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Energy Efficient Control and Optimisation of Distillation Column Using Artificial Neural Network

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This paper presents a neural network based strategy for the modelling and optimisation of 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 was 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 product quality constraints. Applications to Methanol-Water and Benzene-Toluene separation columns demonstrate the effectiveness of the proposed method.

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. For instance there are about 40,000 distillation columns in the US alone. These distillation columns consume about 40 - 60 % of the total energy usage in the chemical and petrochemical industries and 6 % of the total US energy (Emersonprocessxperts, 2010). Distillation unit poses a great challenge to control engineers because of its complexity. It comes in varieties of configurations with different operating objectives, significant interactions among the control loop and specialised constraints. These result in distinct dynamic behaviours and different operational degree of freedom that will necessitate the need for specialised control configurations in order to optimise energy usage. Usually the order of economic importance in the control of distillation column 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 of distillation columns requires accurate process models. A number of distillation process models are available in the published literatures but the complexity of distillation processes has led to a number of assumptions that might limit the universality of the models. 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 (Liang et al., 2006). 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. Furthermore, 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. ANN has been recognised as a powerful tool that can facilitate the effective development of models for highly nonlinear and multivariable systems. ANN can

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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 (Ochoa-Estopier et al., 2013). Often the economic objective in terms of profitability is the focus in the optimisation of such distillation process (Amit et al., 2013). However, with the issues of global warming, GHG effects, and depleting source of energy resources, the issue of energy efficiency of processes has been brought to the limelight. 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 is the heat integrated distillation column HIDC (Suzuki et al., 2012), thermally coupled dividing wall column (Long and Lee, 2014), Petyluk column and intensified distillation column (Kiss et al., 2013). In addition, previous works on the thermodynamic efficiency of the crude distillation unit revealed a high energy and exergy loss of the column (Haragovics and Mizsey, 2012) with the overall efficiency of the column ranging from 5 - 23 % (Al-Muslim and Dincer, 2005). This shows that there is a lot of room for improvement of the distillation column and indicating a high entropy generation within in column that is making the irreversibility of the column to be highly significant. In the past, there have been efforts at devising methods of minimising entropy production rate in distillation column. Though most of these attempts are targeted at diabatic binary distillation systems (de Koeijer et al., 2002)**.** 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 (Kamel et al., 2013). In this work an attempt is made at improving the energy efficiency of the distillation column 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 were used in the decision making.

2. ANN Modelling and optimisation

2.1 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; quantifying sources of inefficiency and distinguishing quality of energy used (Rosen and Dincer, 1997). 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 use evaluation of the process, potentials for efficient energy use of such processes can then be identified and energy use 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 et al. (1988) 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

$$Ex_{total} = Ex_{phy} + Ex_{chem} + Ex_{mixing} \tag{1}$$

Ex_{chem} and Ex_{mixing} are the chemical and mixing exergy, which in the case of a binary and non reactive distillation system are assumed negligible.

$$Ex_{phy} = H - H_0 - T_0(S - S_0) \tag{2}$$

H is the total enthalpy,
S is the total entropy
T_0 is the reference temperature
H_0 and S_0 are enthalpy and entropy measured at reference conditions.
Exergy of the system is calculated as

$$\varphi = \frac{\sum Ex_{out}}{\sum Ex_{in}} \tag{3}$$

It takes a good engineering judgement to determine the streams that qualified as in and those that qualify as out. For a binary system such as the one being considered the in and out are given as

$$TotalEx_{in} = Ex_{feed} + Ex_{reboiler} + Ex_{reflux} + Ex_{boilup} \tag{4}$$

$$TotalEx_{out} = Ex_{distillate} + Ex_{bottoms} \tag{5}$$

2.2 Artificial neural Network Modelling

Here neural networks are used to model exergy efficiency and product composition. The neural networks models are then used for exergy efficiency optimisation subject to product quality constraints. Data for neural network modelling are generated from simulation. The neural network model for exergy efficiency is of the following form:

$$y = f(x_1, x_2, x_3, x_4, x_5, x_6) \tag{6}$$

Where y is exergy efficiency, x_1 to x_6 are feed rate, feed temperature, feed composition, distillate and bottom composition, and reboiler heat duty.

Neural network models for top and bottom product compositions use the same model inputs.

