Osuolale FN, Zhang J.

[Energy efficiency optimisation for distillation column using artificial neural network models.](#)

Energy 2016, 106, 562-578.

Copyright:

© 2016. This manuscript version is made available under the [CC-BY-NC-ND 4.0 license](#)

DOI link to article:

<http://dx.doi.org/10.1016/j.energy.2016.03.051>

Date deposited:

18/03/2016

Embargo release date:

12 April 2017

This work is licensed under a

[Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International licence](#)

Energy Efficiency Optimisation for Distillation Column Using Artificial Neural Network Models

Funmilayo N. Osuolale, Jie Zhang^{*}

School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, UK

e-mail: f.n.osuolale@ncl.ac.uk or funmikorede@yahoo.com; jie.zhang@newcastle.ac.uk

Abstract

This paper presents a neural network based strategy for the modelling and optimisation of energy efficiency in distillation columns incorporating the second law of thermodynamics. Real-time optimisation of distillation columns based on mechanistic models is often infeasible due to the effort in model development and the large computation effort associated with mechanistic model computation. This issue can be addressed by using neural network models which can be quickly developed from process operation data. The computation time in neural network model evaluation is very short making them ideal for real-time optimisation. Bootstrap aggregated neural networks are used in this study for enhanced model accuracy and reliability. Aspen HYSYS is used for the simulation of the distillation systems. Neural network models for exergy efficiency and product compositions are developed from simulated process operation data and are used to maximise exergy efficiency while satisfying products qualities constraints. Applications to binary systems of methanol-water and benzene-toluene separations culminate in a reduction of utility consumption of 8.2% and 28.2% respectively. Application to multi-component separation columns also demonstrate the effectiveness of the proposed method with a 32.4% improvement in the exergy efficiency.

Keywords: Bootstrap aggregated neural network, exergy, modelling, optimisation

1 Introduction

The importance of distillation columns continues to increase both in the traditional petro-chemical industry and in the sustainable sector with renewable resources and energy. The key role they play in the chemical and petrochemical industries and the quest to make them more energy efficient has made distillation processes high priority for all stake holders in the industries. Distillation unit poses a great challenge to process and control engineers because of its complexity. It comes in varieties of configurations with different operating objectives, significant interactions among the control loops and specialised constraints [1]. Usually the order of economic importance in the control and optimisation of

^{*} Corresponding author

distillation columns is product quality, process throughput and utility reductions and often traded off between them has to be made.

Optimisation of distillation column operations is essential in order to achieve energy efficiency while meeting product quality constraints. Optimisation is a major quantitative tool in decision making for the process industries. Rather than large scale expansion, most industries will maximise available resources for maximum profitability. Optimisation of distillation columns requires accurate process models. A number of distillation process models are available in the published literatures [2] but the complexity of distillation processes has led to a number of assumptions that might limit the universality of the models [3]. Most of the mechanistic models of distillation systems have assumed equilibrium cases for the stages. Such models deviate from the reality and will not give a true representation. To overcome this, non-equilibrium stages are assumed [4]. Non-equilibrium models however involve large number of variables, leading to distillation models with differential equations that may exhibit high differential index that could generate stiff dynamics. The development of such mechanistic models is generally very effort demanding as they involve a large number of differential and algebraic equations and a large number of model parameters. Furthermore, the solutions and calculations of such mechanistic models are computationally demanding making them not suitable for real-time optimisation. To overcome these problems, data driven models such as artificial neural network (ANN) models can be utilised [5]. ANN has been recognised as a powerful tool that can facilitate the effective development of data-driven models for highly nonlinear and multivariable systems [6]. ANN can learn complex functional relations for a system from the input and output data of the system. Furthermore, their evaluation is much less computationally demanding making them suitable for real-time optimisation.

Most neural network applications to distillation systems target at modelling the product specification as the model output [7]. Neural network has been applied to the simple cases of binary systems [8] and sometimes targeted at inferential composition control [9] and model predictive control of the column [10]. In some related works, applications to the control of multi-component systems are presented for traditional column [11] and for dividing wall column [12]. Economic objective in terms of profitability is often the focus in the optimisation of such distillation processes [13]. However, with the issues of global warming, greenhouse gas effects, and depleting fossil energy resources, the issue of energy efficiency of distillation processes has been brought to the limelight. The need therefore arise to focus on energy efficiency of the column especially focusing on second law of thermodynamics (exergy analysis) in lieu of first law of thermodynamics. Application of thermodynamics for process energy improvement especially in terms of pinch analysis has been widely reported [14]. However, pinch analysis is restricted to analysing for minimum utility consumption and or minimum number of heating units for heat exchange equipments. Exergy analysis overcomes this restriction and encompasses the

total energy systems in processes. This work attempts to model the exergy efficiency of distillation column using ANN. Previously ANN has been used to model distillation column, but there is a need for robust and accurate model to represent the column within an optimisation frame work irrespective of the complexities of the column. Bootstrap aggregated neural network is introduced in this study to improve the prediction accuracy and reliability of the model. The model is then used for the optimisation of exergy efficiency of the distillation column to reduce the energy consumption while satisfying product quality specifications. Past studies on the exergy analysis of distillation column has been limited to pinpointing and quantifying sources of inefficiencies in the column [15]. A further step away from the usual is to use exergy analysis as a retrofit tool to present several practical options for process energy improvement rather than as an analytical tool. This study develops an optimisation based methodology incorporating exergy analysis for improving the energy efficiency of the column.

Quite a number of publications have been on ways to reduce the energy consumption of distillation processes via alternate energy efficient arrangement. Of note amongst these are the heat integrated distillation column (HIDC) [16], thermally coupled dividing wall column, petyluk column and intensified distillation column [17]. In addition, previous works on the thermodynamic efficiency of the crude distillation unit revealed a high energy and exergy loss of the column [18] with the overall efficiency of the column ranging from 5-23% [19]. This shows that there is a lot of room for improvement of the distillation column and indicates that a high entropy generation within column is making the irreversibility of the column to be highly significant. In the past, there had been efforts at devising methods of minimising entropy production rate in distillation columns, one of such attempt was targeted at diabatic binary distillation systems [20]. Also most often, distillation columns are optimised in terms of energy usage without paying particular attention to the reduction of entropy generation within the column [21]. There is therefore a strong need to focus on reducing column's irreversibility by applying the second law of thermodynamics in column efficiency improvement.

