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Estimation of FCC feed composition from routinely measured lab properties through ANN model

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A B S T R A C T

Realistic kinetic modeling of fluid catalytic cracking (FCC) units requires detailed composition of the feed stream in terms of paraffins, naphthenes and aromatics(PNA) which cannot be analyzed in a field laboratory. This paper presents an artificial neural network (ANN) model to predict detailed composition of FCC feed using routinely measured properties such as density, ASTM distillation temperatures, Conradson carbon residue (CCR) content, sulfur and total nitrogen as inputs to the model. Several feedforward-error back propagation networks with different number of neurons in hidden layers were studied using Levenberg–Marquardt (LM) training algorithm. Among different network architectures investigated, the ANN model with 8 inputs, namely density and ASTM distillation temperatures except IBP, FBP and only one neuron in the output layer to predict paraffin, naphthene and aromatic contents individually showed the best agreement with the experimental results within permissible limit. These compositions when used with a 10-lump kinetic model of FCC unit, successfully simulated plant performance for several different feeds.

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1. Introduction

Modeling of FCC unit becomes complex due to the presence of a large number of hydrocarbons in the feed which undergo a variety of reactions to yield valuable cracking products. Laboratory analysis of these components at their molecular level is not an easy task and therefore, it is not possible to account for each individual feed component and its reactions in any realistic modeling exercise. Use of kinetic lumps has been made extensively by various researchers to model FCC units with varying degree of success. The earliest attempt had only two lumps, one representing the feed and the second component was the product [1]. Three, four and five lump models have successively been used with improved success [2–4]. Clearly, the larger the number of lumps used, the closer we approach to the real system.

In all these models, feed is represented by a single lump of average composition and molecular weight. If instead, feed analysis is available in terms of hydrocarbon groups and their relative proportions, the reaction kinetics can be better accounted for [5]. Ten and twelve lumps have been successfully used to simulate industrial FCC units with better prediction capabilities. Of these lumps, 6 to 8 were used to characterize feed and intermediate product (light fuel oil 221–343 °C)

and remaining four for the final products namely gasoline, LPG, dry gas, and coke [6–9].

1.1. FCC feed characterization

Typically for the above models, the accuracy of model prediction depends on realistic FCC feed characterization in terms of paraffins, naphthenes, aromatic rings and aromatic substituent groups. Different test methods are available for the detection of hydrocarbon classes such as NMR, HPLC and mass spectroscopy. High-performance liquid chromatography (HPLC) has been used successfully in separating different hydrocarbon group types in nonvolatile feedstocks such as residue, and identifying the molecular species in the asphaltene fraction [10,11]. However, a severe shortcoming of most high-performance liquid chromatographic approaches to a hydrocarbon group type of analysis is the difficulty in obtaining accurate response factors applicable to different distillate products. Nuclear magnetic resonance (NMR) has been used frequently for the measurement of aromatics and saturated hydrocarbons (ASTM E-386) as well as hydrogen distribution [12]. Beyond these results, both C and H in various structural groupings in a molecule can be determined [13]. As NMR (1H and 13C) is fast and relatively inexpensive, it has gained a prominent place for the structural group analysis of petroleum fractions particularly in heavy gas oil range [14,15]. Mass spectroscopy has proved to be highly successful in petroleum industry, especially with the use of computerized techniques for the quantitative determination of the percentage of paraffins, cycloparaffins

and aromatics in the heavy gas oil fraction. High-resolution mass spectrometry analysis (HRMS) was used for determining the hydrocarbon types in diesel range samples before and after the hydrocracking process and the results were compared with NMR [16]. Being a very rapid method for obtaining full hydrocarbon type analyses for a wide range of fractions up to and including heavy gas oils, mass spectrometry is considered the most useful technique for the PNA characterization of petroleum fractions. However, such an elaborate analysis for FCC feed which is usually in the range of heavy gas oil, can hardly be undertaken in field laboratories, which are geared to perform only routine measurements on a regular basis. There is a clear need to develop a scheme to relate the detailed composition, desired for a realistic FCC kinetic model, with the routinely measured feed properties in a field laboratory. Therefore, PNA based FCC model application calls for research endeavor to correlate structural feed analysis with simple, routinely available feed properties.

