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# Thermodynamic Optimization of Atmospheric Distillation Unit

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## Abstract

This paper presents a methodology for optimising the exergy efficiency of atmospheric distillation unit without trading off the products qualities and process throughput. The presented method incorporates the second law of thermodynamics in data driven models. Bootstrap aggregated neural networks (BANN) are used for enhanced model accuracy and reliability. The standard error of the individual neural network predictions is taken as the indication of model prediction reliability and is incorporated in the optimization objective function. The economic analysis of the recoverable energy (sum of internal and external exergy losses) reveals the energy saving potential of the proposed method, which will aid the design and operation of energy efficient atmospheric distillation columns.

Keywords: atmospheric distillation, exergy, optimization, neural networks.

## **1. Introduction**

Distillation process has always attracted the interest of researchers and quite a number of work in the literatures are focused on improving its energy efficiency either for binary system [1] or multi-component system [2]. Most success in improving the efficiency of the column are the development of energy integrated schemes such as the petyluk column [3], internally heat integrated column [4], heat integrated distillation column HIDC [5], thermally coupled dividing wall column [6] and intensified distillation column [7]. However, the conventional columns are still dominantly in use in most chemical and petrochemical industries. Most industries will rather maximize available resources for maximum

profitability in place of large scale expansion. One tool that has gained widespread application in this regard is optimization. Optimization is a major quantitative tool in decision making for the process industries [8]. In recent years optimization of crude distillation system has received considerable research interests. This is because the major cost of refinery operation second only to the cost of crude is energy and 35% of these is consumed in the crude distillation unit. Optimization is a well-developed field in chemical engineering and has been applied on a number of processes [9] with a combination of differing objectives [10]. It has also find application in improving the energy efficiency of the crude distillation unit albeit in terms of the utility consumption alone [11].

Previous studies on the energy efficiency of crude distillation units assert the need for the energy improvements methods of the column to be based on second law efficiency [12] and exergy loss profiles of the column [13]. This is because efficiency based on second law provides means of understanding the improvement capability of a system while identifying and quantifying the sources of inefficiency within the system. For example, past works on the second law analysis (exergy) reveals low efficiency of some crude distillation systems. Cornelissen [14] performed analysis on a crude distillation unit with an exergy efficiency of 0.27 for an atmosphere distillation unit (ADU), while Al-Muslim and Dincer [15] came out with a result of 0.433 for an ADU. The first law analysis (energy efficiency) are always higher than the second law analysis in all cases. This could imply that improvement of the efficiency of the column will be better off when it is based on the second law. Even though there have been optimization procedures for the energy improvement of the crude distillation process they are often formulated by using energy consumption [16] and/or plant economic [17] as the objective functions. This might give a fictitious sense of accomplishment since energy based approach relies only on the first law of thermodynamics. The challenge is to develop ways of incorporating exergy in an optimization frame work especially for real time optimization. This work presents a data driven modelling approach for the optimization of an atmospheric distillation column based on first and second laws analysis aimed at minimizing the inefficiencies without compromising the qualities of the products. In addition, in order to improve the optimization reliability

especially for application to real time optimization, minimization of model prediction confidence bounds is incorporated in the objective function in addition to maximize the exergy efficiency of the column.

The paper is organized as follows: Section 2 gives a description of the atmospheric distillation unit and methods of analysis of the system such as exergy analysis and economic analysis. Section 3 deals with bootstrap aggregated neural network (BANN) modeling of the ADU. Section 4 gives the optimization technique and Section 5 concludes the paper.