In this work an attempt is made at improving the energy efficiency of distillation columns using the tool of applied thermodynamics to determine the optimum operating conditions of the column with consideration to energy efficiency and product quality. The energy efficiency is however on the basis of reduction in the irreversibility of the column. Exergy analysis and optimisation are the major qualitative and quantitative tools that are used in the decision making. In order to overcome the difficulties in developing detailed mechanistic models for exergy efficiency calculation and using such models in on-line optimisation, this paper proposes using neural networks to model exergy efficiency in distillation columns from process operational data. The neural network models can be developed quickly as long as process operational data are available and can be used effectively in real-time optimisation. This work extends and modifies ANN model using bootstrap aggregated neural networks to enhance model prediction accuracy and reliability.

The paper is structured as follows. Section 2 presents the second law analysis of distillation columns. Neural network modelling of exergy efficiency is presented in Section 3. Applications of neural network modelling and optimisation of exergy efficiency to binary and multi-component systems are presented in Sections 4 and 5 respectively. Finally Section 6 gives the conclusions.

2 Thermodynamic Analysis

Exergy is from a combination of the 1st and 2nd laws of thermodynamics. It is a key aspect of providing better understanding of the process and quantifying sources of inefficiency and distinguishing quality of energy used [22]. Exergy analysis is a measure of the quality of energy. It is a tool for determining how energy efficient a process is. Exergy analysis of processes gives insights into the overall energy usage evaluation of the process, potentials for efficient energy usage of such processes can then be identified and energy usage improving measures of the processes can be suggested.

The basis of the exergy concept was laid almost a century ago and was introduced as a tool for process analysis in the 1950s by Keenan and Rant. Szargut [23] introduced the concept of chemical exergy and its associated reference states. It is common to use ambient pressure and temperature as $P_0 = 101.325$ kPa and $T_0 = 298.15$ K.

The total exergy of a stream is calculated as

$$Ex_{total} = Ex_{phy} + Ex_{chem} \quad (1)$$

where Ex_{chem} and Ex_{phy} are the chemical and physical exergy respectively.

For a multi-component system, the chemical and physical exergy are calculated as follows.

$$Ex_{chem} = m(h_0 - \sum z_i \bar{h}_{0i} - T_0(s_0 - \sum z_i \bar{s}_{0i})) \quad (2)$$

$$Ex_{phy} = m(h - h_0 - T_0(s - s_0)) \quad (3)$$

where z_i is the mole fraction of the i th component, $\bar{h}_{0i}$ and $\bar{s}_{0i}$ are the partial specific enthalpy and entropy of the component at the reference condition respectively, h is the specific enthalpy, s is the

specific entropy, T_0 is the reference temperature, h_0 and s_0 are specific enthalpy and entropy measured at the reference conditions respectively.

The chemical exergy for a binary and non-reactive distillation system is assumed to be negligible. For a heat source such as the reboiler, the work equivalent of the heat source is calculated as [24]

$$W_Z = \int_{initial}^{final} \left(1 - \frac{T_0}{T_Z}\right) \partial Q_Z \quad (4)$$

where ∂Q_Z is an incremental heat transfer at absolute temperature T_Z and the integral is from initial state to final state.

If the temperature of the heat source is constant, the work equivalent of heat is given by [24]

$$W_Z = Q_Z \left(1 - \frac{T_0}{T_Z}\right) \quad (5)$$

Every real process has an element of irreversibility. Exergy analysis aims at minimising the irreversibility by pinpointing the location of actual losses in processes and the magnitude of the losses. The total exergy balance of the distillation column is

$$\sum Ex_{in} = \sum Ex_{out} + I \quad (6)$$

where $\sum Ex_{in}$ is the total exergy in to the system, $\sum Ex_{out}$ is the total exergy out of the system and I is the quantified irreversibility of the system.

For a typical binary distillation system as shown in Fig. 1, [25]

$$\sum Ex_{in} = Ex_{feed} + Ex_{boilup} \quad (7)$$

$$\sum Ex_{out} = Ex_{distillate} + Ex_{bottoms} + Ex_{condenser} \quad (8)$$

Essentially for a distillation column, Eq(7) and Eq(8) hold except to account for additional streams that may be included due to the nature of the column. For instance, in the case of a multi-component system with multiple feeds and side strippers, the feeds are included in the exergy in and the side strippers are considered in the exergy out.

From Eq(6), the irreversibility of the system is calculated as:

$$I = \sum Ex_{in} - \sum Ex_{out} \quad (9)$$

Efficiency of the system is then given as

$$\varphi = \frac{\sum Ex_{out}}{\sum Ex_{in}} \quad (10)$$

Figure 1: A typical binary distillation column with the in and out streams and the exergy analysis boundary

3 Modelling of Exergy Efficiency

3.1 Artificial neural network modelling

Mechanistic models have been traditionally used in the past for control and optimisation studies. However developing mechanistic models for complex processes especially to incorporate the second

law energy efficiency could be very difficult and time consuming. These difficulties can be readily circumvented by developing neural network models from plant operational data. Neural network models have been proved to be capable of approximating any continuous non-linear functions. Here neural networks are used to model exergy efficiency and product compositions in distillation columns. The neural networks models are then used for exergy efficiency optimisation subject to product quality constraints. In this study, data for neural network modelling are generated from simulation, which is supposed to represent a real distillation column. For practical applications of the proposed method, distillation column operational operation data can be used. The neural network model for exergy efficiency is of the following form:

$$\varphi = f(x_1, x_2, x_3 \dots x_k) \quad (11)$$

where φ is exergy efficiency, x_1 and x_2 are feed rate and feed temperature respectively, while x_3 to x_k are the most volatile composition in each of the outlet stream. Neural network models for the product compositions use the same model inputs. Single hidden layer feed forward neural networks are used to model exergy efficiency and product compositions. The quality of the neural network is dependent on the training data and the training method [26]. The data were divided into training data (50%), testing data (30%), and unseen validation data (20%). The training data is used for network training and the testing data is used for network structure selection (number of hidden neurons) and “early stopping” in network training. With the “early stopping” mechanism, neural network prediction errors on the testing data are continuously monitored during training and training is terminated when the prediction errors on the testing data do not further reduce. A number of networks with different number of hidden neurons are trained and the one giving the lowest sum of squared errors (SSE) on the testing data is considered as having the appropriate number of hidden neurons. The final developed neural network model is evaluated on the unseen validation data. The data for the network training, validation and testing were scaled to the range [-1, 1] because of the different magnitudes of the model inputs and outputs. Levenberg-Marquardt training algorithm is used to train the networks. For the purpose of comparison, linear models are also built using partial least square (PLS) regression.

However, conventional neural networks can lack generalisation capability when applied to unseen data due to over-fitting of noise in the data [27]. The objective in neural network modelling is to build a network which can generalise and not to build a network which simply memorise the training data. Several techniques have been reported for the enhancement of neural network model generalisation capability such as Bayesian learning, regularisation, training with dynamic and static process data, early stopping and combining multiple networks, and bootstrap aggregated neural networks [28].