There are several empirical correlations available in the literature [17,18] which relates hydrocarbon groups of heavy and light fuel oil fractions to properties measured on a regular basis such as specific gravity and refractive index. The most commonly known procedures are the n-d-M method (ASTM D-3238) & API correlation [12,19]. The n-d-M method is used for estimating percentage carbon in aromatic, naphthenic and paraffinic structures with refractive index, density, average molecular weight and sulfur as input [20]. However, this method is very sensitive to refractive index and can only be applied for samples with paraffin content more than 25 wt.%. The API method is a generalized method that predicts the mole fraction of paraffinic, naphthenic and aromatic compounds for an olefin-free hydrocarbon fraction. Other procedures for the estimation of the composition of heavy and light petroleum fractions have been discussed by Waterman et al. [21] and Riazi and Daubert [22]. However, all the existing methods are accurate only for data on which the method is based and cannot be extrapolated for a wide range of properties. Moreover, most of these methods predict PNA composition in terms of mole or volume basis which is difficult to validate with mass spectroscopy, NMR or HPLC analysis obtained on weight basis.

1.2. Artificial neural network (ANN)

Artificial neural networks have been successfully implemented in the chemical industry, especially in the areas of dynamic modeling. Bhat and McAvoy [23] used back propagation neural network for the dynamic modeling of pH in a CSTR and compared the results with traditional ARMA models. They found ANN models to be more accurate than ARMA models. Lately an increasing trend is observed to model the steady state processes also using ANN approach. The height equivalent of theoretical plate (HETP) and pressure drop for columns with structured packing were predicted by neural network model and the results were found to be more accurate than traditional semi-empirical model [24,25]. Neural network models have also been developed for the prediction of heavy gas oil cracking products in hydrocracking [26,27], fluid catalytic cracking and catalytic reforming units [28]. An ANN model was compared with a non-linear statistical model for FCC [29]. The results showed the superiority of the ANN model in terms of prediction accuracy. An ANN model based optimizer to separate gas flow coming out of a hydrocracking reactor was developed [30] and the results were compared with those obtained from the first principle models developed by Bayley et al. [31]. The ANN was trained with data obtained from a commercial simulator (ASPEN PLUS) in the absence of the availability of sufficient plant data.

Neural networks have been used as soft sensors for the estimation of various parameters of crude petroleum column and prediction of product properties [32–34]. Presently, several refineries use ANN models as soft sensors to estimate output stream quality online and use this information to control distillation columns. Its applications are also shown in the online data processing for detecting gross errors due to faulty sensors [35].

2. Model performance evaluation criteria

The following criteria were applied to evaluate the model performance:

$$\text{Mean Square Error(MSE)} = \frac{1}{n} \sum_n \left(y_i^{obs} - y_i^{pred} \right)^2$$

$$\text{Root Mean Square Error(RMSE)} = \sqrt{(MSE)}$$

$$\text{Percent deviation(PD)} = \frac{y_i^{obs} - y_i^{pred}}{y_i^{obs}} * 100.$$

Coefficient of determination (also called R^2) as defined below, was also included here as it reflects the accuracy of prediction. For a perfect model, $R^2 = 1$.

$$R^2 = \left(1 - \frac{SSE}{SST} \right)$$

where,

$$SSE = \sum_n \left(y_i^{obs} - y_i^{pred} \right)^2$$

and

$$SST = \sum_n \left(y_i^{obs} - \bar{y}^{obs} \right)^2.$$

3. ANN model development

The present work aims to develop an artificial neural network based model which can use routinely measured properties of FCC feed such as density, ASTM distillation temperatures, Conradson carbon residue (CCR), sulfur and nitrogen content as inputs and provide detailed composition (wt.% of paraffins, naphthenes and aromatics) as output. Artificial neural network (ANN) type of modeling is most suited for this work since we do not know any functional relationship, even if it exists, between available inputs and desired outputs. Being a black box approach, ANN does not require, nor attempt to develop, any mathematical relation, linear or nonlinear, between input and output and yet can effectively serve as a tool to estimate the detailed composition of the feed required for FCCU modeling.

Conventionally, the desired network architecture is arrived at by a constructive [36] or a destructive method [37]. With the development of evolutionary techniques such as genetic algorithm, it has become possible to design the network architecture optimally and directly [38,39]. In the present study, however, the conventional constructive method has been used to design the networks starting from a small network and expanding it by adding more layers and neurons in the hidden layers.