## 2. Atmospheric distillation unit

## 2.1 Description of the system

Crude at its raw state is a relatively low value material but when refined could yield products whose value is many times that of the original crude. Refining of crude is in two stages of distillation: the atmospheric distillation unit and the vacuum distillation unit. The crude distillation unit under consideration is diagrammatically represented in Figure 1 [18] with a pre-flash column incorporated into the system. Preheated crude at 343°C and 344kPa is introduced at its flash point to the ADU. Superheated steam is injected at the bottom to enhance vaporisation and separation of the crude. The column processes 85,000 barrel/day of crude into 6 products: Light Naphtha, Heavy Naphtha, Kerosene, Diesel, Atmospheric gas oil (AGO) and Residue. Three side stream products are taken from the side strippers. The ADU is equipped with three pump arounds that recover heat for the preheat trains. The bottom product (residue) is the residual liquid material which could not be vaporised under the existing operating conditions of temperature and pressure in the tower. It is further fed to another tower which operates at subatmospheric pressure; the vacuum tower [19]. The side products of the vacuum distillation unit (VDU) are Light vacuum gas oil (LVGO) and Heavy vacuum gas oil (HVGO). The overhead product and the bottom product could serve as inlets to other processing units such as stabilisation and catalytic cracking unit respectively. This paper is focused on the atmospheric distillation unit highlighted in Figure 1.

## 2.2 HYSYS simulation

A process simulation software HYSYS is used for the modelling and simulation of the atmospheric distillation unit. The procedure for the simulation is further highlighted as follows. The crude is described by the TBP distillation curve given in Table 1 and the light ends properties in Table 2. The light ends basis in the assay is 16.8%.

#### Figure 1

Table 1

#### Table 2

#### 2.2.1 Modelling and simulation of the ADU

HYSYS contains a number of components in its data bank. The components are well defined with its thermodynamic and physical properties, temperature dependent properties such as enthalpy and critical properties. The light end components of the refineries were inputted here. It should be noted that the given components are from the laboratory analysis of the raw crude. Other unknown components of the crude are determined from the crude characterization in HYSYS. The property package in HYSYS includes Equation of states (EOSs), activity models, Chao Seadre models and vapour pressure models. One of the property package in EOS is Peng-Robinson. It is chosen as it is properly suited crude oil analysis. The Peng-Robinson method utilises EOS in its enthalpy calculations. Crude oil is a mixture of many identified chemical components and pseudo-components whose chemical identity might be difficult and sometimes impractical to determine. Hence, there is a need for the characterizations of the crude. The crude was characterized using experimental assay that include the bulk crude properties, light end volume percent, ASTM distillation, API gravity and TBP distillation. The result of the characterization is detailed chemical compositions of the identified components and the pseudo-components. The complete and definitive analysis of a crude oil is called *crude assay*. This is more detailed than a crude TBP curve.

## 2.2.2 Building the flow sheet

The modelling of the crude distillation units were done in the HYSYS environment using their operating and design parameters. The simulation was done to be prototype of the actual process as much as possible in terms of these parameters: the number of trays, feed tray, feed temperature, feed flow rates, heat exchangers supply and target temperatures, product specifications, steam flow rates, and pump around flow rates. Data such as entropy, enthalpy, temperatures, pressures, compositions and stream flow rates were extracted from the simulation for exergy analysis.

In the HYSYS simulation, the specifications of the products are added to the streams as given in Table 3 and the quality of the ADU product is maintained by ensuring the temperature difference between the 95% vol. and the 5% vol. of the ASTM D86 of two consecutive products is within the acceptable limit [20]. The ASTM curve for the product of ADU is shown in Figure 2.

## Table 3

## Figure 2

#### 2.3 Analysis of system

## 2.3.1 Exergy analysis

The total exergy of a stream is given as

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

where *Ex<sub>phy</sub>* and *Ex<sub>chem</sub>* are physical exergy and chemical exergy respectively.