3.2 Bootstrap aggregated neural network

When building neural network models from the same data set, there is possibility that different networks perform well in different regions of the input space. Hence, prediction accuracy on the entire input space could be improved when multiple neural networks are combined. In a bootstrap aggregated neural network model, several neural network models are developed to model the same relationship. Individual neural network models are developed from bootstrap re-sampling replications of the original training data. Instead of selecting a single neural work that is considered to be the “best”, several networks are combined together to improve model accuracy and robustness. These models can be developed on different parts of the data set. A diagram of a bootstrap aggregated neural network is shown in Fig. 2.

A bootstrap aggregated neural network can be represented mathematically as

$$f(X) = \sum_{i=1}^n w_i f_i(X) \quad (12)$$

where $f(X)$ is the aggregated neural network predictor, $f_i(X)$ is the i th neural network, w_i is the aggregating weight for combining the i th predicted neural network, n is the number of neural networks and X is a vector of neural network inputs. The overall output of bootstrap aggregated network is a combination of the weighted individual neural network output.

Figure 2: A bootstrap aggregated neural network

The bootstrap aggregated neural network can also be used to calculate model prediction confidence bounds from individual network predictions [26]. The standard error of the i th predicted value is calculated as

$$\sigma_e = \left\{ \frac{1}{n-1} \sum_{b=1}^n [y(x_i; W^b) - \varphi(x_i;)]^2 \right\}^{\frac{1}{2}} \quad (13)$$

where $\varphi(x_i) = \sum_{b=1}^n \varphi(x_i; W^b) / n$ and n is the number of neural networks. The 95% prediction confidence bounds can be calculated as $\varphi(x_i;) \pm 1.96\sigma_e$. A narrower confidence bounds indicates the associated model prediction is more reliable.

4 Application to Binary Distillation Systems

4.1 Modelling of the distillation systems

Two binary distillation systems of methanol-water and benzene-toluene separations are considered. The methanol-water system is to be rectified into a distillate containing 90% methanol and a residue containing 5% methanol [29]. The Benzene-toluene system is to be separated to 95% benzene in the distillate and 5% benzene in the residue [30]. The nominal parameters for simulation are as given in Table 1. At the steady state, based on the data generated in HYSYS, exergy analyses of the streams are performed using Eq(3). Exergies of the reboiler and condenser are calculated using Eq(5). This is because the data in HYSYS are obtained at the steady state and the temperature can safely be assumed to be constant at the prevailing operating conditions. Careful considerations are made to compute the exergy of each stream both at the prevailing operating conditions and at reference states.

In Tables 2 and 3, the data for the streams in and out of the column are given for methanol-water and benzene-toluene respectively. The exergy efficiency and the irreversibility of the system are calculated using Eq(7) to Eq(10). The exergy efficiencies are 83.93% and 82.34% for methanol-water and benzene-toluene respectively while the exergy loss / irreversibility are 7.216×10^5 and 3.691×10^6 respectively for methanol-water and benzene toluene. This reveals that there is room for improvement of energy efficiency in these separation processes.

Table 1: Nominal parameters for the base case simulations

	Benzene-Toluene	Methanol-Water	Unit
Feed temperature	105	53	°C
Feed pressure	1	1	atm
Feed rate	350	216.8	kmol/h
Reflux ratio	3.5	1.028	
Number of trays	11	8	
Feed tray	7	5	
Distillate rate	151.8	88.94	kmol/h

Table 2: Simulated data for exergy analysis of methanol-water system

	$h_0(\text{kJ/kmol})$	$s_0(\text{kJ/kmol}^\circ\text{C})$	$h(\text{kJ/kmol})$	$s(\text{kJ/kmol}^\circ\text{C})$	$m(\text{kmol/h})$	$Ex(\text{kJ/h})$
Feed	-2.66×10^5	26.574	-2.64×10^5	46.21	216	4.53×10^5
Distillate out	-2.42×10^5	11.16	-2.39×10^5	42.83	88.93	1.39×10^5
Bottom out	-2.83×10^5	29.89	-2.77×10^5	71.863	127.06	5.54×10^5
Reflux	-2.42×10^5	11.16	-2.39×10^5	42.823	49.67	7.78×10^4
Boilup	-2.73×10^5	28.58	-2.28×10^5	175.73	138.44	5.63×10^6
Reboiler						4.03×10^6
Condenser						3.07×10^6

Table 3: Simulated data for exergy analysis of benzene-toluene system

	$h_0(\text{kJ/kmol})$	$s_0(\text{kJ/kmol}^\circ\text{C})$	$h(\text{kJ/kmol})$	$s(\text{kJ/kmol}^\circ\text{C})$	$m(\text{kmol/h})$	$Ex(\text{kJ/h})$
Feed	29022.4	-103.739	73150.8	40.76	350	14181516
Distillate	47908.7	-122.424	55163.2	-83.9598	151.75	954911.8
Bottoms	14566.9	-96.5928	28547.7	-29.0841	198.24	2437092
Reflux	47908.7	-122.424	55163.2	-83.9598	497.9	3133213
Boil up	16856.3	-97.1049	63541.8	55.1096	261.2	11201230
Reboiler						6722074
Condenser						13820882

The emphasis is to increase exergy efficiency and increase profitability of existing plants rather than plant expansion. Parametric analysis of the column is conducted to investigate the impacts of a number of variables on the exergy efficiency of the column. For each variable perturbations of the size $\pm 15\%$ of its initial value are added. The initial exergy efficiencies are 83.93% for methanol water and 82.34% for benzene toluene as given for the base cases of the systems. The desired purity specifications of the distillate are maintained for all the variations. The exergy of the material streams and energy streams are calculated at each variation, the corresponding exergy efficiency and reboiler exergy are calculated. Tables 4 and 5 show the sensitivity analysis of the two systems under consideration. For most cases considered, improving exergy efficiency translates to reduction in reboiler energy. However, exception is noticed for condenser pressure and the feed temperature in Tables 4 and 5. This is possibly because there is a significant change in the reboiler energy at these variations without corresponding significant change in the exergy of the streams.

From Tables 4 and 5, some of the variables fail to give a converged solution at the steady state when changed from their initial values. They however give converged solutions in the dynamic state when the distillate and bottom compositions are controlled to be at their reference values. These variables are

considered not feasible because the data to be generated for ANN training are to be taken from the steady state. For most of the variables of the methanol-water system, the change in variable values alters the composition of the bottoms from the initial reference value. This is not seriously considered as the main focus of the sensitivity analysis is to check out the variables that have noticeable impact on the overall exergy efficiency of the column. Reflux rate and reboiler energy even though have effects on the exergy efficiency are not considered. This is because that they are typically used as manipulated variables in the composition control systems [31]. The feed rate has no effect on the exergy efficiency of the column but influences the reboiler energy. It has been previously considered as input in the simulation of distillation column [13].

