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DEVELOPMENT OF NEURAL NETWORK MODELS FOR A CRUDE OIL DISTILLATION COLUMN

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Abstract. This paper discusses the development of artificial neural network (ANN) models for a crude oil distillation column. Since the models were developed for real time optimisation (RTO) applications, they are steady-state, multivariable models. Training and testing data used to develop the models were generated from a reconciled steady-state model simulated in a process simulator. The radial basis function networks (RBFN), a type of feedforward ANN model, were able to model the crude tower very well, with the root mean square error for the prediction of each variable less than 1%. Grouping related output variables in a network model was found to give better predictions than lumping all the variables in a single model; this also allowed the overall complex, multivariable model to be simplified into smaller models that are more manageable. In addition, the RBFN models were also able to satisfactorily perform range and dimensional extrapolation, which is necessary for models that are used in RTO.

1.0 INTRODUCTION

1.1 Background

Mathematical models are important in chemical engineering, both in the design and operation of chemical plants. In plant operation, models are required for analysis, control (particularly advanced control), and optimisation. Real time optimisation (RTO), which is the continuous evaluation and adjustment of process operating conditions to optimise the economic productivity subject to constraints, requires rigorous steady-state plant models.

Good process models are critical for a successful implementation of RTO. Currently, most RTO implementation uses rigorous first principles (FP) mathematical models, which are not only complex and costly to develop, but also cumbersome and difficult to maintain because of skill and time requirements [1]. The high computation time required in solving the models is also a major problem for on-line applications. In fact, developing reliable models for a chemical process is a major obstacle in implementing advanced control and optimisation because of the complexity and cost involved [2]. This leads to the quest for finding other types of suitable models, such as artificial neural network (ANN).

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ANN had generated much interest in the chemical engineering community since the late eighties as an alternate approach to model a process. Many industrial applications have been reported [3, 4, 5, 6, 7]. ANN, a connectionist-based (black box) model, consists of layers of nodes with non-linear basis functions and weighted connections that link the nodes. Using the nodes and weights, the inputs are mapped to the outputs after being trained with a set of training or learning data. Multilayer feedforward ANN were mathematically proven to be a universal approximator [8]. However, since ANN is data driven, the resulting model can only be as good as the data provided to the network.

Recently, there are several studies that report a preference using ANN models eventhough rigorous FP models for the processes are available [9, 10, 11]. The FP models were used to generate data for developing ANN models. ANN models are suitable for on-line applications because of the short computation time to solve the ANN model and its ability to accurately represent the model. In optimisation, this is especially advantageous since the model must be accessed by the optimiser and computed repeatedly. For example, Nascimento *et al.* [9] successfully optimised the operating conditions of a nylon-6,6 polymerisation process. The pure ANN model for the process was developed using data generated from a rigorous semi-mechanistic model that had been fitted to the plant data. Optimisation was performed off-line by mapping all the possible solutions within the region of interest using the ANN model and locating the optimum using a grid-search method.

ANN models developed for RTO are different from those developed for process control or other off-line applications. RTO requires steady-state models that can yield all output variables required by the optimiser. For large, multivariable processes, there can be more than 100 input and output variables. In addition, since the application is on-line, the models must also have short computation times.

A desirable feature of ANN models developed for RTO is to have the ability to extrapolate slightly beyond the training range, especially for applications in optimisation because logical estimates are essential for optimisation algorithms that utilize the infeasible path approach to search for the optimum value. Although ANNs are usually poor extrapolators, there were studies on the development of ANN models that could satisfactorily perform range and dimensional extrapolation. Range extrapolation takes place when one of the input variables to a model is applied outside the range that it was trained for. Dimensional extrapolation takes place when a variable that was not part of the input variable during identification (because it was constant during the training phase) varies during the use of the model [12]. The ability to extrapolate slight beyond the training range is important, especially for applications in optimisation because feasible answers are essential when optimisation algorithms that violate constraints slightly in an effort to reach the optimum value are used.