The physical exergy is calculated as

$$Ex_{phy} = H - H_0 - T_0(S - S_0)$$
<sup>(2)</sup>

where H is the total enthalpy, S is the total entropy and T is the temperature. The subscript 0 denotes reference conditions

For the crude stream considered, standard molar chemical exergy  $Ex_{chem}$  is calculated from the standard molar chemical exergies of all identified components and pseudo-components as

$$Ex_{chem} = m \left[ \sum b_{qk} + \sum b_{chk} + RT_0 \sum lna_k \right]$$
(3)

Where  $b_{chk}$  is the chemical exergy for component k,  $b_{qk}$  is the chemical exergy for pseudo component k, and  $a_k$  is the activity coefficient of component k. The standard chemical exergy for pseudo-components can be determined for heuristic empirical expression as a function of the elementary composition and their heating values [21].

$$b_{qk} = \vartheta_k C_k \tag{4}$$

Where  $\vartheta_k$  is the regression equation to express the ratio H/C, N/C, O/C and S/C for pseudo-component k,  $C_k$  is the net calorific heating value of the pseudo-component k [22]. From Figure 1 the exergy for the inlet and outlet streams for the ADU are given as

$$\sum Ex_{out} = Ex_{LNaphtha} + Ex_{Hnaphtha} + Ex_{kero} + Ex_{diesel} + Ex_{AGO} + Ex_{residue}$$
(5)

 $\sum Ex_{in} = Ex_{Preflash \ liquid} + Ex_{steam} + Ex_{furnace} + Ex_{kero \ steam} + Ex_{diesel \ steam} + Ex_{AGO \ steam}$ 

The exergy efficiency and the irreversibility are then calculated as:

$$\varphi = \frac{\sum Ex_{out}}{\sum Ex_{in}}$$
(7)

$$I = \sum E x_{in} - \sum E x_{out} \tag{8}$$

Table 4 gives the results of the physical exergy of the ADU

## Table 4

## **2.3.2 Economic Analysis**

The total cost of the column is given as

$$Total cost = Energy cost + Capital cost$$
<sup>(9)</sup>

In the above equation,

$$Energy \cos t = \sum Q_x C_x \tag{10}$$

where  $Q_x$  is the duty of utility x and  $C_x$  is the unit cost of utility x.

While assuming that the retrofit of the atmospheric distillation unit might only involve adding or removing heat exchangers as the case may be, the capital cost estimation of the ADU is based on the heat exchanger cost. Hence the capital cost is given as [2]

$$Capital \ cost = Heat \ exchanger \ cost = A + B(area)^c \tag{11}$$

where A is the fixed cost of installation and B is exchanger cost per unit area.

For a stainless steel shell and tube heat exchanger,

Heat exchanger cost = 
$$33422 + 1784(area)^{0.81}$$
 (12)

The method of improvement being proposed here does not include a change in any of the equipment and hence the capital cost remains the same. Basically the economic analysis is based on the operating profit of the column and expressed mathematically as

$$Profit = \sum_{j=1}^{n} M_j C_j - [M_{crude} C_{crude} + M_{steam} C_{steam} + \sum_{x=1}^{n} Q_x C_x]$$
(13)

Where  $M_j$  and  $C_j$  are the flow rate and cost of the *j*th product,  $M_{steam}$  and  $C_{steam}$  are the flow rate and cost of steam respectively,  $Q_x$  and  $C_x$  are the heat requirement of utility and the cost of utility respectively. The

calculation is based on the assumption of 8600 h per year. In Table 5, the feed, products and utility prices are shown [23].

#### Table 5

## 3. Modelling of the Atmospheric distillation unit

#### 3.1 Data collection and processing

The inputs for the data driven model are the flow rates of all the ADU products, the three side strippers flow rates, the pump around rates and change in pump around temperatures. The input are chosen on the basis of being variables that can be manipulated and also impact the heat recovery of the process and hence the energy efficiency. The crude flow rate and hence its stripping steam were not considered as model inputs since they are constant for the case being studied. If the data for the modelling are to be taken from actual plant operating conditions and are found to be varied, then they should be considered as additional model inputs. The outputs are the products qualities and the exergy efficiency of the system.