Table 4: Sensitivity analysis of the methanol-water system

	-15% of initial values			+15% of initial values		
	Exergy eff (%)	Reboiler duty (kJ/h)	Reboiler exergy (kJ/h)	Exergy eff (%)	Reboiler duty (kJ/h)	Reboiler exergy (kJ/h)
Reflux rate	82.15	5.320×10^6	3.905×10^6	85.20	5.700×10^6	4.183×10^6
Feed rate	83.93	4.675×10^6	3.432×10^6	83.93	6.325×10^6	4.643×10^6
Feed temperature	84.14	5.632×10^6	4.135×10^6	83.66	5.367×10^6	3.940×10^6
Reboiler duty	97.5	4.675×10^6	3.430×10^6	77.32	6.325×10^6	4.640×10^6
Condenser pressure	80.92	5.459×10^6	4.008×10^6	86.37	5.536×10^6	4.064×10^6
Reboiler pressure	85	5.417×10^6	3.905×10^6	83.12	5.574×10^6	4.152×10^6
Condenser temperature	Not feasible			Not feasible		
Reboiler temperature	99.9	2.970×10^6	2.042×10^6	Not Feasible		
Distillate rate	97	4.684×10^6	3.335×10^6	Not feasible		
Bottoms rate	Not feasible			98	4.366×10^6	3.081×10^6

The variables that are then considered are the controlled variables (distillate and bottom compositions) and external input variables which can be regulated (feed rates and feed temperatures). Subsequently, data for neural network training are generated by varying these independent variables within their upper

and lower bounds. The bounds are determined from the sensitivity analysis. Corresponding values of the exergy efficiency and irreversibility are calculated based on Eq.(3) to Eq.(10).

4.2 Linear models

PLS regression is used to build the linear models in this study. It is found that 4 latent variables give the smallest SSE on the testing data and, hence, 4 latent variables should be used in the PLS models. Plots of model prediction error (top left), model prediction error versus fitted values (top right), histogram of prediction error (bottom left), and normal probability plots (bottom right) from the two PLS models are given in Fig. 3 and Fig. 4. These plots indicate the linear model prediction errors of the two systems are not normally distributed indicating that the models are not adequate. Table 6 gives the SSE, mean square error (MSE), and the coefficient of determination (R^2) for the models. The very large SSE and MSE values of the linear models and their low R^2 values indicate that there could be strong non-linearity in the relationship between exergy efficiency and process operating conditions. This justifies the need to build nonlinear models using ANN.

Table 5: Sensitivity analysis of the benzene-toluene system

	-15% of initial values			+15% of initial values		
	Exergy eff (%)	Reboiler duty (kJ/h)	Reboiler exergy (kJ/h)	Exergy eff (%)	Reboiler duty (kJ/h)	Reboiler exergy (kJ/h)
Reflux rate	83.95	5.959×10^6	4.568×10^6	82.10	1.121×10^7	8.676×10^6
Feed rate	82.34	7.393×10^6	5.704×10^6	82.34	1.01×10^7	7.721×10^6
Feed temp.	91.53	1.435×10^7	1.107×10^7	82.01	8.491×10^6	6.551×10^6
Reboiler duty	82.86	7.4×10^6	5.694×10^6	74.47	1.00×10^7	7.7296×10^6
Condenser pressure	80.07	8.596×10^6	6.632×10^6	84.14	8.823×10^6	6.807×10^6
Reboiler pressure	82.48	8.224×10^6	6.22×10^6	82.24	9.11×10^6	7.124×10^6
Condenser temp.	Not feasible			Not feasible		
Reboiler temp.	Not feasible			Not feasible		
Distillate rate	85.66	4.477×10^6	3.414×10^6	Not feasible		
Bottoms rate	Not feasible			86.9	3.640×10^6	2.768×10^6

Table 6: Model performance indicators for linear models

	Methanol-water			Benzene-toluene		
	Training	Testing	Validation	Training	Testing	Validation
SSE	186.68	63.86	50.41	109.82	43.42	37.11
MSE	0.4050	0.3414	0.3680	0.1489	0.1336	0.1405
R ²	0.4701	0.3934	0.4871	0.6880	0.6215	0.6908

Figure 3: Linear model validation for the methanol-water system

4.3 ANN models

The neural network structure and training are as described in Section 3.1. Fig. 5 and Fig. 6 show the actual exergy efficiencies (solid curves, blue) and neural network predictions (dashed curves, red) on the training, testing, and unseen validation data sets for the methanol-water column and the benzene-toluene column respectively. The SSEs on the training, testing and unseen validation data sets are given in Table 7. The numbers of hidden neurons that gave the least SSE on the testing data are 21 for methanol-water and 21 for benzene-toluene. The results in Figs. 5 and 6 and Table 7 show that the ANN models give excellent prediction performance. The models can be conveniently used to determine the exergy efficiencies of the distillation processes at different operating conditions. Usually in the calculation of exergy efficiency, the enthalpies and entropies of all streams involved must be determined. The ANN models can be used to predict the exergy efficiencies without the rigours of calculating the enthalpies and entropies of the streams. This will be a valuable tool in the hand of process

design engineers and operators in determining the effects of different operating conditions on the exergy efficiency of the distillation process.

Figure 4: Linear model validation for the benzene-toluene system

Table 7: Model performance indicators for single ANN models

	Methanol-water			Benzene-toluene		
	Training	Testing	Validation	Training	Testing	Validation
SSE	0.0089	0.0039	0.0026	0.0011	0.0010	0.0007
MSE	8×10^{-6}	7×10^{-6}	1.35×10^{-6}	2.95×10^{-6}	4.15×10^{-6}	4.66×10^{-5}
R^2	0.9990	0.9988	0.9987	0.9976	0.9913	0.9913

4.4 Bootstrap Aggregated Neural Network

A bootstrap aggregated neural network (BANN) containing 30 neural networks is developed to predict the exergy efficiency of each system. Each individual network has one hidden layer. The Levenberg-Marquardt training algorithm is used to train the networks. Training data for the individual networks differs. This is due to bootstrap re-sampling to ensure that different individual networks are obtained and their combination lead to that the entire input space being well predicted. A problem in neural

network is over-fitting which means a trained neural network can give excellent performance on the training data but performs poorly when applied to unseen validation data. A combination of multiple non-perfect models improves the prediction accuracy on the entire input space. Figs. 7 and 8 show the MSE of individual network on training, testing and validation data sets. It can be seen that the performances of individual networks on different data sets are inconsistent. A network with low MSE on the training data could have a large MSE on the unseen validation data. This shows the non-robust nature of a single neural network. The MSE values for the aggregated neural networks with different numbers of constituent networks are shown in Fig. 9 and Fig. 10 for the methanol-water column and the benzene-toluene column respectively. The MSE for BANN models on training and validation data sets are 1.20×10^{-6} and 1.00×10^{-6} respectively for the methanol-water system and 2.51×10^{-6} and 2.83×10^{-6} respectively for the benzene-toluene system. This is an improvement on the minimum MSE for the single neural networks given in Table 7. The model accuracy is seen being improved by using bootstrap aggregated neural network model.