Single hidden layer feedforward 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 (Zhang, 1999). The data were divided into training data (50 %), testing data (30 %), and unseen validation data (20 %). Levenberg-Marquardt training algorithm was used to train the networks. The number of hidden neurons was determined by building a number of neural networks with different numbers of hidden neurons and tesing them on the testing data. The network 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 then evaluated on the unseen validation data. For the pupose of comparison, a linear model is also built using multiple linear regression (MLR).

2.3 Optimisation using neural network models

The optimisation objective is to maximise the exergy efficiency of the column subject to distillate composition constraint. The optimisation problem can be stated as

$$\min_{X} J = -y \tag{7}$$

s.t.

$$y = f(x_1, x_2, x_3, x_4, x_5, x_6)$$

$$0.8 \le x_4 \le 0.99$$

$$0.01 \le x_5 \le 0.1$$

Where J is the objective function, x=[x_1,x_2,x_3,x_4,x_5,x_6] is a vector of decision variables, i.e. neural network model inputs, and y is the exergy efficiency. The optimisation problem was solved using the sequential quadratic programming (SQP) implemented by the function “fmincon” in MATLAB Optimisation Toolbox.

3. Case Study

Two binary distillation systems of methanol-water and benzene-toluene separations were considered. 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 systems were performed. The efficiency is 42.43 % and 47.49 % for methanol-water and benzene-toluene. This is revealing there is room for improvement of the process. Subsequently, data for the training of the network were generated by varying the independent variables within their upper and lower bounds. Corresponding values of the exergy efficiency were calculated.

3.1 Linear models

The sums of square errors for the linear models are given in Table 2. The very large SSE values of the linear models indicate that there is strong non-linearity in the relationship between exergy efficiency and process operating conditions. This justifies the need to build nonlinear models using ANN.

3.2 ANN models

The performance of ANN is hinged on the data, the network structure and the training method. Figures 1 and 2 show the actual exergy efficiencies (solid curves, blue) and neural network predictions (dashed curves, red) on the training, testing, and unseen validation data sets. The SSEs on the training, testing and unseen validation data sets are given in Table 2. The numbers of hidden neurons that gave the least SSE on the testing data are 17 for methanol-water and 15 for benzene-toluene. The results in Figures 1 and 2 and Table 2 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.

Table1: Nominal parameters for simulation

	Benzene-Toluene	Methanol-Water
Feed temperature (^{o}C)	95	53
Feed pressure (kPa)	101.325	101.325
Feed rate (kmol/h)	350	216.8
Reflux ratio	3.5	1.028
Number of trays	11	8
Feed tray	7	5
Distillate rate (kmol/h)	153.4	84.4
Bottoms rate (kmol/h)	196.6	216.8

Table 2: SSEs from linear models and ANN models

	Methanol-water			Benzene-toluene		
	Training	Testing	Validation	Training	Testing	Validation
ANN model	0.0060	0.0054	0.0036	0.0031	0.0099	0.0242
Linear model	219.826	129.453	83.2434	42.9812	29.3602	25.5340

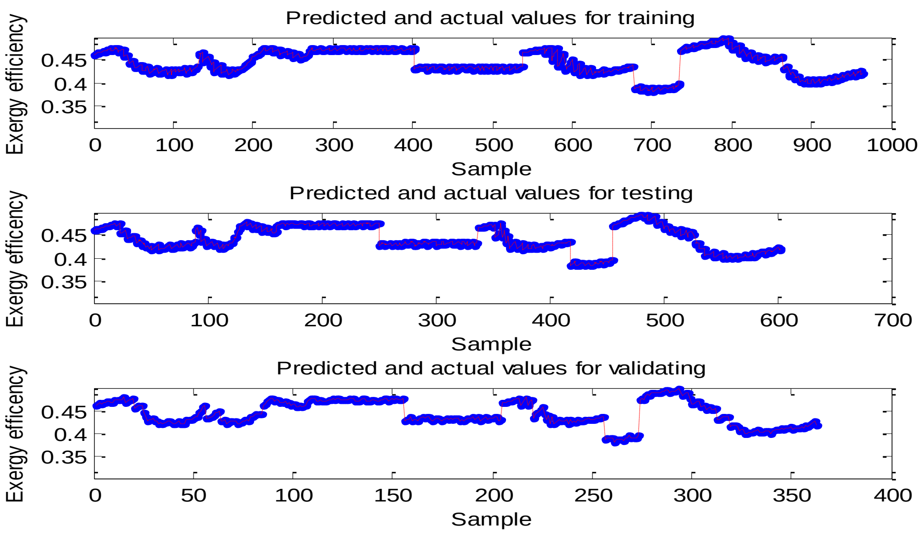

Figure 1: Actual and ANN model predicted exergy efficiency for the methanol-water column

