CONNECTIONIST MODELS OF A CRUDE OIL DISTILLATION COLUMN FOR REAL TIME OPTIMISATION

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ABSTRACT

This study presents the development of connectionist or artificial neural network (ANN) models of a crude oil distillation column that can be utilised for real time optimization (RTO). The column is an actual distillation tower in operation in a refinery in Malaysia. Connectionist models developed for RTO are different than for process control applications because they are steady state, multivariable models. Training data for the network models was generated using a reconciled steady state process model simulated in the Aspen Plus process simulator. All ANN models were coded and simulated in MATLAB. Two types of feedforward network models were developed and compared: multi-layer perceptron (MLP) with adaptive learning rates and radial basis function networks (RBFN). The RBFN models were found to yield better and more consistent predictions with shorter training times than the MLP models. Grouping suitable output variables in a network model were found to give better predictions, and allow the complex, multivariable model of the crude tower to be more manageable.

Keywords: connectionist, neural network, modelling, crude oil distillation.

1.0 INTRODUCTION

Connectionist or artificial neural network (ANN) models are black box models, consisting of layers of nodes with nonlinear basis functions and weighted connections that link the nodes. The inputs to the model are mapped to the outputs after being trained with a set of training or learning data to optimise the weights and biases of the nodes. Multilayer feedforward ANN were mathematically proven to be a universal approximator [Hornik, et. al., 1989].

Connectionist models have generated much interest in the chemical engineering community since 1980's. They are widely applied in chemical industries as substitutes for dynamic mathematical models, especially in the area of fault diagnosis, dynamic process modelling and process control. Applications in chemical engineering include those in petroleum refineries [Cheung, et. al., 1992; Thompson et. al, 1996; Zhao et. al., 1997], chemical plants [Turner, et. al., 1996; Baratti, et. al., 1995], polymerisation processes [Nascimento, et al., 2000], biotechnology [Thibault, et. al, 2000, Schubert, et. al., 1994], metallurgical processes [Meghlaoui, et. al, 1998; Reuter, et. al., 1993], wastewater treatment [Gontarski, et al., 2000; Syu and Chen, 1998], and oil recovery [Elkamel, 1998].

RTO, which is the continuous evaluation and adjustment of process operating conditions to optimise economic productivity, traditionally requires mathematically rigorous steady-state plant models. These models are difficult and expensive to develop and maintain because of skill and time requirements [Naysmith, 1997]. Currently, there are efforts to seek other types of suitable models, such as off-the-shelf commercial simulation packages, or purely black box models like connectionist or artificial neural networks (ANNs) models. A previous research found using commercial simulation packages for RTO to be impractical [Naysmith, 1997]. Several works suggested the use of ANN as the process model for real time optimisation (RTO) [Thompson, et al., 1996; Thompson and Kramer, 1994]. In one study, an important variable was estimated using an ANN model as part of a larger rigorous model for use in on-line supervisory optimisation [Sabharwal, 1997]. In the work of Nascimento and Giudici [1998], rigorous first principle models were used to generate training and testing data to develop ANN models for a chemical process to be used for optimisation. In the studies, the ANN models were found to be accurate and were able to cut down computation time.

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 practical candidate due to variations in operating conditions and its complex, multivariable nature. The ANN models developed are different from those used for process control or other off-line applications because steady-state models are required, instead of dynamic models that are usually discussed in the literature. In addition, the models developed are for the complete process, rather than for just specific variables, which is the case in most published works.

2.0 MODEL DEVELOPMENT

2.1 Process Description and Data Generation

Figure 1 shows a schematic diagram of the crude distillation column, which is currently in operation. The column has four pumparounds (p/a), four side strippers and six product streams, which are the distillate, heavy naphta, 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. Feed going into the column consists of a mixture of two different feed streams: Bintulu condensate stream, of which the light components were first flashed off, and Tapis crude, a sweet crude oil stream. The feed composition depends on the mixture of the oil being fed to the column.

Product from the side draws must meet certain specifications. Operators obtain these from the production planning section and adjust the tower operating conditions to ensure on-spec 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 of the products and the corresponding manipulated variables.

