Research Article GU J Sci 37(1): 427-441 (2024) DOI: 10.35378/gujs.1143087

Gazi University

Journal of Science

http://dergipark.gov.tr/gujs

ANN and RSM Modelling and Optimization of Paraffins and Aromatics in Crude Oil Distillation Products' Properties in Iraq

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Highlights

- Properties of Iraqi oil were investigated using Back-Propagation ANNs and RSM-DOE techniques.
- The effect of both Aromats and Paraffins on product quality (e.g. MON, RON) differs considerably.
- Aromatics increases the octane number of the products and lowers its boiling point limits.
- Aromatics decreases the calorific value and sulfur content of the products.
- Optimization showed that the best percentage of aromatics should not exceed 97%.

Article Info

Received: 11 July 2022
Accepted: 30 Mar 2023

Keywords

RSM
DOE
Petroleum distillation
Artificial neural networks
Aromatics and paraffin

Abstract

Back-Propagation neural networks, as well as RSM-DOE techniques, were used to predict the properties of various compositions of Iraqi oil, which were presented in this study. Paraffin and Aromatics' effect on petroleum properties, e.g., yield, density, calorific value, and other essential properties, were studied. The input-output data to the neural networks were obtained from existing local refineries in Iraq. Several network activation functions to simulate the hydrocracking process were tested and compared. the network function that gave satisfactory results in terms of convergence time and accuracy was adopted. The data were divided into training and testing parts. The results of the trained artificial neural network models for each one of the tested functions have been cross-validated with the experimental data. The network that compared well against this new set of data (i.e. testing data), with an average percent error always less than 3% for the various products of the hydrocracking unit were chosen for the study. Aromatics showed to have more profound effect on the Octane number at low concentrations of paraffin, while, for specific gravity and calorific value they have similar effects. As for boiling points and sulfur contents, aromatics have almost no effect at lower levels of paraffin.

1. INTRODUCTION

The crude oil industry owes its existence and continuity to continuous and increased consumption due to the high demand for hydrocarbon fuels and other petrochemical products [1].

Modern petroleum refining planta involves several complicated units and processes e.g. Crude Distillation Units (CDU), Catalytic Reforming Processes (CRU), Hydro-treating Units (HDT), Fluid Catalytic Cracking (FCC) ...etc. [1-3].

Most refineries regularly enhance and modify their operational units by implementing new technology in order to comply with environmental requirements and the required quality of petroleum products from a refinery. Utilizing Hydrotreating (HDT) machines to eliminate inorganic pollutants like sulfur, nitrogen, oxygen, etc. is one such example. The HDT process should take into account a number of process factors, including charge, pressure, temperature, liquid hourly space velocity (LHSV), and hydrogen to hydrocarbon (H_2/HC) ratio. In the literature, this wasn't really explored all that much. One further illustration of such alterations is the use of hydrogen [2,4].

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Significant advancements in computational techniques (e.g., simulation modeling, optimization, control, etc.) and computational power have become significant aid to improve petrochemical industries. Aspen HYSYS (Version 11), Bryan Research and Engineering ProMax 2.0, ChemCAD (Version 7), EPCON CHEMPRO 9.2, and many others are among the software available for simulating petroleum refining processes. This software depends on the availability of data for modeling. Another mathematical technique for modeling the outcome of the refining process is Artificial Neural Network (ANN), Genetic Algorithm (GA), and Design of Experiments (DOE).

Neural network (NN) is an effective tool for capturing the process's non-linearities based on the data available from the refinery plant. After selecting the model, training it to capture the system behavior, and testing it, NN can predict the needed simulation variables with a good degree of accuracy and quickly [5-6].

Reviewing the literature, one finds that a great deal of research was conducted on the effect of petroleum constituents on their end-use application (e.g., IC Engines, gas turbines, etc.).

Kidoguchi et al. [7] showed, experimentally, that increasing aromatic content for high cetane number fuel caused high Oxides of Nitrogen (NOx) and particulate emissions. While, for low cetane fuel, it resulted in high Total Hydrocarbon (THC) emission at retarded injection timing.

Tsurutani et al. [8] also found that aromatic content has a significant influence on the NOx emissions from the Indirect Injection Diesel Engine (IDI) diesel engine.

Karonis et al. [9] also found in their attempt to correlate fuel properties with engine-out emissions that the aromatic content is strongly correlated with the cetane number, density, and the 90% distillation point of diesel fuel.

According to Sienicki et al. [10], sulfur content, aromatic content, and 90% distillation temperature were the greatest predictors of particle emissions. They also stated that multi-ring aromatics had a greater impact on hydrocarbon and particle emissions than total aromatics content.