Data for ANN models can be either obtained from process operation parameters [24] or from other models [25]. In this case study, simulated process operational data were generated from HYSYS (V8.2). Variables were varied within their lower and upper bounds in a nested loop. A total of 2048 data samples were generated. The chemical and physical exergies of all the inlets and outlets streams for each generated data were calculated (equations 1-4) and the corresponding exergy loss and exergy efficiency were evaluated (equations 7 and 8). 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 futher reduce. The number of hidden neurons was determined by building a number of neural networks with different numbers of hidden neurons and testing 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 Levenberg-Marquardt optimization trainning algorithm with regularisation and cross validation based "early stopping" was used to train the network. The final developed neural network model is evaluated on the unseen validation data. Because of the different magnitudes of the input and output data of the model, the data for the training, testing and validating were scaled to be in the range [-1, 1].

For enhanced model accuracy, boostrap aggregated neural network [26] is used in this study. 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 robutsness. These models can be developed on different parts of the data set. One further advantage of BANN is that model prediction confidence bounds can be calculated from individual network predictions. The confidence interval gives an indication of the prediction reliablity. The standard error of the *i*th predicted value is calculated as

$$\sigma = \left\{ \frac{1}{n-1} \sum_{b=1}^{n} \left[ y(x_i; W^b) - y(x_i; ) \right]^2 \right\}^{\frac{1}{2}}$$
(14)

where  $y(x_i) = \sum_{b=1}^n y(x_i; W^b) / n$  and *n* is the number of neural networks. The 95% prediction confidence bounds can be calculated as  $y(x_i;) \pm 1.96\sigma$ . It indicates a 95% certainty level that the interval will contain the true process output with a probability of 0.95. A narrower confidence bounds indicates the associated model prediction is more reliable.

#### 3.2 BANN model of the column

Bootstrap aggregated neural network models each containing 30 neural networks were developed for predicting the exergy efficiency and the product qualities of the ADU. Each network has a single hidden layer with 20 hidden neurons. It has been proved that a single hidden layer neural network with the sigmoid activation function in the hidden layer can approximate any continuous nonlinear function as long as the

number of hidden neurons is sufficient [27]. Sigmoid activation function was used for the hidden neurons and linear activation function for the output neuron. The 30 neural networks are different in that they are trained with different training data sets, which are obtained as bootstrap re-sampling replications of the original training data set, and they have different initial weights during training. Figure 3 shows the predicted and the actual values. The predicted and the actual values are super imposed on each other. This shows the BANN model almost perfectly mimic the actual data for the training, testing and validation. This gives a measure of confidence on the reliability of the model. In Figure 4, the prediction error between BANN model and actual process data is shown for the training, testing and validation data set. BANN model predictions can be said to be very accurate.

Figure 4 shows the scaled MSE of the individual networks. It can be seen from Figure 4 that a network with small training MSE may have quite large MSE on the validation data. This indicates inconsistency and non-robust nature of the individual networks. Table 6 shows the MSE of the bootstrap aggregated neural network models and the standard errors from the individual network predictions on the tarining and validation data sets. The model accuracy is seen to be improved by combining the imperfect models.

It can be seen that individual networks give inconsistent performance on the training and unseen validation data indicating the non-robust nature of single networks. BANNs give consistent and more accurate prediction performance on the training and unseen validation data sets.

## Figure 3

## Figure 4

## Table 6

## **4.1Optimization Techniques**

## 4.1 Optimization of exergy efficiency based on BANN model

The objective of the optimization here is to maximize the exergy efficiency of the atmospheric distillation unit. There are a number of decision variables in the ADU which finding their optimal can significantly improve the exergy efficiency of the ADU. The model prediction confidence bound, which depends on model input variables, is incorporated in the optimization problem. By penalizing wide model prediction confidence bounds, the optimization results are forced into the region where model predictions are reliable. The optimization formulation is given as

$$\max_{X} J = \varphi - \beta \sigma \tag{15}$$

s.t.