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 sensitivity analysis feature in Aspen Plus was used to generate training and testing data for the crude tower. The model for the crude tower are divided into the following sections: 1) top (T), 2) heavy naphta stripper (HN), 3) kerosene stripper (K), 4) diesel stripper (D), 5) AGO stripper (AG), and 6) bottom (B).

Only variables associated with the particular section were included in the network model. 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. Table 2 lists the input and output variables of the network models for each section of the crude distillation column. Nomenclature for the input and output variables is given in the nomenclature section at the end of this paper.

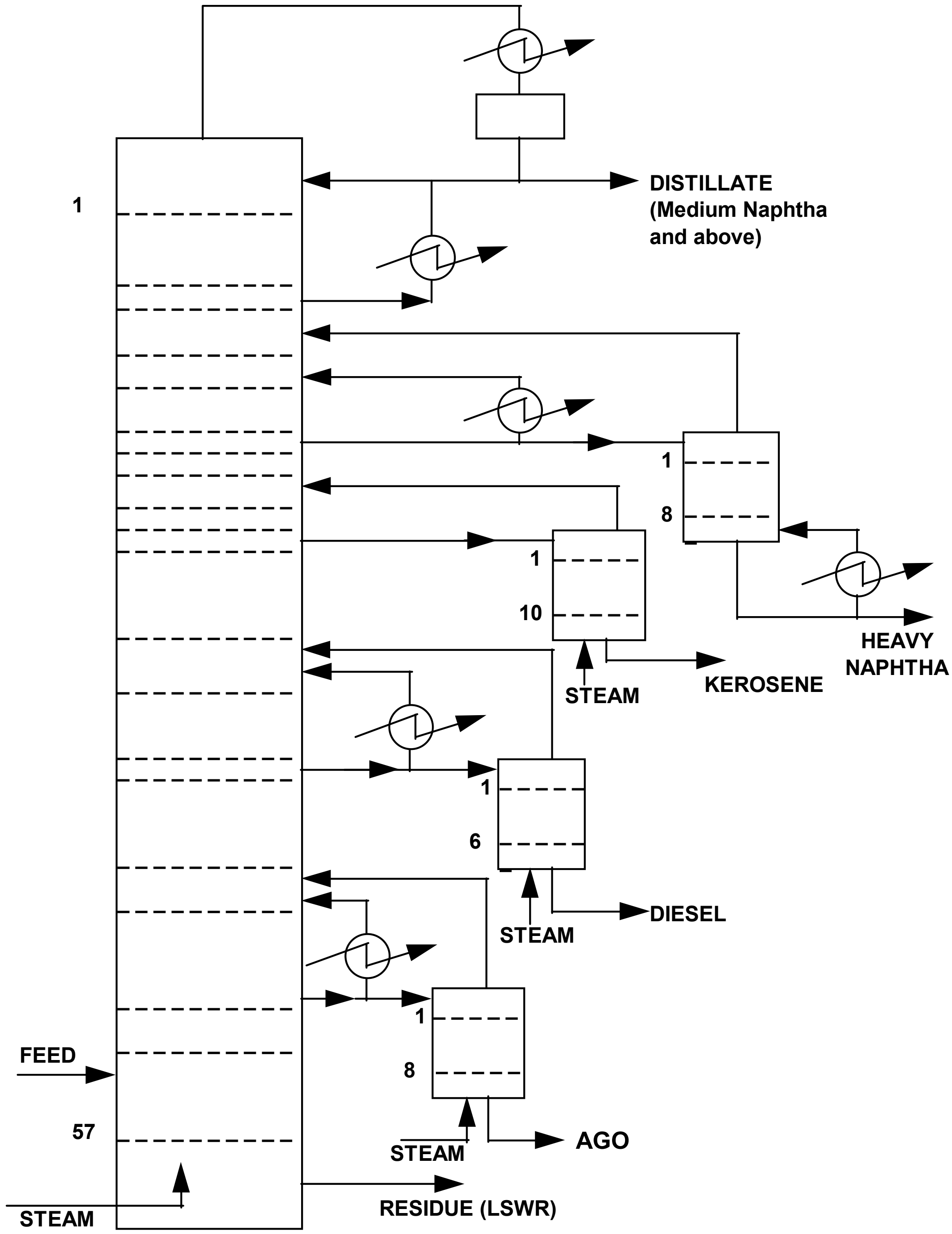

Fig. 1. Schematic diagram of the crude oil distillation tower.