Shekhawat et al. [11] also found that the fuel constituents (paraffin, naphthenes, and aromatics), as well as their chemical structure (e.g., branched versus linear paraffin) and consequently the sulfur content of the fuel, have a significant influence on the H_2 yield of fuel cells.

Rodríguez et al. [12] revealed more exceptional soot from paraffinic and, significantly, oxygenated biofuels to be oxidized under lower temperature conditions.

Soriano et al. [13-14], found that paraffinic fuels were very beneficial in reducing THC than other alternatives. In their experiments on gas turbines, Ruslan et al. [15] found that the amount (mass%) of biphenyls, monocycloparaffin, alkylbenzene, fluorenes, distillation temperature (90%), carbon content (mass %), naphthalene, and the composite density, benzocycloparaffin content, liquid density at 15°C, aromatics content (vol %) and net heat of combustion has an apparent direct effect on the smoke number. In contrast, other fuel properties such as iso-paraffin content and flashpoint have less impact on the smoke number.

The effect of aromatic concentration in gasoline fuel on the engine's emissions was studied by Georgios et al. [16]. They reported significant increase in the THC with Aromatics content of the fuel. NOx, however, was not affected by the Aromatics content of the fuel as reported in the research work. They also reported good correlation between PM index and PM mass and number with Aromatics.

The main goal of this work is to find the effect of paraffin and aromatics on the quality of the products of the refining process in Iraq. The effect of those two components on the high sulfur content [17], low octane number, and calorific values need to be investigated and optimized. This will help the officials in Iraq

modify the petroleum refining process to solve the high-sulfur, low-calorific value and low octane gasoline problem as a result of the current distillation process followed in their refineries.

2. MATERIAL METHOD

In this study, experimental data were collected from various Iraqi petroleum refineries at different intervals of the year, and the effect of aromatics and paraffin on the properties was modeled using the ANN technique. Further, the interaction between those two factors was done using the DOE technique. Three types of neural activation functions were tested to find the most accurate and quickest network that can model the properties of the distillation process.

2.1. Artificial Neural Networks

A multilayered perceptron (MLP) with back-propagation (BP) ANN algorithm was chosen and trained in this study to develop a predictive regression model with scaled crude oil properties such as paraffin, aromatics as input, and the rest of the distillation output gasoline properties, e.g., Motor Octane Number (MON) and, Research Octane Number (RON), density, etc. as output to the model. This technique is well-established have been used earlier by other researchers [18-20]. The schematic diagram of the MLP-BP-ANN technique is shown in Figure 1.

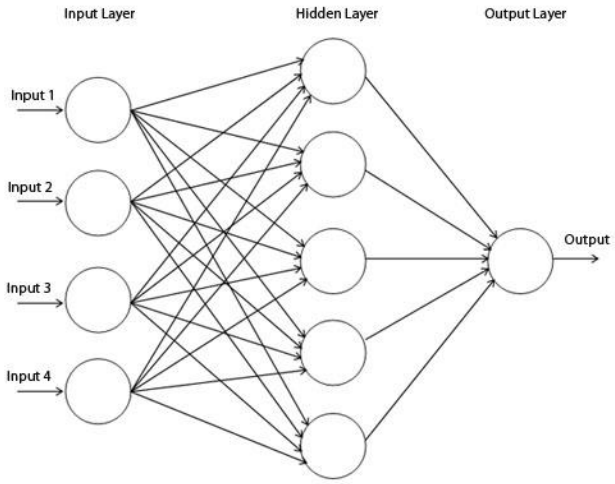


Figure 1. *Schematic diagram of the MLP-BP-ANN method*

The number of input neurons is fixed by the number of input factors, and in the output layer by the number of outputs variables to be predicted [21].

The experimental data obtained for different Iraqi oil refining plants were divided into 80% for training, 10% for validation, and another 10% for testing of the model. The data presented in Table 1 represents a sample of the complete data obtained from the oil refineries.

The activation functions used in this study were the Sigmoid, Tan Hyperbolic, and Gaussian functions. The sigmoid function is of the form $(x) = \frac{1}{1+e^{-kx}}$, Tan Hyperbolic is of the form $F(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}}$, and that for the Gaussian function $F(x) = e^{-\frac{1}{2}x}$ [22]. After finding the proper activation function, the distillate properties' mathematical modeling was found, and the optimum mixture (input) needed for the desired properties was done.