A feed forward error back propagation type of modeling approach has been followed in the present work which is most suited for numerical NN modeling. The number of neurons for feed forward neural networks is approximately proportional to the number of learning data sets [40,41]. All neurons in the input layer carry information to the neurons in the hidden layers after multiplying each with corresponding synaptic weights. Each layer has mapping function (somatic operation) to be suitably chosen. Fig. 1 shows a typical neural unit (neuron) with linear synaptic operation. Normally, one or two hidden layers are sufficient to estimate any function [42]. The hidden layer may consist of one
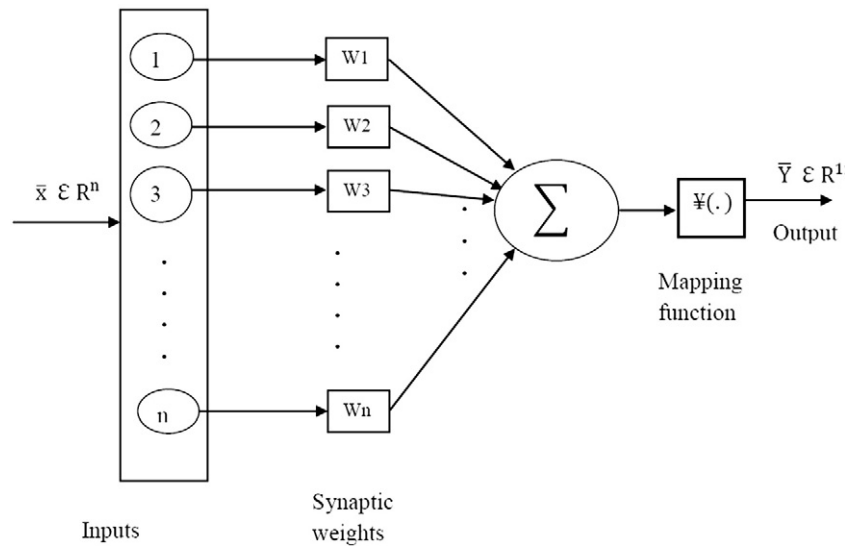
Fig. 1. A typical neuron with linear synaptic operation.

or more layers which may be connected in series or parallel or a combination with the output layer.

In the present work, trial and error method was used to find near optimum ANN architecture for the estimation of detailed feed composition (PNA). Neural Network Toolbox in MATLAB was used for the purpose. Various activation functions were investigated using different combinations for the hidden and the output layers. The number of neurons was also varied systematically in the hidden layers. The least square error

Fig. 2. a. Model 1: ANN architecture with three output neurons. b. Model 2: ANN architecture with one output neuron.

Table 1
Mass spectrometry analysis for different samples (wt.%).