 $\varphi = U(x)$ 

where J is the objective function,  $\varphi$  is the exergy efficiency, U is the BANN model of the ADU,  $x = (x_1, x_2, ..., x_n)$  is a vector of decision variables which are the flow rates of light naphtha, heavy naphtha, kerosene, diesel, AGO, residue, AGO SS steam, Diesel SS steam, Kero SS steam, PA1, PA2, PA3, and PA1 $\Delta T$ , PA2 $\Delta T$ , PA3 $\Delta T$ ,  $\sigma$  is standard prediction error for BANN prediction, and  $\beta$  is the weighting factor of  $\sigma$ . Here PA represents pump around and PA1 $\Delta T$  represents the change in temperature in the pump around.

The optimisation problem was solved using the sequential quadratic programing (SQP) implemented by the function "fmincon" in MATLAB Optimisation Toolbox. Table 7 shows the optimum and HYSYS validated results with varying weighting factors of the confidence bounds. The approach in this work is to improve model prediction reliability using BANN and to provide a model prediction confidence bounds which is then penalized in the optimization objective function. The effect of penalization of the wide model prediction confidence bounds during the optimization can be clearly seen in Table 7. The result of the optimization without including the confidence bounds is included for the purpose of comparison. The relative error is calculated as the difference between BANN and HYSYS model predictions divided by the HYSYS model prediction. The method results in much less relative error between the BANN model and HYSYS model. This indicates the reliability of the proposed model because the performance on the actual process (HYSYS simulation) is close to that predicted by the neural network model. The improved reliability of the optimization results is due to the incorporation of model prediction confidence bounds in the optimization objective function. The selection of the weighting parameter,  $\beta$ , depends on the relative magnitudes of the two terms in the objective function. It should be selected so that a tradeoff between the two terms can be achieved. One could start with a small value and gradually increase it until the reduction in the standard error become small.

#### Table 7

Crude distillation operations are often bounded by product quality specifications. An optimal efficiency procedure without consideration to the quality specification might not be feasible in practice. For petrochemical system where it is not possible to give a discrete component specifications as a measure of the product quality, the 95% vol and 5% vol of the ASTM distillation is often use as a guide [28]. The quality of the products as %vol of the ASTM distillation for the base case and optimized case are given in Table 8. Quite often, optimization of distillation process is performed subject to one or two distillate qualities [29]. The method proffered here allows for inclusion of as many product qualities as desired. A number of methods exist in literature for online monitoring of chemical processes [30] especially crude distillation process qualities [31]. The method as proposed here could predict the product qualities and as well predict the optimum operating exergy efficiency of the column. Stringent requirement of petroleum quality demands the need to monitor and control the quality at all times. One approach is to use off-line laboratory analysis at periodical intervals. This could result in massive time delay and sometimes manual efforts. The other approach of online analyser could be expensive and difficult to predict its exactness.

a possibility of developing this method further to monitor the product quality with the added advantage of predicting the efficiency of the system. It could have applications in process monitoring, advanced control and fault diagnosis. In Table 8, the 95% vol and 5% vol of the ASTM distillation for the base case and the optimized cases are shown.

## Table 8

#### Table 9

In Table 7, the least relative prediction error is at when the weighting on confidence bounds is 0.5. Using this optimum case for the economy analysis of the optimization result, the optimization resulted in 76.71 % increment of the exergy efficiency as shown in Table 9. This translates to 44.8 % decrease in irreversibility loss in the column and 7.6 % reduction in energy costs of the column with reference to their initial values. Every real process has an element of irreversibility and often time the performance of engineering system is degraded by their presence. With the methodology proffered from this study, ways of considerably reducing the irreversibility of the system as well as determining the efficiency of the process is made easy. This will be a good tool in the hand of process and design engineers for the operation of energy efficient column. It could equally find relevance in the control of the column for improving efficiency.

The total profit is increased by  $26.3 \times 10^4$ /year. The increment is mainly due to the optimum operating conditions from the exergy based analysis of the column. The reduction in the cost of energy contributed to about 0.8% in the total profit. The results show that considerable economic benefit of the column can be achieved at no additional cost of equipments.

