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Energy efficiency optimisation for distillation column using artificial neural network models

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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 multicomponent separation columns also demonstrate the effectiveness of the proposed method with a 32.4% improvement in the exergy efficiency.

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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 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

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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 focussing 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 framework 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 to 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

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

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.

$$Ex_{chem} = m\left(h_0 - \sum z_i \overline{h}_{0i} - T_0\left(s_0 - \sum z_i \overline{s}_{0i}\right)\right) \tag{2}$$

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

where z_i is the mole fraction of the ith component, $\overline{h}_{0i}$ and $\overline{s}_{0i}$ 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]

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