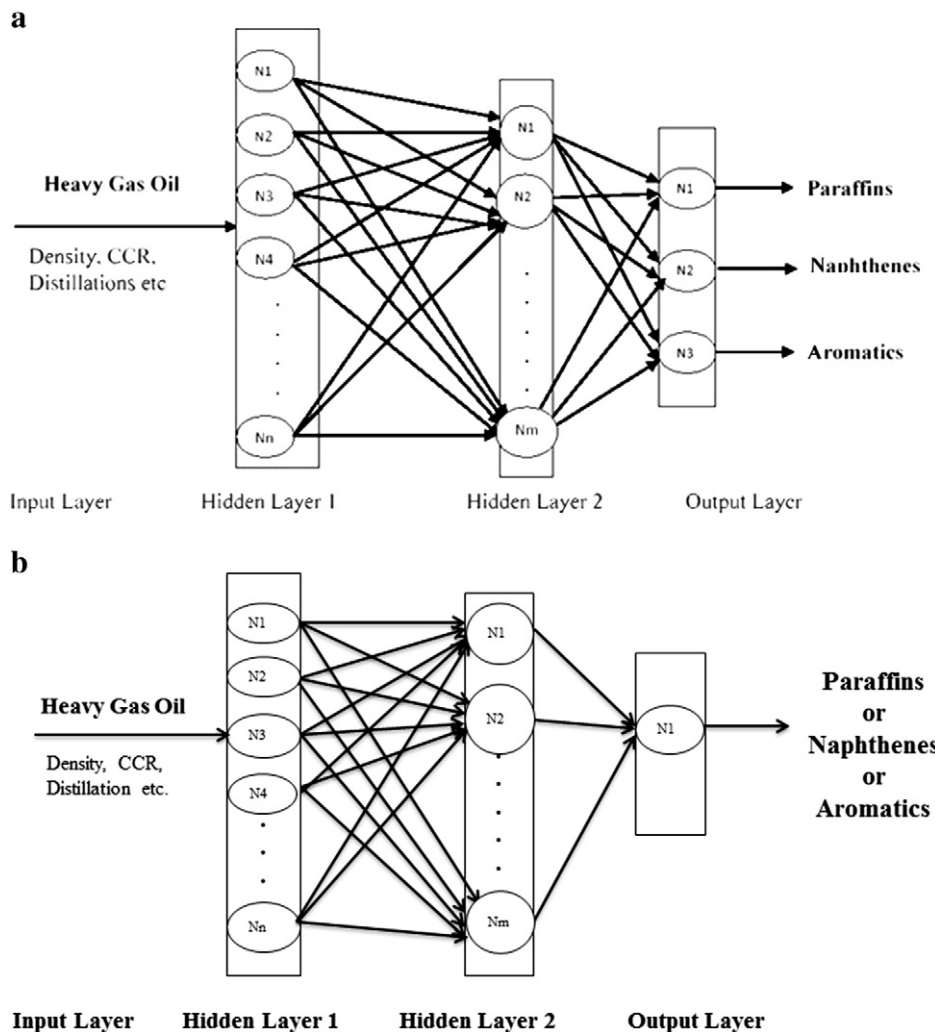| FCC feed	HSVGO	Mixed feed	OHCU bottom	HVGO
Paraffins	10.9	10.4	31.4	33.8
Monocycloparaffins	9.8	4.6	23.8	9.3
Dicycloparaffins	7.3	4.7	15.3	5.5
Tricycloparaffins	5.8	5.3	10.5	5.1
Tetracycloparaffins	0.0	1.8	3.6	0.3
Pentacycloparaffins	0.0	0.0	0.0	0
Hexacycloparaffins	0.0	0.0	0.0	0
Heptacycloparaffins	0.0	0.0	0.0	0
Saturates	33.8	26.8	84.6	54.0
Alkylbenzenes	9.2	5.3	6.3	6.3
Benzocycloparaffins	4.7	5.0	4.2	5.1
Benzodicycloparaffins	3.7	4.9	1.6	3.7
Naphthalenes	3.2	9.3	2.2	5.8
Acenaphenes, biphenyls	2.4	6.9	0.0	3.0
Acenaphthylenes, fluorenes	4.3	12.9	0.7	8.6
Phenanthrenes	3.8	9.0	0.1	6.1
Pyrenes	5.4	9.5	0.1	4.2
Chrysenes	2.7	3.4	0.0	0.1
Benzopyrenes	3.1	0.1	0.0	0.0
Aromatics	42.5	66.3	15.2	42.9
Thiophenes	0.3	0.0	0.0	0.0
Benzothiophenes	12.8	4.6	0.1	2.6
Dibenzothiophenes	10.5	2.2	0.0	0.4
Naphthobenzothiophenes	0.0	0.0	0.0	0.0
Sulfur compounds	23.6	6.8	0.1	3.0

was optimized by the addition of the neurons in the hidden layer. Finally, two hidden layers were found to be optimum.

In this algorithm, all information moves in the forward direction from input to output through the hidden layers. Initial weights are arbitrarily assigned. During ANN training, the output is compared with the desired (experimental) known output and the error is back propagated to adjust the weights. Any non-linear optimization method whether local or global one can be used to optimize feed-forward neural network by changing the synaptic weights. The most popular optimization method has been Levenberg Marquardt algorithm based on variants of gradient method which was used in the present work. The training performance varies depending on the objective function and underlying error for a given problem and network configuration. After the network was fully trained and validated with new data sets, the network was used to calculate the response to different inputs. Standard connections were used i.e.; network was fully connected between adjacent layers only. Two different ANN models (Model-1 and Model-2) have been developed in the present study. Model-1 predicts three output parameters: weight percent of paraffin, naphthene and aromatic content of FCC feed from a single ANN architecture having three neurons in the output layer (Fig. 2a). Model-2 predicts the paraffin, naphthene and aromatic content

Table 2
Range of input data used in ANN model development.