This paper presents the development of ANN models for an industrial crude oil distillation column that is suitable for an RTO application. The crude tower is a prac-

tical candidate due to variations in operating conditions and its complex, multivariable nature. The ANN models developed are steady-state, multivariable models for the complete process. Thus, they are different from ANN models for process control, which are dynamic models used to predict one or two variables that are usually pub-

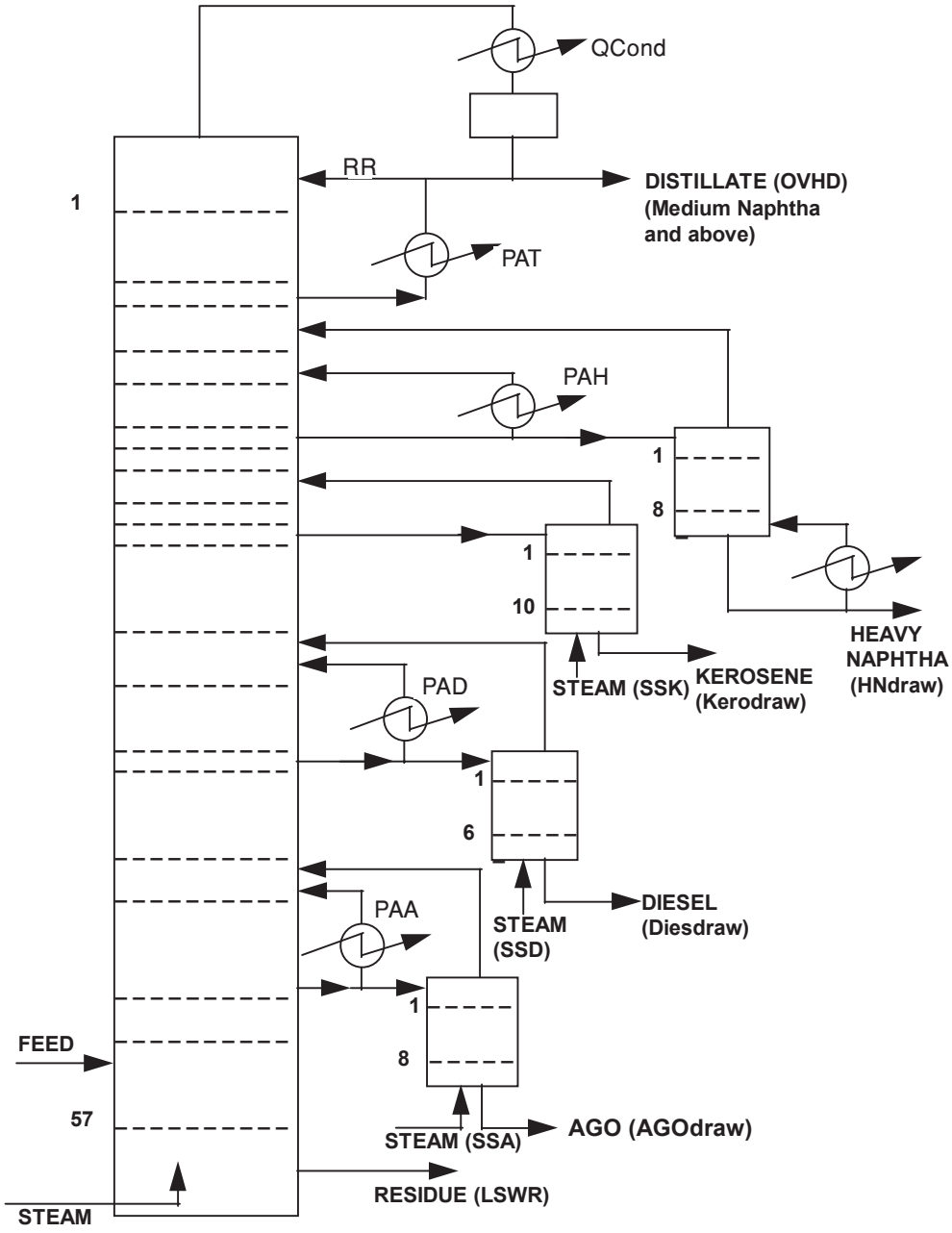

Figure 1 Schematic diagram of the crude oil distillation tower

lished in the literature. In addition, the ANN models developed were tested for range and dimensional extrapolation.

1.2 The Crude Oil Distillation Column

The crude oil distillation tower used in this study is an actual operating column. The tower (Figure 1) was designed to process sweet crude oil (crude oil with low sulfur content) and condensate. This process faced problems brought about by the varying composition and fractions of the crude oil and condensate feed.

The column has four pumparounds (p/a), four side strippers, and six product streams, which are the distillate, heavy naphtha, kerosene, diesel, atmospheric gas oil (AGO), and low sulphur waxy residue (LSWR) streams. In actual operation, the product draw-off flowrates are adjusted to ensure on-specification products and to achieve the targeted production rate. The feed flow rate is adjusted according to the production target. The feed entering the column consists of a mixture of two feed streams, namely the condensate stream, of which the light components were flashed off, and the crude oil stream. The feed composition depends on the mixture of the oil and condensate being fed to the column.

