|---|---|---|---|
| No. of hidden neuron | 3.0 | 4.0 | 7.0 |
| Parameter 1 | 0.4 | 0.3 | 0.2 |
| Parameter 2 | 0.5 | 0.2 | 0.2 |
| Dynamic order | First | Second | Second |
| Residual error | 14.1813 | 10.4754 | 13.9777 |
| Correlation coefficient | 0.9759 | 0.9749 | 0.9643 |
| Validation SSE | 7.9774 | 5.9661 | 6.8569 |

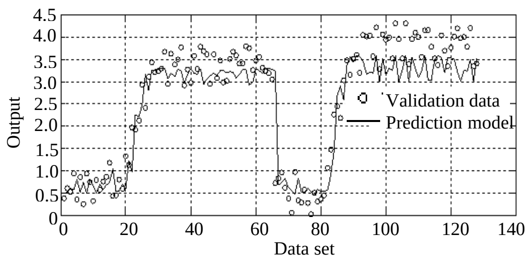


Fig. 11: Neural network validation performance for top end point composition (y1) in highly uncertain system

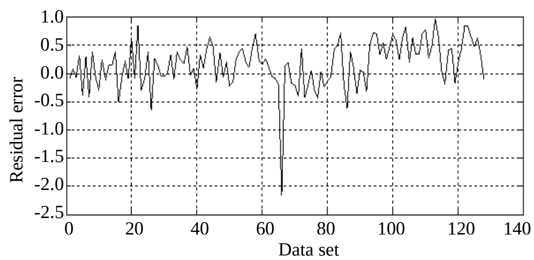


Fig. 12: Residual between actual and predicted validation data for multiple-input single-output system for top end point composition (y1) in highly uncertain system.

The second order dynamics network is again proven to be useful in predicting MISO system for bottoms reflux temperature.

In addition, the prediction for the first step change is not noted to be sufficiently excellent when the model fails to precisely fit the data points. However, the discrepancy is still acceptable and the model could closely capture the second step change with unnoticeable error.

From the summary as tabulated in Table 8, the network performance is fairly well in all of the 3 controlled outputs with the validation sum squared error less than 10.0 and correlation coefficient greater than 0.96. The chosen parameter values, for instance number of hidden neurons and network dynamics order, are moderate in value instead of exceedingly high.

**Network prediction on highly uncertain system:** From previous analysis, it is perceived that the extent of random noise would substantially influence the network performance whilst the network is capable in capturing the dynamics for MISO system even if the manipulated variables are introduced separately. In combining all of those features to the dynamics of top end point composition, the network ability is examined and this analysis is important since the actual dynamics of composition in real distillation column might most probably elusive and complicated.

In this case, the random noise being introduced ranges from 0 to 1.0 while the step time is applied randomly from 0 to 50 min. Previously, there are 8 uncertainties exist in this system which encompass 5 process gain uncertainties, 2 disturbance variables and 1 random measurement noise. But in this system, another 3 uncertainties will be added, which are the 3 unpredictable step time for manipulated variables. Under this circumstance, the network is assessed on its performance in handling this inherently complex system to where it might happen in real application of distillation operation. As shown in Fig. 11, the validation data itself are scattered in an unusual yet highly oscillated trend and the prediction model fits it roughly in nonlinear manner. The network prediction on the second step change is somewhat worse than the former as the model is slightly lower than the actual data and approximately 0.5 is deviated.

The network performance is deemed to be acceptable especially in handling the system with high level of uncertainties to which the trend is intractable with possibly large deviation from one point to another. The prediction model is observed to be maintaining and oscillating within the scattered points in capturing the data trend. In this case, the first order dynamics network with 4 hidden neurons is chosen as the best-trained neural network model for this nonlinear system. As summarized from Table 6, the validation sum squared error for first order dynamics network is rather the greatest than second and third order dynamics albeit it's training and testing performance are outperforming to the latter. Instead, third order dynamics network can validate better than first order system with validation error as 19.1375 and however, this is deemed to be taken place coincidentally since the reference on training and testing performance is more reliable. The changing trend of model on steady state portion, which is sufficiently stable, and without unduly oscillation has exhibited its robustness in capturing the system dynamics.

Explicitly, the validation error is computed as 24.6629 while the total residual error is 43.6760 as elucidated in Table 9 and Fig. 12. Figure 12 clearly imply that the network performance is not as good as previous cases but

Table 9: Summary on neural network parameter values for multiple-input single-output (MISO) systems of top end point composition (y1) in highly uncertain system

| Component | First order | Second order | Third order |
|---|---|---|---|
| No. of hidden neuron | 4.0 | 11 | 5.0 |
| Parameter 1 | 0.5 | 0.1 | 0.2 |
| Parameter 2 | 0.3 | 0.2 | 0.2 |
| Residual error | 43.6760 | 39.2548 | 37.1705 |
| Correlation coefficient | 0.9428 | 0.9493 | 0.9451 |
| Validation SSE | 24.6629 | 20.5796 | 19.1375 |

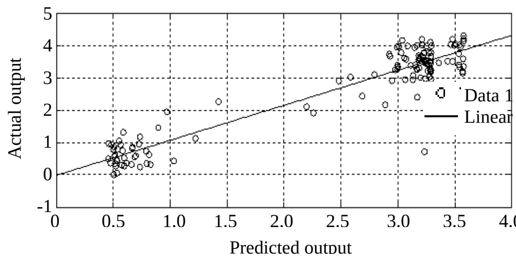


Fig. 13: Proportionality between actual and predicted validation data for multiple-input single-output system for top end point composition (y1) in highly uncertain system

it still reliable in predicting the system dynamics since the model virtually tends to fit into the nonlinearly scattered data points. This is proven by the linearity analysis where the correlation coefficient is sufficiently high and acquired as 0.9428 as illustrated in Fig. 13. In here, this single layer neural network with the simplest processing architecture starts showing its incapability in highly uncertain case. Multiple neural networks with more complicated algorithm would be suggested to improve the network prediction accuracy and robustness.

The overall result is quite similar in terms of trending and also the behavior of the predicted output as what been explained in the research from Meneguelo *et al.* (2009), Chen *et al.* (2004), Ali *et al.* (2008) and Georgieva *et al.* (2007). It is clearly shown that the neural network modeling was able to capture the dynamics of the highly nonlinear system even though it is in high uncertainty scenario.

## CONCLUSION

For the network modeling on single-input single-output (SISO) system, the network performance is moderately satisfying since the prediction model shows ability to capture the immediate step change response but poses pitfall on steady state prediction. The assessment analysis should focus on one validation step change since the system transition and delay error would substantially create confusion on the real prediction error. From the performance optimization via parameter iteration method, it is hypothesized that those influential parameters are intimately tied to the specified system dynamics. The overall neural network performance for the cases such as SISO system, perfect case, high noise-influencing system, MISO system and uncertain system, are fairly satisfying where the network able to capture the nonlinearity and complexity of the system. The trained single layer neural network is good in learning and predicting even with the presence of disturbances and process gain uncertainties. This network is also perceived to be sensitive towards the magnitude of random noise which inflicts significant nonlinearity to the system dynamics and the associated prediction error is known to be proportional to the extent of random noise. The network will always customize itself in nonlinear system and shows its ability in understanding the complex system dynamics with great learning efficiency.

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