Parameters	Minimum	Maximum
Density, g/cc	0.8386	0.996
CCR (wt.%)	0.04	1.61
Total sulfur (wt.%)	0.01	4.35
Total nitrogen (ppm)	5	2089
SIMTBP (wt.%)		
0% (°C)	37	325
5% (°C)	224	409
10% (°C)	263	428
30% (°C)	337	458
50% (°C)	380	481
70% (°C)	407	506
90% (°C)	427	538
95% (°C)	436	552
100% (°C)	460	581
Paraffins (wt.%)	4.9	27.7
Naphthenes (wt.%)	15.4	55.9
Aromatics (wt.%)	16.5	76.5

Table 3
Summary of ANN model architectures for 13 input variables.

Output parameters	Model 1	Model 2		
	PNA	P	N	A
No. of inputs variables	13	13	13	13
No. of hidden layers	2	2	2	2
No. of neurons in layer-1	14	13	12	9
No. of neurons in layer-2	14	14	14	10
Activation function of layer-1	Tansig	Tansig	Logsig	Tansig
Activation function of layer-2	Logsig	Logsig	Logsig	Logsig
Activation function output layer	Purelin	Purelin	Purelin	Purelin
Performance function	Mse	Mse	Msereg	Msereg
Training function	Trainlm	Trainlm	Trainlm	Trainlm

individually from three different ANN architectures each with a single output neuron followed by normalization (Fig. 2b).

4. Experimental

The purpose of this work is to develop a predictive ANN model for the detailed composition of FCC feeds. In the present study, the different FCC feed samples as well as individual blend constituents such as VGO, HVGO, and OHCU bottom samples were obtained from various Indian refineries processing indigenous crudes as well as low sulfur and high sulfur crudes from other sources such as Arab, Iran mix (Iran heavy & Iran light), and Nigerian and a mix thereof.

All the samples were analyzed for their hydrocarbon compositions through HC22 (22-hydrocarbon component class) analysis based on the high-resolution mass-spectrometric method. An Autospec Ultima high-resolution mass spectrometer from Micromass UK was used for analysis. 5 μl of the sample was introduced into the mass spectrometer using the All Glass Heated Inlet System (AGHIS) and heated to desired temperature. The sample vapors were then allowed to homogenize in the bulb before being introduced into the source of the mass spectrometer.

The high-resolution mass spectra of the samples were acquired using OPUS software. A mass spectrometer with 5000 resolution is sufficient to distinguish masses up to 470 and to separate ions that differ in composition by +1 carbon and +2 hydrogen. The spectral data of minimum 7 or 8 scans were averaged and the averaged data were processed by Teeter's PCMASPEC — HC22 software for hydrocarbon type analysis [43]. The method provides the quantification of 22 classes of hydrocarbons based on the number of hydrogen atoms relative to the number of carbon atoms as expressed by the letter z. The principal fragments formed from paraffin class in a mass spectrometer are at odd masses with z + 1. The seven saturated molecular species considered in this analysis have z values of 0, −2, −4, −6, −8, −10 and −12 respectively which correspond to cycloalkanes with one to seven rings (mono to heptacycloparaffins). The aromatic hydrocarbon groups start with the alkyl benzene that has z number of −6 till z = 28 representing ten classes of aromatics. Four classes of sulfur-aromatics were also reported. This classification widely covers the hydrocarbon classes present in the VGO

Table 4
Summary of ANN model architectures for 8 input variables.

Output parameters	Model 1	Model 2		
	PNA	P	N	A
No. of inputs variables	8	8	8	8
No. of hidden layers	2	2	2	2
No. of neurons in layer-1	8	12	12	9
No. of neurons in layer-2	9	13	12	9
Transfer function of layer-1	Logsig	Tansig	Tansig	Tansig
Transfer function of layer-2	Logsig	Logsig	Logsig	Logsig
Transfer function output layer	Purelin	Purelin	Purelin	Purelin
Performance function	Mse	Mse	Mse	Msereg
Training function	Trainlm	Trainlm	Trainlm	Trainlm

Table 5
Comparisons of model predictions with experimental observations for two different ANN models with 13 input variables (validation set).