Figure 5: Actual and BANN model predicted exergy efficiency for the methanol-water column

Figure 6: Actual and BANN model predicted exergy efficiency for the benzene-toluene column

Figure 7: Model errors of individual networks for methanol-water system

Figure 8: Model errors of individual networks for benzene-toluene system

Figure 9: Model errors of aggregated networks for methanol-water system

Figure 10: Model errors of aggregated networks for benzene-toluene system

4.5 Optimisation of exergy efficiency

The optimisation problem can be stated as

$$\begin{aligned}
 &\min_x J = -\varphi \\
 &\text{s.t.} \\
 &\varphi = f(x_1, x_2, x_3, x_4) \\
 &0.8 \leq x_3 \leq 0.99 \\
 &0.01 \leq x_4 \leq 0.1
 \end{aligned} \tag{14}$$

where J is the objective function, $x=[x_1, x_2, x_3, x_4]$ is a vector of neural network model inputs which are feed rate, feed temperature, distillate composition and bottom composition respectively; and φ is the exergy efficiency. As changing feed temperature would require pre-heating of the feed which can have impact on the overall energy efficiency, in this study the feed temperature is kept constant, i.e. removed from decision variable list. Thus the decision variables in this case are feed rate, distillate composition and bottom composition.

The sequential quadratic programming (SQP) method is used for the optimisation. The exergy efficiency is maximised subject to the distillate composition constraints. Table 8 and Table 9 give the results of the optimisation procedure for the two systems. In Tables 8 and 9, case 1 refers to the solution

of Eq(14). It can be seen that exergy efficiency is improved with the bottom composition at its upper bound. When the bounds on the product compositions are altered (cases 2 and 3), the optimal exergy efficiencies increases when the bounds are narrowed and it reduces when the bounds are widen. However, there is a limit for the purity specification of the products beyond which increasing the exergy efficiency has the added clause of increase in energy of the reboiler. This is shown in case 4 and gives a caution on placing consideration on the exergy efficiency while specifying the product purity.

Table 8: Summary of optimisation results for methanol-water system

	Base case	Optimum case 1	Optimum case 2	Optimum case 3	Optimum case 4
Feed rate (kmol/h)	216.8	216.8	216.79	180.7	216.79
Feed temp.(°C)	53	53	53	53	53
Distillate composition	0.90	0.90	0.90	0.90	0.92
Bottom composition	0.05	0.1	0.08	0.01	0.05
ANN predicted efficiency (%)	83.95	93.28	89.77	74.98	85.59
HYSYS validated efficiency (%)	83.93	93.31	89.29	77.9	85.59
Reboiler energy (kJ/hr)	5.5×10^6	5.02×10^6	5.23×10^6	6.74×10^6	5.77×10^6
Reboiler exergy(kJ/hr)	4.04×10^6	3.61×10^6	3.78×10^6	5.05×10^6	4.24×10^6
Utility cost (\$/yr)	1.70×10^4	1.56×10^4	1.62×10^4	2.09×10^4	1.79×10^4

The optimum efficiency as given in each case shows that there is a reduction of entropy generation within the systems at these operating conditions and that is why there are corresponding increases in the exergy efficiencies of the systems. The distillate composition is not compromised for the first case showing that the desired purity can be maintained with a corresponding increase in the exergy efficiency of the system. This increment translates to an increase in the energy efficiency of the systems considering the fact that there is a decrease in the reboiler energy even though the feed rate is maintained. Other varying compositions specifications are shown with their corresponding exergy efficiencies.

Taking the optimum case 1 as an example, the improvement in the exergy efficiency of the system is 11.17% for methanol-water system and 1.79% for benzene-toluene system when compared to the base case. The utility cost of the cases based on the assumption of 8600 h per year are calculated and shown in Tables 8 and 9. For the optimum case 1, the increase in exergy efficiency translates to 8.2% reduction

in utility cost for methanol water and 28.2% reduction in utility cost for benzene toluene over a year period. The cumulative effect of this could be of great economic value.

Table 9: Summary of optimisation results for benzene-toluene system

	Base case	Optimum case 1	Optimum case 2	Optimum case 3	Optimum case 4
Feed rate (kmol/h)	350	350	350	350	350
Feed temp.(°C)	105	105	105	105	105
Distillate composition	0.95	0.95	0.90	0.90	0.97
Bottom composition	0.05	0.1	0.08	0.01	0.05
ANN predicted efficiency (%)	82.34	83.82	83.22	80.86	82.88
HYSYS validated efficiency (%)	82.34	83.86	83.15	81.78	83.25
Reboiler energy (kJ/hr)	8.712×10^6	6.05×10^6	6.92×10^6	1.87×10^7	2.07×10^7
Reboiler exergy(kJ/hr)	6.72×10^6	4.64×10^6	5.31×10^6	1.44×10^7	1.71×10^7
Utility cost (\$/yr)	2.94×10^4	2.11×10^4	2.38×10^4	3.04×10^4	3.68×10^4

The optimum operating conditions given by the optimisation procedures are simulated in HYSYS. It can be seen from Tables 8 and 9 that actual (HYSYS simulated) exergy efficiencies are very close to the BANN model predicted values. This shows that the optimal predicted conditions of the BANN model can give the optimal operating conditions on the actual process. This further demonstrates the suitability of the Bootstrap aggregated neural network models at the modelling and optimisation of the exergy efficiency of the distillation columns. The method as applied on the binary system might seem trivial but the accuracy of the predictability of BANN model of the exergy efficiency cannot be over emphasised. For a much complex system, the relevance of the method will be much more pronounced.

As seen in Tables 8 and 9, BANN model is able to predict what the exergy efficiency of the system will be at different quality specifications. In a processing plant, the relevance of this cannot be over emphasised especially in the area of decision making for the most energy efficient operating conditions of the system. This could serve as guide for process operators and process engineers. It could also find relevance in the design of a new system. The caution in the application is that the system to be investigated should be fully trained. A BANN model for a particular system, might not work for another.