Training of the MLP-BP-ANN proposed model was done till the minimum value of the mean square error (MSE) was achieved during the validation phase. The effectiveness of the model was judged based on the overall accuracy of the predicted data at this stage. For better performance (both from a time and accuracy point of view), the data used was scaled down to 0-1 form with 0 as the new x_{min} and 1 as the new x_{max} using Equation (1) below [23]:

$$x_{i-n} = \frac{x_i - x_{min}}{x_{max} - x_{min}} (new\ x_{max} - new\ x_{min}) + new\ x_{min}\ . \quad (1)$$

In Equation (1), x_i is the input/output data (data of independent and dependent variable variables), x_{max} and x_{min} are the maximum and minimum values of the particular variable, respectively.

Table 1. *Sample results obtained from Al-Doura Refinery in Baghdad*

Properties items	Test methods	LSRN	Reformate	Al Doura Pool	Power Formate
Sp.gr.	IROX test	0.659	0.755	0.715	0.757
RVP bar	ASTM D323	0.94	0.38	0.6	0.37
Distillation Temp. ºC	ASTM D86				
IBP		32	43	36	40
10%		43	68	54	58
20%		52	82	64	77
30%		58	98	72	95
40%		63	110	82	117
50%		68	121	92	135
60%		74	134	102	152
70%		80	146	115	168
80%		86	161	129	186
90%		97	182	148	198
EBP		115	215	187	219
T.D.ml		98	98	98.5	98.5
Max.S.content ppm	ASTM D4294	74.90	91.40	43.8	34.80
Water content ppm	ASTM D4928	35.60	67.22	131.95	42.00
Existent gum mgm/100ml	ASTM D381	0.60	Nill	1.2	Nill
Calorific value kcal/kgm		11488	11203	11326	11197
MON	ASTM D2700	64.60	86.00	80	84.80
RON	ASTM D2699	69.20	90.50	84.5	89.30
Aromatics	IROX test	4.30	41.66	24.25	39.23
Olefins	IROX test	0.00	0.00	0	0.00
Paraffins & Naphthenes	IROX test	95.70	58.34	75.75	60.77

2.2. Response Surface Methodology

The polynomial model was selected in this study to show the interaction between the different experimental factors. This model is shown in Equation (2) below:

$$y = \beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{1 \le i \le j}^{k} \beta_{ij} x_i x_j + \epsilon\ . \quad (2)$$

In Equation (3), β_{ij} represents the coefficients of the interaction parameters. To determine a critical point (maximum, minimum, or saddle), the polynomial function must contain quadratic terms according to Equation (3) presented below:

$$y = \beta_o + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{1 \le i \le j}^{k} \beta_{ij} x_i x_j + \epsilon \quad (3)$$

where β_{ii} represents the coefficients of the quadratic relationship. To estimate the parameters in Equation (4), the experimental design is to assure that all studied variables are carried out at least three-factor levels.

The use of the RSM and ANN methods to simulate the petroleum refining process has been well-established and used by several researchers.

Anish et al. [24] used the RSM methodology to optimize the operation of the fluid catalytic cracking (FCC) unit. Their results showed that statistical techniques can be effectively used to simulate and optimize complex chemical engineering operations

Festus et al. [25] used the RSM method to study the effect of time and temperature on the desulfurization of crude oil using NaOH solution concentration. They reported an accuracy of about 97.5% which shows the suitability of such statistical methods in the simulate-related processes.

Nalini et al. [26] used the ANN method to predict the crude oil pricing which they reported to perform excellently in predicting the oil price.

The ANN method was also used by Lluvia et al. [27] to improve heat-integrated crude oil distillation systems. They claimed that the neural network model could solve convergence issues caused by rigorous or simplified models, and that using neural networks, as opposed to rigorous models, the simulation time was significantly reduced with almost no loss in model accuracy.

The artificial neural network (ANN) technique was used by Vo Thanh et al. [28] to forecast the oil recovery and CO2 storage capacity in residual oil zones. (ROZs). Their findings showed that the ANN model could forecast CO2 storage and oil recovery with exceptional accuracy and that it could be used as a reliable tool to assess the viability of CCUS in ROZs at an early stage.

An extensive review on the use of ANN in petroleum-related processes (e.g. Oil/gas exploration, drilling, production, and reservoir management …etc), Alkinani et al [29].

3. THE RESEARCH FINDINGS AND DISCUSSION

The data used in the study was collected from several oil refineries across Iraq. A sample of the data collected from other refineries for different oil wells and different qualities is shown in Table 2. A statistical summary of the data used in this research is shown below in Table 3.