Sample ID	Paraffins			Naphthenes			Aromatics		
	EXP	Model 1	Dev%	EXP	Model 1	Dev%	EXP	Model 1	Dev%
1	15.8	14.6	7.71	35.9	36.7	−2.17	48.3	48.7	−0.91
2	14.4	15.1	−5.12	23.3	23.2	0.53	62.2	61.7	0.83
3	4.9	5.0	−1.56	21.1	22.2	−5.09	74.0	72.8	1.55
4	10.9	16.7	−52.74	29.9	26.9	9.90	59.2	56.4	4.71
5	10.4	9.2	11.40	18.5	24.6	−33.21	71.0	66.1	6.84
6	6.3	6.5	−3.96	26.2	30.6	−16.75	67.5	62.9	6.87
Sample ID	Paraffins			Naphthenes			Aromatics		
	EXP	Model 2	Dev%	EXP	Model 2	Dev%	EXP	Model 2	Dev%
1	15.8	16.9	−6.95	35.9	31.7	11.63	48.3	51.4	−6.37
2	14.4	12.6	12.50	23.3	26.9	−15.47	62.2	60.5	2.74
3	4.9	5.4	−9.15	21.1	23.8	−12.75	74.0	70.9	4.24
4	10.9	11.9	−9.75	29.9	29.5	1.19	59.2	58.5	1.20
5	10.4	12.1	−16.23	18.5	19.1	−3.23	71.0	68.8	3.08
6	6.3	6.4	−1.18	26.2	26.6	−1.47	67.5	67.0	0.68

RMS error: Model 1 = 2.97, Model 2 = 2.04.
R^2 value: Model 1 = 0.98, Model 2 = 0.993.

range of samples. Representative analyses for four different samples are shown in Table 1.

Routine laboratory measurements for density, ASTM distillation temperatures, CCR, total sulfur and total nitrogen were also made for all the samples. ASTM D4052 and ASTM D4530 test methods were used to calculate specific gravity and carbon residue content respectively. Distillation temperatures are measured by simulated distillation (SIMTBP) using the ASTM D2887 test method (55–538 °C). Total sulfur was measured by the ASTM D2622 test method using the X-ray fluorescence spectrometry (XRF) and total nitrogen was measured by the ASTM D4629 method (CHNS).

A total of 28 samples were analyzed in the laboratory, of which 16 data sets covering the entire range of data (data range given in Table 2) were used for the development of ANN models. Another six data sets were used for the testing of the models. The developed ANN models were validated with remaining six data sets representing FCC feeds with wide variation in compositions (paraffinic, naphthenic or aromatic in nature).

5. Results & discussion

In ANN modeling there is always the question about what should constitute the input parameters and there is no straight forward way to answer. One, therefore, tends to cautiously choose all possible inputs that are likely to influence the output. But this comes at a cost. Besides increasing computation load, particularly during training, it calls for larger data sets. All experimental data are prone to measurement errors, a ± 5% window is a standard norm for the uncertainty in all experimental data and present measurements are no exception. While training a neural net with experimentally measured data, learning rates are usually kept low resulting in further slowing down the training. It is therefore, desirable to use an optimal set of input parameters where the contribution of each input is more significant than the noise it adds. In the present study a learning rate of 0.01 was used for all the cases investigated (default option in MATLAB).

In the present study, initially all the 13 measured properties were chosen as input, namely: density, ASTM distillation temperatures —
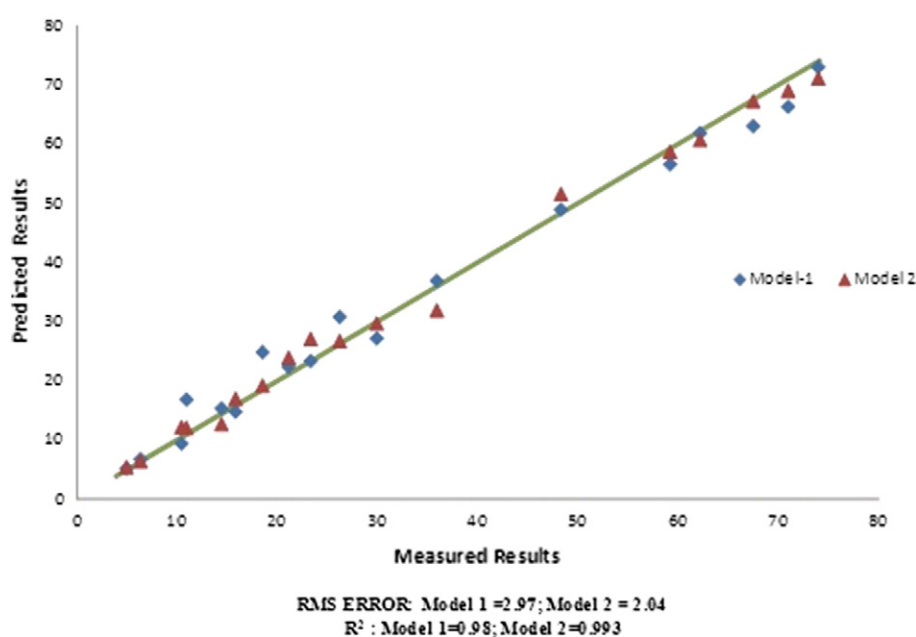

RMS ERROR: Model 1 =2.97; Model 2 = 2.04
R^2 : Model 1=0.98; Model 2=0.993

Fig. 3. Parity plot between ANN predicted compositions and experimental values for models using 13 input variables.