#### 4 Conclusions

The challenge for the design and optimization of crude distillation system involves developing models that are reliable and computationally efficient. ANN models of distillation column has been developed, however, the reliability might be questionable especially for real time optimization of the process. The BANN models were found to predict optimum operating conditions of the ADU. The historic data of a plant can be utilized to build a neural network model. If a system is generated based on real conditions of operation of a plant, the system can be constantly improved. This is because new operating conditions from the plant can be used to train and adjust the neural network. This will guide operators and design engineer to operate the plant at the most energy efficient conditions. Product quality constraints on the column also introduced a measure of penalization on the optimization result to give as close as possible to what obtains in reality. The proposed technique can significantly improve the second law efficiency of the system with an additional economic advantage. Most methods found in the literature are based only on the first law analysis of the column. This might give a fictitious sense of achievement. The proposed modeling and optimization strategy can aid in the operation and design of energy efficient column. The proposed method can also be applied to other systems as long as the operational data of the systems are available and the exergy efficiency of the systems can be modelled and then optimized.

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## Nomenclature

- API American petroleum Institute
- Ex Exergy rate, kJhr<sup>-1</sup>
- H Total enthalpy, kJhr<sup>-1</sup>
- m Molar flow, kmolhr<sup>-1</sup>

PA	Pump	around
----	------	--------

## PA $\Delta$ T Change in pump around temperature

- P<sub>0</sub> Reference pressure, kpa
- S Specific entropy, kJhr<sup>-1</sup>K<sup>-1</sup>
- SS Side stripping
- TBP True boiling point
- T<sub>0</sub> Reference temperature, K
- *W<sup>b</sup>* Network weight for bootstrap sample
- $x_i$  Neural network input
- $\sigma \sigma_e$  Standard prediction error
- $\varphi$  Exergy efficiency, %

## Subscript

- 0 Reference conditions
- phy Physical
- chem Chemical

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# **FIGURES**



Figure 1: Schematic diagram of the atmospheric distillation unit



Figure 2: ASTM D86 of end products of the ADU



Figure 3: BANN model of the ADU



Figure 4: BANN predicted vs. actual exergy efficiency (left) and prediction errors (right) for training, testing and validation data



Figure 5: Model error of individual networks for the crude distillation unit

# TABLES

Assay Percent	Temperature (K)
2.68	309
7.2	366.5
15	422
24.5	477.6
33.31	533.1
44.70	588.7
49.60	616.5
59.14	672
75.22	783
84.46	866.5
95.81	1023

Table 1: TBP distillation curve

Light ends	Composition (mass%)
Propane	0.7595
i-Butane	0.5622
n-Butane	0.1567
i-Pentane	1.173
n-Hexane	4.203
n-Heptane	1.308
n-Octane	5.475
n-Nonane	2.939
n-Pentane	0.2167

Table 2: Light ends assay

Table 3: ADU product specifications

Products	Specifications (K)
Light Naphtha	ASTM D86 95% =384
Heavy Naphtha	ASTM D86 95% =455
Kerosene	ASTM D86 95% =541
Diesel	ASTM D86 95% =599
AGO	ASTM D86 95% =710