5 Application to multi-component system

5.1 The system

A multi-component system as depicted in Fig. 11 [32] is simulated in HYSYS. The 3 products from the fractionation process are a vapor distillate rich in C_2 and C_3 , vapor side stream rich in nC_4 and bottoms rich in nC_5 and nC_6 . SRK equation of state is used for the K values and enthalpy departure.

The enthalpy and entropy at the stream conditions and at reference conditions are shown in Table 10. The physical exergy of the inlet and outlet streams as calculated using Eq.(3) are shown in Table 11. The system being a multi-components system with 5 components necessitate the calculation of the chemical exergy of each stream to determine the contribution of the chemical exergy to the total exergy the stream. Eq.(2) is used in calculation of the chemical exergy. Exergy of the component at reference states of 298 K and 101.325 kPa are taken from the literature for each of the component [23].

Figure 11: The multi-component separation system

The total exergy in and out of the system is given by Eq(15) and Eq(16).

$$\sum Ex_{in} = Ex_{feed} + Ex_{reboiler} \quad (15)$$

$$\sum Ex_{out} = Ex_{distillate} + Ex_{bottoms} + Ex_{sidestream} + Ex_{condenser} \quad (16)$$

Each stream exergy is a sum of the physical and chemical exergy. The exergy efficiency and the irreversibility of the unit is calculated using Eq(9) and Eq(10).

In Table 11, the exergy efficiency, exergy loss and the reboiler energy of the unit is shown. Two measures of efficiency are presented. Efficiency 1 is based on the physical exergy of the streams and efficiency 2 is a combination of the physical and chemical exergy of the streams. As can be seen in Table 11, the reboiler energy and reboiler exergy for the two measured efficiencies are the same. There is a slight difference in the exergy loss. The contribution of the chemical exergy to the total exergy of the unit is 0.53%. This is attributed to the fact that the distillation process as described here is a physical process. A reactive distillation column might possibly have a significant contribution from the chemical exergy. The contribution of chemical exergy to this process can be reasonably assumed to be negligible [33].

Table 10: Simulated data for exergy analysis of multi-component system

	h_0 (kJ/kmol)	s_0 (kJ/kmol ⁰ C)	h (kJ/kmol)	s (kJ/kmol ⁰ C)	m (kmol/h)	Ex (kJ/h)
Feed	-129865	160.51	-150891	84.12	45.36	7.88×10^4
Distillate	-102864	168.95	-115493	104.36	10.43	5.75×10^4
Side stream	-130216	141.87	-121966	139.39	16.79	1.19×10^5
Bottom	-171395	74.984	-147889	143.99	18.14	7.89×10^4
Reflux	-102864	168.95	-115493	104.36	68.03	3.75×10^5
Boilup	-160416	96.11	-129710	177.29	117.8	1.02×10^6
Reboiler duty						1.865×10^6
Condenser duty						9.932×10^5

Table 11: Exergy analysis of the multi-component system

	Efficiency 1 (%)	Efficiency 2 (%)
	64.29	64.63
Reboiler energy (kJ/hr)	1.983×10^6	1.983×10^6
Reboiler Exergy (kJ/hr)	1.865×10^6	1.865×10^6
Exergy loss (kJ/hr)	6.940×10^6	6.885×10^6

As discussed in Section 4.1, the decision variables are the feed temperature, the feed rate and the key component in each of the product stream which are propane in the distillate, npentane in the bottom and nbutane in the side stream. The decision variables are varied in their upper and lower bounds and the

corresponding exergy analysis of the inlet and outlet streams are calculated both at the prevailing operating conditions and at reference conditions. Subsequently data generated in HYSYS simulation are used in the ANN modeling of the column. The software generated data can be easily replaced with plant operating data over a period of time for an industrial column. The methodology as developed could be generic.

5.2 Bootstrap aggregated neural network modelling

A bootstrap aggregated neural network is developed from process operational data based on the simulated data from HYSYS. The BANN contains 30 neural networks for predicting the exergy efficiency of the system. Each individual network has a single layer with 30 hidden neurons. Hidden neurons use sigmoid activation function and the output neuron uses the linear activation function. Levenberg-Marquardt training algorithm is used to train the individual networks. Fig. 12 shows the predicted and actual values of the exergy efficiency as well as the confidence bounds. The prediction error lies between -4×10^{-3} and 6×10^{-3} as shown in Fig. 13. An advantage of BANN model is that it can offer model prediction confidence bound. A narrower confidence bound indicates that the associated model prediction is more reliable.

Figure 12: Actual values, predictions, and confidence bounds of multi-component BANN model

5.3 BANN model of a modified multi-component system

A further modification of the system is made based on the given specification in Fig. 14. The number of stages is increased to 25, the feed stage at stage 7 and the sidestream is drawn from stage 17. The

modifications are intended for a change in the design of the column to investigate the contribution it could have on the exergy efficiency.

Figure 13: Error of prediction of multi-component BANN model

The subsequent thermodynamic analysis of the modified system is made as described in Section 5.1. Table 12 shows the simulated data and the exergy calculation of the streams in and out of the modified system. Exergy efficiency, exergy loss and reboiler exergy of the system are shown in Table 13. As is the case for the previous multicomponent system, the reboiler exergy and exergy loss for the two measured efficiencies are the same. The contribution of the chemical exergy to the total exergy of the system is 0.25% and hence can be considered negligible here as well. There is an increment in the exergy efficiency of the modified system by 2% corresponding to an improvement of 3.2% as compared to the initial system. There is a corresponding decrease in the reboiler energy and the exergy loss of the system. This signifies a reduction in entropy generation within the column resulting from increasing the stage number. It should however be noted that the improvement in efficiency comes with the added expenses of capital cost.

Fig. 15 shows the predictions of the BANN against the true energy efficiency on the training, testing, and unseen validation data sets. It can be seen that the model predictions are very accurate.