Table 2. *The data used for the study*

Aromatics	Paraffins	RON	MON	Sp.Gr	S	H_2O	Qcv	RVP	IBP	EBP	Recovery
% vol	% vol				(ppm)	(ppm)	(kcal/kg)	(bar)	(C)	(C)	%
4.3	95.7	69.2	64.6	0.659	74.96	35.6	11488	0.94	32	115	98
8.85	89.26	60.31	55.71	0.71	45	40	11341	0.56	45	174	98
10.8	86.5	56.5	51.2	0.733	32	43	11272	0.4	62	203	98.5
23.1	76.9	80.5	76	0.637	86.6	44	11547.9	0.62	37	190	98
23.4	76.6	81.5	77	0.63	84.2	43.5	11566.5	0.62	34	187	98
32.99	67.01	89.7	85.1	0.733	44.5	45.4	11972	0.44	49	179	98
33.63	66.37	95.4	90.9	0.744	34.3	43.4	12058.6	0.48	47	179	99
38.67	61.33	89.6	85	0.761	35.2	39.4	11229	0.42	51	184	98
39.12	59.88	89.3	85.8	0.756	35.3	41.9	11209.8	0.385	50	185	98
39.23	59.77	89.3	84.8	0.757	35.8	42	11197	0.382	49	185	98
41.66	58.34	90.5	86	0.755	91.4	67.22	11050	0.38	43	205	98

Table 3. *Statistical summary of the data used in the analysis*

	Aromatics	Paraffin	RON	MON	Sp.Gr	S	H_2O	Qcv	RVP	IBP	EBP	Recovery
	% vol	% vol				(ppm)	(ppm)	(kcal/kg)	(bar)	(C)	(C)	%
Number	33	33	33	33	33	33	33	33	33	33	33	33
Mean	43.09	56.77	113.08	110.51	0.76	41.65	93.35	11252.91	0.46	95.40	203.03	98.4
Median	39.12	60.88	86.06	86.23	0.75	57.8	48.26	11225.35	0.44	45.62	186.80	98
Standard Deviation	28.13	27.97	50.45	55.06	0.095	249.75	84.97	401.86	0.28	111.75	63.85	0.9774

Figure 2 shows three main activation functions (Sigmoid, TanH, and Gaussian) that were tested in this study. The aim was to use the one that gives the best performance in reaching the best solution with the least epochs and time.

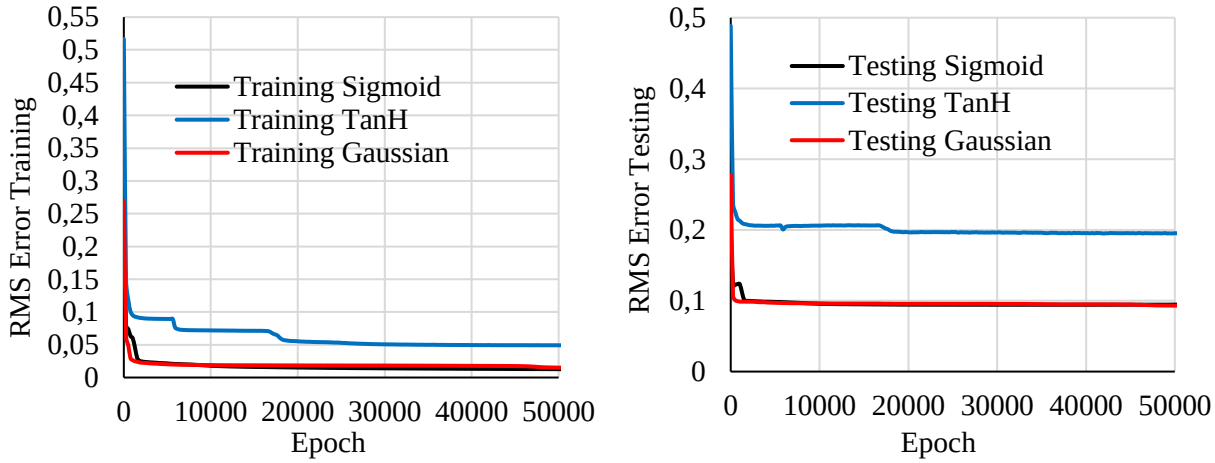


Figure 2. *Performance comparison between activation functions*

It was clearly shown in the figure that the Tan Hyperbolic functions failed to give the same performance as the other activation functions. There was a slight edge in favor of the Gaussian function over the sigmoid for both training and testing. This is shown in the figure by the RSM error for each activation function at a steady state or after a certain number of runs. Therefore, the Gaussian activation function was chosen. The detailed model properties and their accuracy are summarized in Table 4.