Products from the side draws must meet certain specifications. Operators obtain these specifications from the production planning section and adjust the tower operating conditions to ensure on-specification products. The quality specifications are checked, off-line, once during each shift - twice a day - at 06:00 and 18:00, and are thus called "cold" properties. Table 1 lists the specifications and the corresponding products and manipulated variables. It is important to take note of the cold properties because these are the variables that would be predicted in the model output.

Table 1 Product specifications and manipulated variables of the crude tower

Specifications/Properties	Manipulated	Variables
Heavy Naphtha	IBP	Top temperature or Q
	FBP	HN draw
Kerosene	Flash Point/IBP	HN draw
		SS
	Freeze Point/FBP	Kerosene draw
Diesel	Pour Point/Colour IBP	Diesel draw
	FBP	Kerosene draw
		Diesel draw
AGO	Pour Point/Colour	AGO draw
	IBP	Diesel draw
	FBP	AGO draw
LSWR	Pour Point	AGO draw

Note: IBP is initial boiling point
FBP is final boiling point
Q is reboiler duty
SS is stripping steam rate

2.0 METHODOLOGY

2.1 Data Generation

To develop the ANN model, data were first generated for the purpose of training and testing. A reconciled steady-state simulation of the crude tower was developed in Aspen Plus using the PETROFRAC model, a rigorous tray by tray equilibrium based distillation column model designed specifically for petroleum applications. The main column, side strippers, pumparounds, and condenser were all modelled as part of the column with PETROFRAC.

To obtain an accurate feed composition for the simulation, the products of the crude tower section were back-mixed and analysed in the plant. The feed assay information provided to Aspen Plus included the true boiling point (TBP) curve, light ends analysis, stream specific gravity, and average molecular weight. All these information were obtained from the laboratory analyses conducted in the plant. In Aspen Plus, the feed stream compositions were approximated with seven conventional components ranging from C2 to C5, and about 50 pseudo-components. The Peng-Robinson equation of state, which is recommended for refinery applications [13], was used to calculate all thermodynamic properties.

Table 2 Input and output variables for each section of the crude distillation column

Crude tower section	Input variables	Output variables
Top of main column	Bintolt, Htfeed, HNdraw, Kerodraw, Qreb	Ttop, Ovhd, RR, Qcond, PAT
HN stripper	Bintolt, Htfeed, HNdraw, Kerodraw, Qreb	TtopH, TbotH, PAH, IBPH, FBPH, RhoH
Kerosene stripper	Bintolt, Htfeed, HNdraw, Kerodraw, Diesdraw, SSK	TtopK, TbotK, FPKero, IBPK, FBPK
Diesel stripper	Bintolt, Htfeed, Kerodraw, Diesdraw, AGOdraw, SSD	TtopD, TbotD, IBPD, FBPD, PourD, PAD
AGO stripper	Bintolt, Htfeed, Diesdraw, AGOdraw, SSA	TtopA, TbotA, IBPA, FBPA, PourA, PAA
LSWR (Bottom of main column)	Bintolt, Htfeed, AGOdraw, SSM	TBot, PourL

The sensitivity analysis feature in Aspen Plus was used to generate training and testing data for the crude tower. Input variables for the ANN models include the feed flow rates for the two feed streams, and the specified variables of a particular section for the tower operation. The output variables are the dependant variables that were

needed by the optimiser and were calculated due to changes in the input variables. Ranges for the variables were within the operating region of the column. Within this region, the variables in each section of the column have negligible influence on other sections in the column, except the sections that are immediately above and below it. This allowed data to be generated one section at a time. However, any section of the column that had more than five independent variables was simulated one at a time for each value of the sixth independent variables because the sensitivity analysis feature of Aspen Plus only allows a maximum of five independent variables.

Table 2 lists the input and output variables of the network models for each section of the crude distillation column. Only variables associated with the particular section were included in the network model.

2.2 ANN Model Development

In this work, all ANN models were developed in MATLAB environment. Radial basis function networks (RBFN) were chosen to model the crude tower because of the short training times. RBFNs are multilayer feedforward networks. The networks have an input layer, a hidden layer, and an output layer. The RBF network has a single hidden layer of nodes with Gaussian density function. MATLAB uses the orthogonal least squares (OLS) algorithm by Chen *et al.* [14] to solve for the RBF centers and weights for the connections between the nodes in the hidden and output layers.