Figure 14: Modified multi-component system

Table 12: Simulated and thermodynamic data of the modified system

	h_0 (kJ/kmol)	s_0 (kJ/kmol ⁰ C)	h (kJ/kmol)	s (kJ/kmol ⁰ C)	m (kmol/h)	Ex (kJ/h)
Feed	-129865	160.5106	-150891	84.12	45.36	7.88×10^4

Distillate	-102864	168.9596	-115491	104.36	10.20	7.03×10^4
Side stream	-130216	141.8794	-121965	139.38	16.86	1.56×10^5
Bottom	-171395	74.98403	-147889	143.99	18.30	5.44×10^4
Reflux	-102864	168.9599	-115491	104.36	77.62	5.35×10^5
Boilup	-160416	96.10724	-129710	177.30	124.2	8.12×10^5
Reboiler duty						1.95×10^6
Condenser duty						1.06×10^6

Table 13: Exergy analysis of the modified multi-component system

	Efficiency 1 (%)	Efficiency 2 (%)
	66.52	66.84
Reboiler energy (kJ/hr)	2.072×10^6	2.072×10^6
Reboiler Exergy (kJ/hr)	1.949×10^6	1.949×10^6
Exergy loss (kJ/hr)	6.788×10^5	6.733×10^5

Figure 15: Predicted and actual exergy efficiency

5.4 Optimisation using neural network models

The optimisation objective is to maximise the exergy efficiency of the column subject to products composition constraints. The products are the most volatile in the distillate, side stream and bottom composition.

$$\min_x J = -\varphi \quad (17)$$

s.t.

$$\varphi = f(x_1, x_2, x_3, x_4, x_5)$$

$$0.75 \leq x_3 \leq 0.95$$

$$0.6 \leq x_4 \leq 0.9$$

$$0.7 \leq x_5 \leq 0.95$$

where x_1 is the feed rate, x_2 is the feed temperature, x_3 is propane composition in the distillate, x_4 is n pentane composition in the bottom and x_5 is n butane composition in the side stream.

In addition to the process operation objective, minimising the model prediction confidence bounds can be incorporated as an addition optimisation objective. To improve the reliability of the optimisation strategy, a modified objective function is proposed. The optimisation problem can be stated as

$$\min_x J = -(\varphi - \beta\sigma)$$

s.t.

$$\varphi = f(x_1, x_2, x_3, x_4, x_5) \quad (18)$$

$$lb \leq x_{prod} \leq ub$$

where J is the objective function, $x=[x_1, x_2, x_3, x_4, x_5]$ is a vector of decision variables, i.e. neural network model inputs, y is the exergy efficiency, σ is standard prediction error, and β is a weighting factor for σ .

The optimisation problem was solved using the SQP method implemented by the function “fmincon” in MATLAB Optimisation Toolbox. The optimisation framework presented in this work is illustrated in Figure 16. Exergy analysis is carried out on distillation column operation data (or simulated distillation column operation data). Then the nonlinear relationship between process operating conditions and exergy efficiency is modelled by a neural network using the exergy analysis data. The

neural network model is used in an optimisation framework to find the distillation column operating conditions leading to the highest exergy efficiency subject to product quality constraints. The optimised operating conditions are further validated on the distillation columns or their simulation.

Table 14 shows the optimum results without confidence bounds for the initial system and the modified system. The prediction errors of the optimum results and the HYSYS validated exergy efficiency are 0.00165 and 0.0058 for the initial and modified cases respectively. The results further confirm the predictability accuracy of BANN. Also without modifying the design, optimum operating conditions that led to 32.38% increment in exergy efficiency of the system were found using the proposed methods. This is without sacrificing the purity of the product specifications. This further justifies the suitability of the method in determining energy efficient operating conditions for the distillation column. However, with the modification, the exergy efficiency has increased from 64.29% to 66.52% this is just about 2% increment in the exergy efficiency as compared to 32.38% from the method proffered here. This increment for the modified case is at an additional capital cost (increasing number of trays and change in location of feed and side stream). The tools described here can aid in decision making of what trade off should be made in the design and operation of energy efficient column. The modified system is further improved as shown in Table 14 and there is an increase in its exergy efficiency of about 31% of its initial value.

In Table 15, the results of the optimisation of the base case with model prediction confidence bounds are shown. The effects of some values of the weighting factor of the standard prediction error on exergy efficiency are also investigated. Narrowing the confidence bound to a weighting factor of 0.01 improves the prediction accuracy and reliability of the model. Incorporating confidence bound in the optimisation can ensure the reliability and the generalisation of the associated model especially for complex cases.

Figure 16: Description of the optimisation procedure

Table 14: Summary of optimisation results for multi-component systems

	Multi-component System		Modified System	
	Base case	Optimum case	Base case	Optimum case
Feed rate (kmol/h)	45.36	45.36	45.36	45.36
Feed temperature (K)	308.1	308.1	308.1	308.1
Propane in distillate	0.8080	0.85	0.8562	0.85
n Pentane in Bottom	0.6778	0.71	0.7310	0.82

n Butane in sidestream	0.7393	0.85	0.8280	0.92
Exergy efficiency (%)	64.29	96.67	66.84	97.62
ANN predicted exergy efficiency (%)	66	96.51	63.20	97.05

6 Conclusions

This study shows that ANN can accurately model exergy efficiency in distillation columns from process operational data. The ANN models are then used in obtaining optimal distillation operation conditions that can maximise the energy performance of distillation systems while maintaining the product quality and throughput. A reliable strategy based on BANN for improved generalisation of the predicted model is also presented. BANN enhances model prediction accuracy and also provides model prediction confidence bounds. Exergy analysis is a much effective way of determining the energy efficiency of processes and hence the importance of this study to process and design engineers. Applications to two binary systems and a multi-component system demonstrate the proposed methods can significantly increase the exergy efficiency of distillation columns. The optimisation resulted in 11.2% increment of the exergy efficiency of methanol water and 1.8% for benzene toluene. This brings about a reduction in the consumption of utility of the systems to 8.2% for methanol water and 28.2% for benzene toluene. The improvement is based on changing the operating conditions of the system and has no additional capital costs. The multi-component system has an improvement in the exergy efficiency to be 32.4%. This is without incurring any additional capital costs as well. The modified multi-component system has an exergy improvement of about 31%, but the column structure has to be redesigned creating an additional capital costs. The advantage of incurring these further costs can be weighed and informed decisions can then be made. The ANN and BANN model based modelling and optimisation can aid the decision making of energy efficient operations and control of distillation columns.

Table 15: Summary of optimisation results with confidence bounds

Confidence bounds	Base case	0	1	0.1	0.01
Feed rate (kmol/h)	45.36	45.36	45.36	45.36	45.36
Feed temp (K)	308	308	308	308	308
Propane comp	0.808	0.85	0.85	0.85	0.85
n Pentane comp	0.6778	0.71	0.71	0.71	0.71

n Butane comp	0.7393	0.85	0.85	0.85	0.85
HYSYS validated					
efficiency (%)	64.29	96.67	96.68	96.66	96.66
Optimum efficiency					
from ANN (%)	66	96.51	95.78	96.44	96.60
Error of prediction	0.0265	0.00165	0.009	0.0022	0.0006

Acknowledgement

The work was supported by the Commonwealth scholarships commission in the UK and partially supported by the EU FP7 (Ref: PIRSES-GA-2013-612230).