Table 4. *Summary of the model accuracy*

	Network Structure	R^2		RMSE	
		Training	Testing	Training	Testing
Motor Octane Number	2-5-1	0.9941	0.9948	1.0308	3.2340
Research Octane Number	2-5-1	0.9978	0.9942	1.6676	1.0635
Specific Gravity	2-5-1	0.9985	0.9939	0.0023	0.0047
Reid Vapor Pressure	2-5-1	0.9948	0.9812	0.0011	0.0321
Initial Boiling Point	2-5-1	0.9953	0.9833	3.094	1.3971
End Boiling Point	2-5-1	0.9995	009942	0.3304	2.2597
Sulfur Content	2-5-1	0.9971	0.9955	10.7901	21.4072
H_2O	2-5-1	0.9800	0.9720	1.3893	10.9067
Calorific Value	2-5-1	0.9996	0.9676	6.5302	69.3384
Recovery percent	2-6-1	0.9998	0.9949	0.0021	0.03089
		Percentage Evaporated			
10%	2-6-1	0.9914	0.7185	3.6707	4.9676
20%	2-6-1	0.9960	0.7831	2.3352	4.9431
30%	2-6-1	0.9913	0.9843	3.1673	1.7777
40%	2-6-1	0.9657	0.8639	5.8150	6.1525
50%	2-6-1	0.9335	0.7252	7.6619	9.8718
60%	2-6-1	0.8880	0.9227	9.3857	5.9883
70%	2-6-1	0.8314	0.9757	11.4391	3.7262
80%	2-6-1	0.7374	0.9774	13.8828	4.0909
90%	2-6-1	0.7168	0.9424	14.2822	7.3431

As shown in Table 4 the values for the R^2 are close to unity for all predicted variables. This means that the model predicted by ANN for these variables is accurate.

As for the model equations, a generic form of the final equation taking that for MON as an example is presented below, and the rest are tabulated in Table 4. The hidden layer neurons' equations were in the form, as shown below in Equation (4):

$$H_i = e^{-\frac{1}{2}(a_{i_o} + b_i * \text{Aromatics} + c_i * \text{Paraffins})^2} \quad (4)$$

where a_{i_o} is the bias for every neuron (i), b is the weight between the input aromatics and the hidden neuron, and c is the weight between paraffin and the hidden neuron.

The equation relating the output to the inputs through the hidden neurons is expressed as in Equation (5):

$$Output = a_{j_o} + \sum_{j=1}^{n} w_j H_j \quad (5)$$

where n is the number of hidden neurons.

An example of the first equation for the MON values is shown in Equations (6) and (7). The rest of the hidden neuron equations are tabulated in Table 5. The weights between the hidden layer and the output parameter used in Equation (4) for all 18 parameters are given in Table 6. The above equations were then used to generate the data needed for the design of experiment analysis and optimization using RMS. This part was conducted using Minitab R19 software. The hidden layer equations obtained by the ANN model are shown below in Equation (6) below:

$$\left.\begin{aligned}
H_1 &= e^{-\frac{1}{2}(0.504900275409111 + 0.0539234532539091 * \text{Aromatics} - 0.0538847299842973 * \text{Paraffins})^2} \\
H_2 &= e^{-\frac{1}{2}(6.24519435953332 - 0.0902377857918179 * \text{Aromatics} - 0.0405453422855877 * \text{Paraffins})^2} \\
H_3 &= e^{-\frac{1}{2}(4.45590735958828 + 0.0525719636776719 * \text{Aromatics} - 0.0830521615463908 * \text{Paraffins})^2} \\
H_4 &= e^{-\frac{1}{2}(-1.9832002315875 + 0.0500896838484564 * \text{Aromatics} + 0.00578451692137609 * \text{Paraffins})^2} \\
H_5 &= e^{-\frac{1}{2}(-1.71141059795421 - 0.00937848011682443 * \text{Aromatics} + 0.0593037417991988 * \text{Paraffins})^2}
\end{aligned}\right\} \quad (6)$$

From these hidden layer formulas, the equation predicting the output parameter, here MON is shown, for example, can be written as:

$$MON_{Predicted} = 89.2466049 - 252.80038310 * H_1 + 412.846307 * H_2 - 90.495782965 * H_3 - 180.801673681 * H_4 + 7.2448114436 * H_5 \quad (7)$$