To develop the RBFN models, other than specifying an error goal, the spread constant, σ, which determines the width of the receptive fields must also be specified. σ should be large enough for the receptive fields to overlap one another for ample coverage of the whole input range. Nevertheless, it should not be too large that there is no distinction between the output of different nodes in the same area of the input space. The values of s for the models were found through systematic trial and error. Since the spread of data for each section of the crude tower was approximately equal, the suitable value of σ, between 0.15 and 0.20, was found to be almost equivalent for all the models.

Once the error goal for training and σ had been specified, the RBFN model was trained using the set of training data for the section. The OLS algorithm used by MATLAB added one node at a time to the model until the error goal was satisfied. The model was then verified with a set of training data for the particular section.

Evaluations of the models are based on root mean squared (RMS) error from each model prediction. Error is defined as the difference between desired (or actual value provided by the testing data) output value and the predicted output value. Training time was also taken into consideration, mainly because of the convenience in developing models with short training times. Nevertheless, this was not as important as RMS error because once trained, the execution of the model was very fast. The training time was only a major concern if the model was periodically updated on-line. For all the models, the results presented in this paper were the best ones obtained after numerous trials of different training error tolerance and spread constant.

The crude tower model was not developed as a single lumped system. Changes within the operating range for a section in the crude distillation tower affected only the sections that were immediately above and below the section. Therefore, it allowed the crude tower model to be divided into sections where the related variables were grouped together, and thus made the model more manageable.

The ANN model for the crude tower was divided into the following sections:

1. top (T),
2. heavy naphta stripper (HN),
3. kerosene stripper (K),
4. diesel stripper (D),
5. AGO stripper (A), and
6. bottom (B).

Input and output variables of the network models for each module of the crude distillation column are listed in Table 2. Each section had 300 training data and 150 testing data.

3.0 RESULTS AND DISCUSSION

3.1 Prediction of Variables

Several techniques may be used to predict all the output variables. One way would be to predict all the variables in the crude tower using a single RBFN model, which would result in a single, large model. On the other hand, the variables may also be predicted individually such as one at a time, which would result in many RBFN models, each with a single output. The variables may also be grouped either randomly or according to the respective sections.

To determine if the grouping of output variables had a strong influence on the prediction, the variables in the first two sections at the top of the column were predicted individually and in different groups. The results are shown in Table 3, where the first 11 output variables (from Ttop to RhoH) were predicted individually. This means that each output variable had a RBFN model where the input variables comprised of the input variables of the corresponding section. For example, the model for predicting Ttop, which was an output variable in the top section of the crude tower, had Bintolt, Htfeed, HNdraw, Kerodraw, and Qreb as the input variables. Table 2 listed the input and output variables for each section of the tower.

From Table 3, it can be seen that for almost all the variables, the RMS errors are smaller when the variables are grouped together in a suitable combination. For example, the RMS errors for variables at the top of the column, Ttop, Ovhd, RR, Qcond and PAT are 0.0048, 0.0029, 0.0046, 0.0033, and 0.0140 respectively when predicted individually, compared to 0.0014, 0.0015, 0.0025, 0.0017, and 0.0075 respectively when predicted together. This is also true with the variables in the HN section.

Table 3 RMS errors of variables of top and HN sections of the crude tower

Outputs	Overall RMS Error	Individual RMS Error
Ttop	0.0048	
PAT	0.0140	
RR	0.0046	
Ovhd	0.0029	
Qcond	0.0033	
TtopH	0.0039	
TbotH	0.0039	
PAH	0.0099	
IBPH	0.0046	
FBPH	0.0046	
RhoH	0.0076	
IBPH, RR, Qcond	**0.0134**	**0.0051, 0.0042, 0.0041**
Ttop, RR, Qcond	**0.0067**	**0.0023, 0.0035, 0.0009**
Ttop, Ovhd, RR, Qcond, PAT	0.0146	0.0014, 0.0015, 0.0025, 0.0017, 0.0075
TtopH, TbotH, PAH, IBPH, FBPH, RhoH	0.0292	0.0021, 0.0028, 0.0121, 0.0029, 0.0019, 0.0074

The results also show that it is not advisable to combine unrelated variables. For example, comparing the two variable combinations that are highlighted in bold letters in Table 3, the combination with IBPH, which is in a different section than RR and Qcond, the RMS error for RR and Qcond are higher than when the variables were combined with Ttop.