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

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

2.2 The ANN Models

In this work, all ANN models were developed in MATLAB environment and utilizes MATLAB neural network toolbox. Two different types of feedforward ANN models were developed and compared for the top section of the column: multi-layer perceptron (MLP) and radial basis function networks (RBFN). MLP and RBFNs are multilayer feedforward networks. The networks have an input layer, a hidden layer and an output layer.

The MLP models had one hidden layer with the sigmoid function as the activation function. The models are trained using backpropagation algorithm with adaptive learning rates. Adapting the learning rate, μ, to the current position on the error surface during training improves the performance of the backpropagation algorithm in optimizing the weights and biases. To develop an MLP model, the number of nodes in the hidden layer and the maximum acceptable error during training were varied. The results given in this paper are the best found during the study.

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. [1991] 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 to amply cover 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. For the RBFN models, the OLS algorithm calculated the number of hidden nodes.

The selection of the number of training data points are based on several trial runs to find the number that gives the best result. A number that is too small will give poor estimation of the test data, while too many data points will over fit the model.

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 is not as important as RMS error because once a connectionist model is trained, the execution of the model is very fast. The training time will only be a major concern when the model is periodically updated on-line. For all the models, the results presented in this paper are 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. As mentioned in the previous section, changes within the operating range for a section in the crude distillation tower affects only the sections that are immediately above and below the section. This therefore allows the crude tower model to be divided into sections where the variables that are related are grouped together, and thus make the model more manageable.

3.0 RESULTS AND DISCUSSION

3.1 Comparison between RBFN and MLP

A comparison on the RMS error and training times is made between RBFN models and MLP models. The MLP model has 15 nodes in the hidden layer. Table 3 shows the results of the two different networks using two different groups of training data for the top section of the crude tower. From the results, it can be seen that RBFN is superior both in prediction of the test data and training times. The rest of the sections will therefore use RBFN.

3.2 Grouping of Variables

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 4.

From Table 4, 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. The same is also true with the variables in the HN section.

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.

Table 3. Overall results for the top section of the crude distillation column

	Average RMS Error	CPU Time (sec)
RBFN w/ 300 training data	0.0037	22.85
RBFN w/ 150 training data	0.0063	9.83
MLP w/ 300 training data	0.0338	1397
MLP w/ 150 training data	0.0383	691

Table 4: 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		0.0021,0.0028,0.0121,0.0029,0.0019, 0.0074

3.2 Overall Prediction

The RMS errors for all output variables of the crude tower are given in Table 5. Output variables in the same section are 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.

4.0 CONCLUSIONS

The results obtained in this study showed that RBFN is suitable for modelling the crude oil distillation column.

It can also be concluded that to develop ANN models large, multivariable systems for RTO, 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.

Table 5: Overall result for all sections in the crude distillation tower.

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

5.0 NOMENCLATURE

- Bintolt is the condensate feed from the storage tank.
- FBPH, FBPK, FBPD, FBPA are the final boiling point of HN, kerosene, diesel and AGO produced respectively.
- FPKero is the flash point of kerosene.
- HNdraw, Kerodraw, Diesdraw and AGOdraw are heavy naphta (HN), kerosene, diesel and AGO product draw off respectively.
- Htfeed is the crude oil feed from the storage tank.
- IBPH, IBPK, IBPD and IBPA are the initial boiling point of HN, kerosene, diesel and AGO produced respectively.
- Ovhd is the overhead draw off rate.
- PAT, PAH, PAD, and PAA are the p/a at the top of the main column, and the HN, diesel and AGO strippers respectively.
- PourD, PourA and PourL are the pour points of diesel, AGO and LSWR produced.
- Qcond is the condenser duty of the main column.
- Qreb is the reboiler duty of the HN side stripper.
- RR is the reflux ratio.
- RhoH is the density of HN.
- SSK, SSD, and SSA are the stripping steam rates for the kerosene, diesel, and AGO side strippers respectively, and SSM is the main column stripping steam rate.
- 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.

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