Table 6
A comparison of model predictions with experimental observations for two different ANN models with 8 input variables (validation set).

Sample ID	Paraffins			Naphthenes			Aromatics		
	EXP	Model 1	Dev%	EXP	Model 1	Dev%	EXP	Model 1	Dev%
1	15.8	15.3	2.83	35.9	36.2	−0.71	48.3	48.5	−0.40
2	14.4	14.3	0.61	23.3	23.3	0.08	62.2	62.4	−0.33
3	4.9	4.8	2.31	21.1	20.8	1.20	74.0	74.4	−0.49
4	10.9	13.3	−22.03	29.9	26.2	12.40	59.2	60.5	−2.21
5	10.4	10.7	−3.27	18.5	23.3	−26.19	71.0	65.9	7.16
6	6.3	6.9	−9.92	26.2	24.6	6.17	67.5	68.5	−1.47

Sample ID	Paraffins			Naphthenes			Aromatics		
	EXP	Model 2	Dev%	EXP	Model 2	Dev%	EXP	Model 2	Dev%
1	15.8	15.8	0.19	35.9	36.4	−1.47	48.3	47.8	1.03
2	14.4	13.5	6.25	23.3	22.6	2.91	62.2	63.9	−2.70
3	4.9	4.5	7.64	21.1	23.3	−10.46	74.0	72.2	2.48
4	10.9	13.4	−22.99	29.9	32.3	−8.08	59.2	54.3	8.31
5	10.4	9.4	9.74	18.5	18.9	−2.14	71.0	71.7	−1.01
6	6.3	6.8	−7.25	26.2	26.7	−1.93	67.5	66.5	1.43

RMS error: Model 1 = 2.04, Model 2 = 1.71.
R^2 value: Model 1 = 0.992, Model 2 = 0.994.

IBP, 5%,10%,30%, 50%, 70%, 90%, 95% and FBP, Conradson carbon residue (CCR), total sulfur and total nitrogen. Subsequently the sensitivity of each variable was examined. Based on the sensitivity study and intuitive reasoning, five of the 13 variables were dropped. IBP and FBP can be seldom determined with any amount of certainty while CCR, sulfur and nitrogen content in VGO are unlikely to influence its PNA composition. Remaining 8 − variables were used as inputs. Results are presented for both 13 as well as 8 inputs.

Tables 3 and 4 provide the details of ANN model architecture used in the present study along with activation functions for the 13 and 8 inputs respectively. Table 5 gives a comparison between experimental values and model predictions of gas oil composition for 13 inputs using both the models. Also included in this table are the percent deviations of the predicted valued from the measured ones, root mean square error and R^2 values. While both the models have acceptable levels of error, Model 2 scores over Model 1 in all respects. This is in line with the common knowledge that it is better to develop architectures with only one neuron in the output layer i.e. each model should predict only one parameter. For Model 1, maximum deviation is 52.7% whereas it is only 16.2% for Model 2. Fig. 3 shows a parity plot between predicted and measured percent compositions for Model 1 and 2 using 13 input parameters. Table 6 and Fig. 4 provide similar information when only 8 inputs were used in place of 13.

A comparison of Model 1 results for the two cases (with inputs 13 and 8) shows that input parameters lead to less RMS error (2.04 against 2.97) and higher coefficient of determination, R^2 (0.992 against 0.98). Similar trend is observed for Model 2 also, however, less prominent. RMS error for Model 2 with 13-inputs was 2.04 which got reduced to 1.71 for 8 inputs, but R^2 values were nearly the same for 13 as well as 8 inputs. Clearly the dropped input parameters namely IBP, FBP, total sulfur, total nitrogen and CCR do not have noticeable role in predicting the FCC feed compositions but their associated measurement errors affect the network model performance.