3.2 Overall Prediction

The RMS errors for all output variables of the crude tower are given in Table 4. Output variables in the same section were grouped and predicted together. The results, as seen in the table, are very good. All the RMS errors are in the order of 10^{-3}, and some are even smaller. This is because the model is continuous within the operating range. The results also show that RBFN is suitable for predicting the output variables of the crude tower.

Table 4 Overall result for all sections in the crude distillation tower

Outputs (y1,y2,y3,y4,y5,y6)	Total RMS Error	Individual RMS Error
Top column section Ttop, Ovhd, RR, Qcond, PAT	0.0146	0.0014, 0.0015, 0.0025, 0.0017, 0.0075
HN stripper section TtopH, TbotH, PAH, IBPH, FBPH, RhoH	0.0292	0.0021, 0.0028, 0.0121, 0.0029, 0.0019, 0.0074
Kerosene stripper section TtopK, TbotK, FPKero, IBPK, FBPK	0.0174	0.0018, 0.0017, 0.0021, 0.0021, 0.0097
Diesel stripper section TtopD, TbotD, IBPD, FBPD, PourD, PAD	0.0210	0.0037, 0.0036, 0.0052, 0.0054, 0.0030, 0.0001
AGO stripper section TtopA, TbotA, IBPA, FBPA, PourA, PAA	0.0133	0.0005, 0.0007, 0.0021, 0.0050, 0.0012, 0.0038
LSWR section (Bottom of main column)TBOT, PourL	0.0098	0.0038, 0.0060

3.3 Range and Dimensional Extrapolation

The ability to extrapolate slightly beyond the training range is essential, especially for applications in optimisation because logical predictions are essential when infeasible path optimisation algorithms are used. Range extrapolation is defined as having one of the input variables to a model being applied outside the range that it was trained for, while dimensional extrapolation is defined as having a variable that was not part of the input variable during identification varying during the use of the model [12]. A well-known weakness of some types of ANN models, like the commonly-used multilayer perceptrons, is the inability to extrapolate outside the training range. Therefore, to ensure that the RBFN model can perform satisfactorily in both range and dimensional extrapolation, the kerosene section of the column was tested. A model for the kerosene section was developed with five input variables instead of six, leaving out the kerosene stripping steam in the input to test for dimensional extrapolation. The stripping steam rate was fixed at the normal operating point. A test data set was developed with the stripping steam at the maximum and minimum operating range.

To test for range extrapolation, a test data set was developed with the stripping steam at 10% above the maximum and 10% below the minimum steam rate. Although this condition is avoided in practice, developing a model that would be feasible just outside its range is important because certain optimisation algorithms crosses over

constraints slightly in an effort to find a path to reach the optimum value.

Table 5 shows the results for both range and dimensional extrapolations. The results obtained for range extrapolation was close to the original results. There is less than 15% increase in the total RMS error. Thus it shows that the RBFN model is able to provide a reasonable prediction should the optimiser crosses over a constraint slightly. There was, however, a nearly three-fold increase in total RMS error for the dimensional extrapolation case. Nevertheless, the predictions are still satisfactory and can be accepted for use because all the individual RMS errors are around 1% or less. Therefore, the RBFN model is suitable for modelling the crude tower for RTO.

Table 5 RMS errors for range and dimensional extrapolation

Outputs (y1,y2,y3,y4,y5)	**Total RMS Error**	**Individual RMS Error**
Original result TtopK, TbotK, FPKero, IBPK, FBPK	0.0174	0.0018, 0.0017, 0.0021, 0.0021, 0.0097
Dimensional extrapolation TtopK, TbotK, FPKero, IBPK, FBPK	0.0515	0.0110,0.0242,0.0024,0.0034,0.0105,
Range extrapolation TtopK, TbotK, FPKero, IBPK, FBPK	0.0200	0.0028,0.0026,0.0027,0.0029,0.0090

4.0 CONCLUSIONS

The results obtained from this study showed that RBFN is suitable for modelling the crude oil distillation column. In addition, the RBFN model for the crude tower was able to satisfactorily perform range and dimensional extrapolation, which are essential for RTO applications.

It can also be concluded that to develop ANN models for large, multivariable systems, output variables that are related should be grouped together, as this would lead to better predictions. Decomposing multivariable systems into smaller modules is also necessary, so that the developed models are more manageable. In addition, grouping unrelated variables together degenerates the model, and as such is not advisable.