Stream Name	h(kJ/kmol)	h <sub>0</sub> (kJ/hr)	s(kJ/hrK)	s <sub>0</sub> (kJ/hrK)	m(kmol/hr)	Ex
Inlet streams						
Crude inlet	-271082	-463266	730.2	309.4	2227	$1.487 \times 10^{8}$
Crude Steam	-230832	-286232	186.5	53.66	125.9	1.993×10 <sup>6</sup>
Kero Steam	-230832	-286232	186.5	53.66	88.13	1.395×10 <sup>6</sup>
Diesel Steam	-230832	-286232	186.5	53.66	62.95	9.964×10 <sup>5</sup>
AGO steam	-230832	-286232	186.5	53.66	18.88	2.988×10 <sup>5</sup>
Furnace duty						6.792×10 <sup>7</sup>
TOTAL IN						2.213×10 <sup>8</sup>
Outlet streams						
L Naphtha	-162826	-194812	187.17	96.83	594.99	3.013×10 <sup>6</sup>
H Naphtha	-219225	-261920	218.21	103.10	504.00	4.228×10 <sup>6</sup>
Kerosene	-286630	-356746	338.35	158.68	423.00	7.010×10 <sup>6</sup>
Diesel	-346029	-476298	578.41	267.78	177.00	6.674×10 <sup>6</sup>
AGO	-386917	-599476	871.93	396.66	184.00	1.305×10 <sup>7</sup>
Residue	-586313	-992013	1677.13	805.88	479.27	7.001×10 <sup>7</sup>
TOTAL OUT						1.040×10 <sup>8</sup>

 Table 4: Simulation data for exergy analysis

Table 5: Feed, products and utility prices

Item	Cost	Unit
Crude oil	80	\$/bbl
Light Naphtha	44.3	\$/bbl
Heavy Naphtha	136	\$/bbl
Kerosene	122.7	\$/bbl
Diesel	121.7	\$/bbl
Atmospheric gas oil	95.29	\$/bbl
Residue	89.71	\$/bbl
Fired heating	150	\$/kJ
Cooling water	5.25	\$/kJ
Stripping steam	0.14	\$/kmol

Table 6: Bootstrap aggregated neural network prediction accuracy for the ADU

	Mean square error	Standard prediction error
Testing data	4×10 <sup>-6</sup>	6×10 <sup>-6</sup>
Validation data	1.6×10 <sup>-5</sup>	1.9×10 <sup>-5</sup>

Items	Base	β=0	β=1	β=0.5	LB	UB	Unit
AGO	184	170	170	170	165	190	barrel/hr
Diesel	177	160	160	160	160	184	barrel/hr
Kerosene	423	410	410	410	405	435	barrel/hr
L Naphtha	595	585	585	585	585	605	barrel/hr
H Naphtha	504	490	490	490	480	510	barrel/hr
PA1	1588	1587	1587	1454.7	1349	1826	barrel/hr
ΡΑ1ΔΤ	50	40	55	40	40	60	°C
PA2	997	995.7	997.4	848	848	1147	barrel/hr
ΡΑ2ΔΤ	70	60	76.2	60	60	80	°C
PA3	451	449.8	450	383	383	518	barrel/hr
ΡΑ3 ΔΤ	70	60	60	60	60	80	°C
AGO steam	18.8	15	19	15		25	kmol/hr
Diesel steam	62.9	55	57	55		70	kmol/hr
Kero steam	88.1	80	80	92		95	kmol/hr
Optimum		79.83	69.01	83.67			%
efficiency							
HYSYS	46.99	77.47	69.61	83.04			%
validated							
Error		0.0304	0.0087	0.0075			

Table 7: Summary of optimization results with different weightings on confidence bounds

 Table 8: ASTM distillation of ADU products

	A5%°C	D5% °C	K5% °C	L5% °C	H5% °C	R5% °C
Base case	266.3	230.9	155.5	-46.62	93.67	775
Optimised	259.5	225	153.8	-46.84	86	772

A, D, K, L, H, R are AGO, Diesel, Kerosene, Light Naphtha, Heavy Naptha and Residue respectively.

 Table 9: Optimisation results (efficiency and profit)

	Exergy (%)	Irreversibility	Steam cost	Energy cos	st Profit (\$/yr)
		(kJ/hr)		(\$/yr)	
Base case	46.99	$1.174 \times 10^{8}$	3.562×10 <sup>5</sup>	$3.456 \times 10^{6}$	3.030×10 <sup>9</sup>
Optimum	83.04	6.478×10 <sup>7</sup>	3.322×10 <sup>5</sup>	3.193×10 <sup>6</sup>	3.055×10 <sup>9</sup>