Table 5. *Weights between the hidden layer and output parameter*

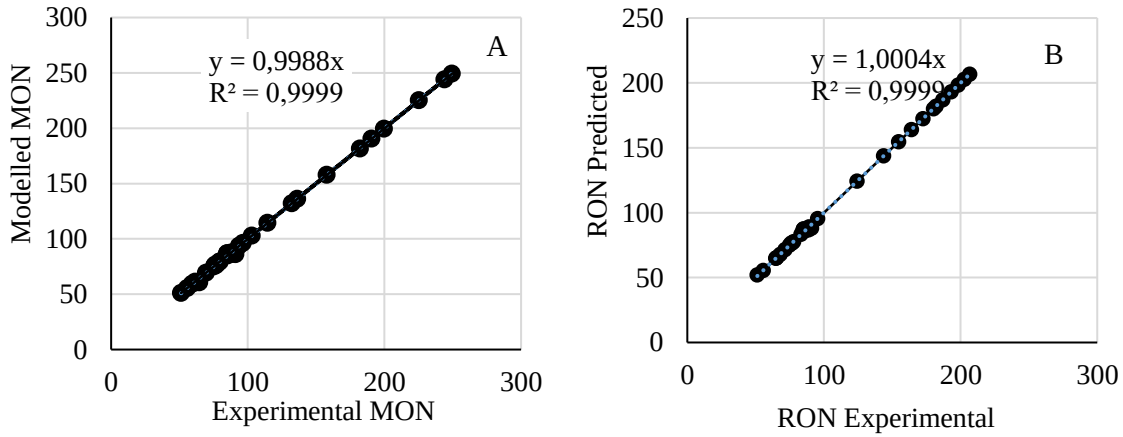
	Bias	W1	W2	W3	W4	W5	W6
Research ON	61.6098	-131.4367	329.142	-30.43344	-11.3627	1.32367	0
Specific Gravity	0.18318	-0.289059	0.17286	-0.500751	1.10782	-0.00476	0
RVP	2.99806	-0.802974	4.91549	-2.063749	0.03685	-4.65714	0
Sulfur Content	-8819.71	977.6782	-40.5743	7208.3001	-498.267	9631.27	0
Initial Boiling Point	565.579	-23.89793	-967.374	510.99078	-339.494	137.137	0
End Boiling Point	9672.12	-327.1301	823.032	208.61216	-9787.34	-535.607	0
H_2O content	48.45565	215.6331	-323.722	431.11729	-263.259	-190.159	0
Calorific Value	11471.55	2889.992	-727.835	2634.5364	-1219.09	-2086.98	0
Recovery (%)	148.2146	-49.65141	-67.2807	-22.11997	89.03423	2.169937	-12.687
10% Evaporated	146.5731	-43.21388	-2.60746	-26.21899	-92.97669	57.11532	-41.210
20% Evaporated	177.6610	-0.161014	-17.5524	-77.36252	-41.08247	41.01890	-90.634
30% Evaporated	122.5311	-63.32803	-35.0521	-46.50951	-47.75886	114.3280	19.1379
40% Evaporated	106.9317	-42.71848	-58.1178	-53.23196	-17.39421	148.5502	-1.2641
50% Evaporated	102.2420	-20.40738	-71.3581	-51.45216	-0.074565	164.6898	-29.179
60% Evaporated	117.2108	-24.79134	-73.9769	-53.88544	7.164428	155.3027	-26.370
70% Evaporated	130.0545	-19.40446	-67.5508	-49.83736	7.315496	143.3186	-32.099
80% Evaporated	145.1035	-22.48214	-57.4266	-42.93229	2.874205	128.0462	-38.490
90% Evaporated	145.7793	-10.31829	-47.8016	-24.59089	0.515717	114.9782	-49.991