REFERENCES

[1] Naysmith, M., Ph.D. Thesis. 1997. Dept. of Chemical Engineering. University of Waterloo.

[2] Hussain, M. 1999. "Review of the Applications of Neural Networks in Chemical Process Control - Simulation and Online Implementation". *Artificial Intelligence in Engineering.* 13: 55-68.

[3] Zhao, J., B. Chen, and J. Shen. 1997. "A Hybrid ANN-ES System for Dynamic Fault Diagnosis of Hydrocracking Processes". *Computers in Chemical Engineering*. 21, Supplement, S929-S933.

[4] Turner, P., G. Montague, and J. Morris. 1996. "Dynamic Neural Networks in Non-linear Applications (an

Industrial Application)". *Computers in Chemical Engineering*. 20, Supplement, S937-S942.
[5] Baratti, R., G. Vacca, and A. Servida. 1995. "Neural Network Modelling of Distillation Columns". *Hydrocarbon Processing*. 35-38.
[6] Cheung, T., O. Kwapong, and J. Elsey. 1992. "Building Empirical Models of Process Plant Data By Regression or Neural Network". *Proceedings of American Control Conference.* Chicago. 1922-1925.
[7] Thibault, J., and B. Grandjean. 1991. "Neural networks in Process Control – A Survey". *Proceedings of IFAC Advanced Control of Chemical Processes*. Toulouse, France. 251-278.
[8] Hornik, K., M. Stinchcombe, and H. White. 1989. "Multilayer Feedforward Neural Networks are Universal Approximators". *Neural Networks*. 2: 359-366.
[9] Nascimento, C., R. Giudici, and R. Guardani. 2000. "Neural Network Based Approach for Optimization of Industrial Chemical Processes". *Computers and Chemical Engineering*. 24: 2303-2314.
[10] Altissimi, R., A. Brambilla, A. Deidda, and D. Semino. 1998. "Optimal Operation of a Separation Plant using Artificial Neural Networks". *Computers in Chemical Engineering*. Vol. 22, S939-S942.
[11] Sabharwal, A., N. Bhat, and T. Wada. 1997. "Integrate Empirical and Physical Modelling". *Hydrocarbon Processing*. 105-112.
[12] te Braake, H., H. van Can, and H. Verbruggen. 1998. "Semi-mechanistic Modeling of Chemical Processes with Neural Networks". *Engineering Applications in Artificial Intelligence*. 11: 507-515.
[13] Aspen Technology Inc., Cambridge, Massachusetts. 1995. *ASPEN PLUS User Guide*. Volume 1, release 9.2 edition.
[14] Chen, S., C. Cowan, and P. Grant. 1991. "Orthogonal Least Squares Learning Algorithm for Radial Basis Function Networks". *IEEE Transactions on Neural Networks*. 2(2): 302-309.

NOMENCLATURE

- Bintolt is the condensate feed from the storage tank.
- Htfeed is the crude oil feed from the storage tank.
- HNdraw, Kerodraw, Diesdraw and AGOdraw are heavy naphta (HN), kerosene, diesel, and AGO product draw off, respectively.
- Qreb is the reboiler duty of the HN side stripper.
- SSK, SSD, and SSA are the stripping steam rates for the kerosene, diesel, and AGO side strippers respectively, and SSM is the main column strping steam rate.

The following lists the nomenclature of the output variables used in Table 2:

- TtopH, TtopK, TtopD, and TtopA are the top temperatures of the HN, kerosene, diesel, and AGO strippers, and Ttop is the top temperature of the main column.
- TbotH, TbotK, TbotD, and TbotA are the bottom temperatures of the HN, kerosene, diesel, and AGO strippers, and Tbot is the bottom temperature of the main column.
- PAT, PAH, PAD, and PAA are the p/a at the top of the main column, and the HN, diesel, and AGO strippers respectively.
- Ovhd is the overhead draw off rate.
- RR is the reflux ratio.
- Qcond is the condenser duty of the main column.
- IBPH, IBPK, IBPD, and IBPA are the initial boiling point of HN, kerosene,

diesel, and AGO produced respectively.
- FBPH, FBPK, FBPD, and FBPA are the final boiling point of HN, kerosene, diesel, and AGO produced respectively.
- RhoH is the density of HN.
- FPKero is the flash point of kerosene.
- PourD, PourA, and PourL are the pour points of diesel, AGO, and LSWR produced respectively.