Nomenclature

Ex	Exergy rate, kJhr^{-1}
h	Specific enthalpy, kJkmol^{-1}
m	Molar flow, kmolhr^{-1}
P_0	Reference pressure, kPa
Q_z	Heat, kJhr^{-1}
s	Specific entropy, $\text{kJkmol}^{-1}\text{K}^{-1}$
SRK	Soave Redlich Kwong (equation of state)
T_0	Reference temperature, K
x_{ji}	The mole fraction of ith component in the liquid state on stage j
y_{ji}	The mole fraction of ith component in the vapour state on stage j
Z_j	Mole fraction of component j
φ	Exergy efficiency, %

Superscript

k	Number of inputs
n	Number of neural networks

Subscript

0	Reference conditions
phy	Physical
chem	Chemical

References

- [1] White DC. Optimise energy use in distillation. Chem Eng Prog 2012; 35-41.
- [2] Gadalla MA, Abdelaziz OY, Kamel DA, Ashour FH. A rigorous simulation-based procedure for retrofitting an existing Egyptian refinery distillation unit. Energy 2015; 83:756-65.

- [3] Ochoa-Estopier LM, Jobson M, Smith R. The use of reduced models for design and optimisation of heat-integrated crude oil distillation systems. *Energy* 2014; 75: 5-13.
- [4] Liang YC, Zhou Z, Wu YT, Geng J, Zhang ZB. A nonequilibrium model for distillation processes. *AIChE J* 2006; 52 : 4229-39.
- [5] Uzlu E, Kankal M, Akpinar A, Dede T. Estimates of energy consumption in Turkey using neural networks with the teaching–learning-based optimization algorithm. *Energy* 2014; 75: 295-303.
- [6] Osuolale FN, Zhang J. Energy efficient control and optimisation of distillation column using artificial neural network. *Chem Eng Trans* 2014; 39: 37-42.
- [7] Ochoa-Estopier LM, Jobson M, Smith R. Operational optimization of crude oil distillation systems using artificial neural networks. *Comput Chem Eng* 2013; 59: 178-85.
- [8] Singh AK, Tyagi B, Kumar V. Application of neural network based control strategies to binary distillation column. *Control Eng App Informatics* 2013; 15, 47-57.
- [9] Osman M, Ramasamy M. Neural network based soft sensor for inferential control of a binary distillation column. *J Appl Sci* 2010; 10: 2558-64.
- [10] de Canete JF, Gonzalez S, del Saz-Orozco P, Garcia I. A harmonic balance approach to robust neural control of MIMO nonlinear processes applied to a distillation column. *J Process Control* 2010; 20: 1270 -77.
- [11] Bahar A, Özgen C, Leblebicioğlu K, Halıcı U. Artificial neural network estimator design for the inferential model predictive control of an industrial distillation column. *Ind Eng Chem Res* 2004; 43: 6102-11.
- [12] Ge XL, Yuan XG, Ao C, Yu KK. Simulation based approach to optimal design of dividing wall column using random search method. *Comput Chem Eng* 2014; 68: 38-46.
- [13] Amit KS, Barjeev T, Vishal K. Application of Feed Forward and Recurrent Neural Network Topologies for the Modeling and Identification of Binary Distillation Column. *IETE J Res* 2013; 59: 167-175.
- [14] Ochoa-Estopier LM, Jobson M. Optimization of heat-integrated crude oil distillation systems. Part III: Optimization framework. *Ind. Eng. Chem. Res.* 2015; 54 : 5018-36.
- [15] Oni AO, Waheed MA. Methodology for the thermoeconomic and environmental assessment of crude oil distillation units. *Int J Exergy* 2015; 16(4):504-32.
- [16] Suzuki Y, Yamaki T, Matsuda K, Takahashi K, Endo A, Nakaiwa M. Energy saving performance of internal heat-integrated batch distillation. *Chem Eng Trans* 2012; 29 : 277-82.
- [17] Kiss AA, Flores Landaeta SJ, Infante Ferreira CA. Towards energy efficient distillation technologies – Making the right choice. *Energy* 2012; 47: 531-42.
- [18] Araujo BA, Brito RP, Vasconcelos LS. Exergetic analysis of distillation processes-A case study. *Energy* 2007; 32: 1185-93.
- [19] Al-Muslim H, Dincer I. Thermodynamic analysis of crude oil distillation systems. *Int J Energy Res* 2005; 29: 637- 55.
- [20] De Koeijer GM, Kjelstrup S, Salamon P, Siragusa G, Schaller M, Hoffmann KH. Comparison of entropy production rate minimization methods for binary diabatic distillation. *Ind Eng Chem Res* 2002; 41: 5826-34.
- [21] Kamela D, Gadallaa M, Ashourb F. New retrofit approach for optimisation and modification for a crude oil distillation system. *Chem Eng Trans* , 2013; 35:1363-68
- [22] Rosen MA, Dincer I. On exergy and environmental impact. *Int J of Energy Res* 1997; 21: 643-54.
- [23] Szargut J, Morris DR, Steward FR. Exergy analysis of thermal, chemical and metallurgical processes. , New York, Hemisphere Publishing Corporation; 1988.
- [24] Dincer I, Rosen MA. Exergy:energy, environment and sustainable development. 2nd ed. London: Elsevier science; 2012.
- [25] Le Goff P, Cachot T, Rivero R. Exergy analysis of distillation processes. *Chem. Eng. Technol.* 1996; 19: 478-485.
- [26] Zhang J. Developing robust non-linear models through bootstrap aggregated neural networks. *Neurocomputing* 1999; 25: 93-113.

- [27] Zhang J. A reliable neural network model based optimal control strategy for a batch polymerization reactor. *Ind Eng Chem Res* 2004; 43: 1030-1038.
- [28] Mukherjee A, Zhang J. A reliable multi-objective control strategy for batch processes based on bootstrap aggregated neural network models. *J Process Control* 2008; 18, 720-34.
- [29] Treybal RE. *Mass-transfer operations*, New York, McGraw-Hill; 1980.
- [30] McCabe WL, Smith JC. *Unit operations of chemical engineering*, Dubuque, Iowa, McGraw-Hill; 2005.
- [31] Skogestad S. The Dos and Don'ts of Distillation Column Control. *Chem Eng Res Des* 2007; 85: 13-23.
- [32] Green DW, Perry RH. (eds.) *Perry's chemical engineering handbook*, China, McGraw-Hill; 2006.
- [33] Anozie AN, Osuolale FN, Osunleke AS. Exergy analysis of binary plate distillation column operations. *Int J Exergy* 2009; 6: 715-28.