Table 6. *The weights between the inputs and hidden layer neurons*

		H1	H2	H3	H4	H5	H6
RON	ao	1.218026	-4.94525	8.360285	-7.179424	1.755552	0
	b	0.010861	0.037146	-0.20458	-0.028626	0.042612	0
	c	-0.01302	0.036048	0.008115	0.114751	-0.041395	0
Specific Gravity	ao	2.622068	1.692600	-3.79097	-4.361374	-0.966850	0
	b	-0.07238	0.061045	0.031017	0.045232	-0.043283	0
	c	-0.00874	-0.053559	0.022211	0.053061	0.012820	0
RVP	ao	1.881966	2.087132	1.248031	-0.140765	-4.506550	0
	b	0.039084	-0.049098	-0.00738	0.000379	0.023737	0
	c	-0.04036	-0.009155	-0.01449	-0.001209	0.056266	0
Sulfur	ao	-5.89542	3.006306	-2.69400	7.351241	0.117395	0
	b	0.088187	-0.072316	0.028506	-0.001515	-0.023144	0
	c	0.035287	0.010593	0.009427	-0.121017	0.008526	0
Initial BP	ao	5.684775	2.414354	0.363873	-6.210412	-2.469675	0
	b	-0.15164	-0.044078	0.027827	0.012303	-0.018286	0
	c	-0.01679	-0.012636	-0.01700	0.066931	0.034090	0
End BP	ao	-1.59213	1.963313	2.240794	-1.369122	0.984382	0
	b	-0.03705	0.005430	0.043127	0.016013	0.042853	0
	c	0.028272	-0.034382	-0.05041	0.0121751	-0.040710	0
H_2O	ao	2.744160	4.607682	-1.98252	1.519695	2.709939	0
	b	0.090289	-0.05619	0.004618	0.070056	0.063986	0
	c	-0.08292	-0.058165	0.036473	-0.065886	-0.064092	0
Calorific Value	ao	0.866205	-3.488047	1.539958	-4.764899	-2.889805	0
	b	-0.05729	-0.099014	0.025971	-0.061963	0.008233	0
	c	0.015366	0.072321	-0.00617	0.119508	0.035484	0
Recovery	ao	-2.80766	0.221966	1.482031	2.337206	3.839143	1.999809
	b	-0.00295	0.016259	-0.02289	0.001913	0.07216	-0.026381
	c	0.035694	-0.011789	0.001182	-0.034137	-0.071206	-0.017069
Evaporation Percent	ao	-2.39343	-6.853717	4.243779	-5.585484	-27.57259	22.03325
	b	0.162172	0.085469	-0.01346	0.024171	0.2642982	-0.165187
	c	0.024029	0.0421755	-0.05505	0.073282	0.2973759	-0.21551

4. RESULTS AND DISCUSSION

The results of the modeling study are shown in Figures (3 A through J). The models obtained for the data were accurate to an acceptable limit of 3-5%. These figures clearly show that the models were able to predict the properties of petroleum with a reasonable degree of accuracy.