3.3 Optimisation

Sequential quadratic programming (SQP) method was used for the optimisation. The objective function maximised was the exergy efficiency subject to the distillate composition constraint. Table 3 gives the results of the optimisation procedure for the two systems. The optimum conditions and the base case conditions are shown. As a consequence of the optimisation, more feed flow rate and slight change in the feed temperatures and feed compositions are required. 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 efficiency of the systems.

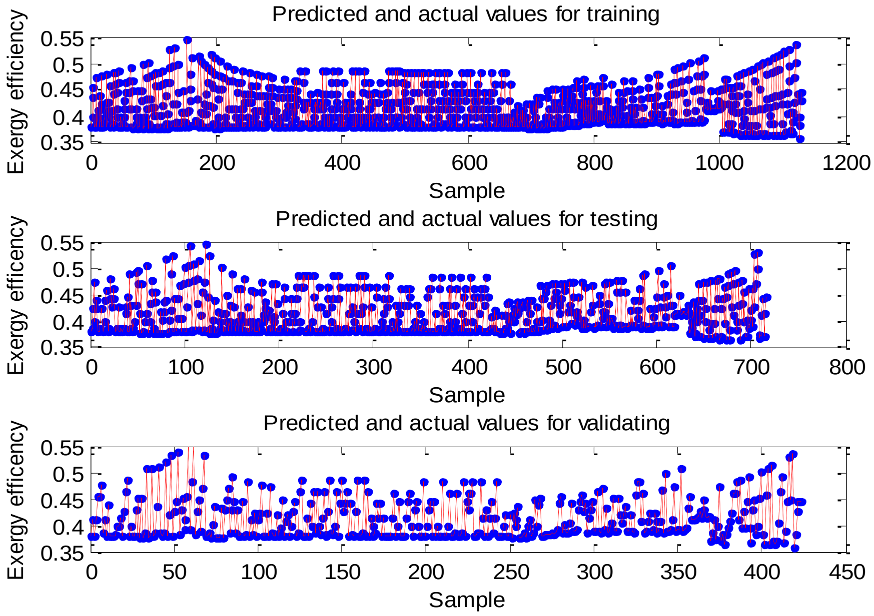

Figure 2: Actual and ANN model predicted exergy efficiency for the benzene-toluene column

The distillate compositions were not compromised 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 an increase in the feed flow rate and the reboiler energy was maintained. The optimum operating conditions given by the optimisation procedures were simulated in HYSYS. It can be seen from Table 3 that actual (HYSYS simulated) exergy efficiencies are very close to the ANN model predicted values. This further demonstrates the suitability of the ANN models at the modelling and optimisation of the exergy efficiency of the distillation columns.

Table 3: Summary of optimisation results

	Methanol-water		Benzene-Toluene	
	Base case	Optimum case	Base case	Optimum case
Feed rate (kmol/h)	216.8	260	350	450
Feed temperature(^{o}C)	53	60	95	90
Feed composition(methanol)	0.4	0.3		
Feed composition(benzene)			0.4402	0.35
Reboiler duty(kJ/h)	6.156e6	6.156e6	7.5e6	7.5e6
Distillate composition	0.95	0.95	0.95	0.95
Bottom composition	0.08	0.05	0.19	0.21
Exergy efficiency (%)	42.43	48.9	47.29	56. 56
ANN predicted Exergy efficiency (%)		48.63		57. 65

4. Conclusions

This study shows that ANN can accurately model exergy efficiency in distillation columns. The ANN models are then used in obtaining optimal distillation operation conditions that can maximise the energy performance of distillation systems. 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. The ANN model based modelling and optimisation can aid the decision making of energy efficient operations and control of distillation columns.

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