5.1. Usefulness of the present study

Steady state FCC modeling and plant simulation have been tried since 1970 with varying degrees of success. For a reactor, reaction kinetics is perhaps the most important part of such studies and the present investigation can enable the process engineer to build kinetic models more accurately. These steady state models are valuable tools for the design of new plants, and analysis and optimization of operating units.
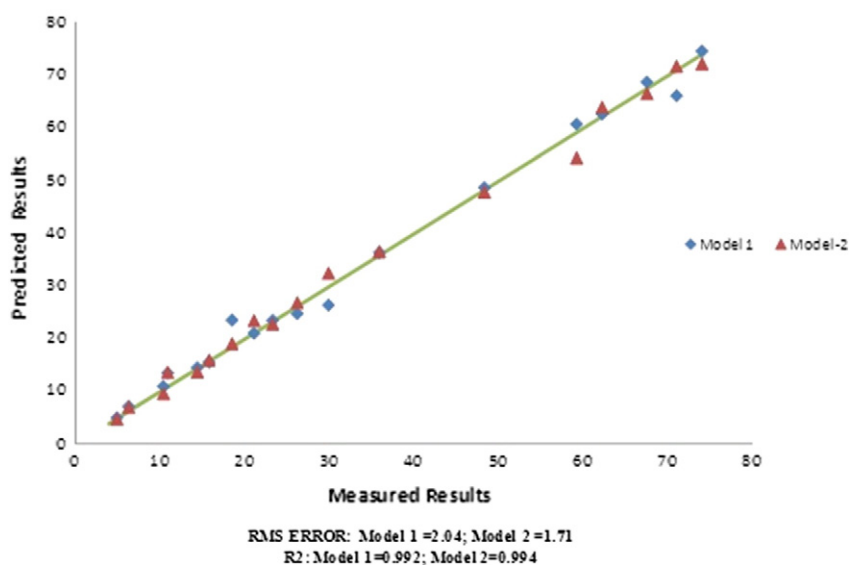

RMS ERROR: Model 1 =2.04; Model 2 =1.71
R2: Model 1=0.992; Model 2=0.994

Fig. 4. Parity plot between ANN predicted compositions and experimental values for models using 8 input variables.

As mentioned earlier, for a more detailed kinetic model of FCC unit such as a 10- and 12-lump model, a detailed feed characterization is required. The present work provides such a scheme without having to actually embark on a detailed laboratory investigation. The present model was used to characterize several gas oil samples which provided a basis for the development of a new 10-lump kinetic model. The model calculated product yields were comparable to predictions made with ASPEN FCC simulator and also matched well with plant observations for all the cases investigated, thus vindicating the usefulness of the present study. Some of these results were presented at the Energy System Modeling & Optimization Conference and are available in the conference proceedings [44].

6. Conclusion

The present work aimed to predict detailed composition of heavy gas oil feeds to FCCU in terms of hydrocarbon types such as weight percent of paraffins, naphthenes and aromatics. ANN models were developed and tested using 13 inputs and also with a subset of 8 inputs. The latter models were found to perform better resulting in a lower RMS error and a higher R^2 coefficient. The eight input parameters included density and ASTM distillation temperatures (at 5, 10 30,50,70,90 and 95%). The other 5 input parameters included in 13 inputs were IBP, FBP, total sulfur, total nitrogen and CCR which did not seems to have any significant effect on the output in terms of the improvement of accuracy. The experimental errors in these 5 parameters, however, increased the error. Model-2, which used three different architectures with only one neuron each in the output layer to separately predict paraffins, naphthenes and aromatics, performed better than Model-1 with multiple neurons in the output layer. Model-2 with 8 input parameters predicted gas oil compositions with ± 10% of the experimental values with more than 50% values being within ± 3%.

Nomenclature

CCR	Conradson carbon residue, wt.%
FBP	finial boiling point, °C
HSVGO	high sulfur vacuum gas oil
HVGO	heavy vacuum gas oil
IBP	initial boiling point, °C
MSE	mean square error
n	number of data points
OHCU	overhead hydrocracker unit
PD	percent deviation
R^2	coefficient of determination
RMSE	root mean square error
SSE	sum square error
SST	total sum of squares
VGO	vacuum gas oil
y_i^{obs}	observed value from laboratory analysis
y_i^{pred}	predicted value from ANN model
$\overline{y}^{obs}$	mean of the observed values.

Acknowledgment

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