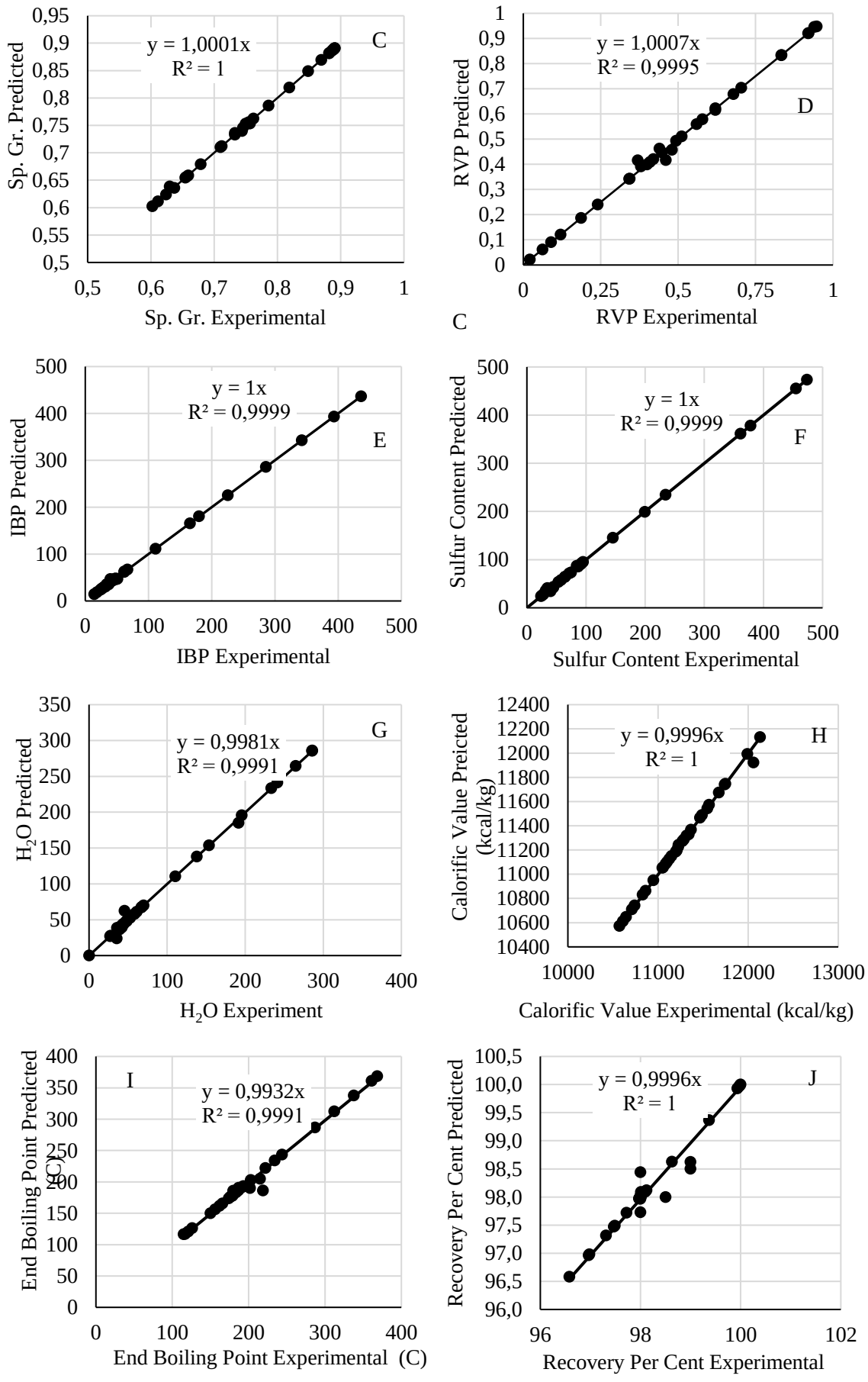


Figure 3. *Predicted versus experimental data for distillate properties*

Figures 4 show the results of the simulation study based on the models obtained above. The effect of presence of Aromatics and Paraffin on various fuel properties is shown in the figures (4.a through d). Based on Figure 4-a, it is noticed that the effect of both components causes the fuel's Octane Number (ON) to increase. The effect is higher for lower concentrations of Paraffins. This is expected because ON for aromatics is much higher than those for paraffins [30]. Hence, as shown in the figure, the effect of aromatics is more pronounced at lower levels of paraffins tat at higher levels. This is one reason for petroleum refineries to add aromatics to the fuel to improve its ON.

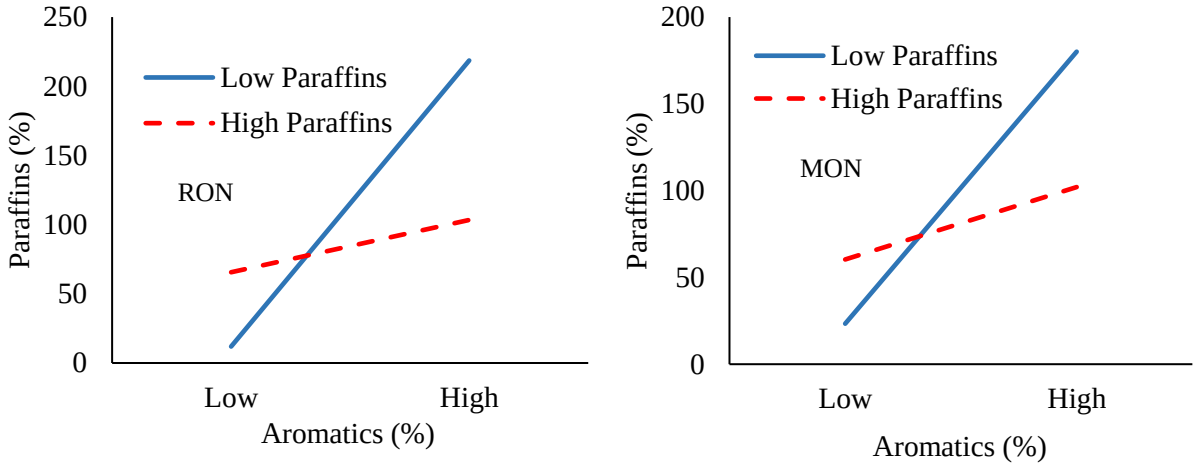


Figure 4-a. *Effect on fuel Octane Number*

Figure 4-b shows the effect of both aromatics and paraffins on specific gravity and calorific value of the fuel. The calorific value of a fuel (or called heat of combustion) based on the (ASTM D240, ASTM D1405, and others) is a direct measure of energy content of the fuel. It is measured by the quantity of heat liberated by the combustion of a unit quantity of fuel with oxygen in a standard bomb calorimeter. A high calorific value is obviously desirable in oil used for heating purposes. Specific gravity of the fuel, on the other hand, is also important since fuels are sold on a volume basis; hence more energy content (kJ/m^3) is available in one liter of fuel if the specific gravity increases. A proposed correlation between the calorific value and specific gravity can be given by [31]:

$$Q_{CV} = 12400 - 2100 * SG^2 \tag{8}$$

where Q_{CV} is the heat of combustion and SG is the specific gravity. Any method used to compute such a property, however, is not guaranteed to be accurate and should only be used as a guide or an approximation to the measured value.

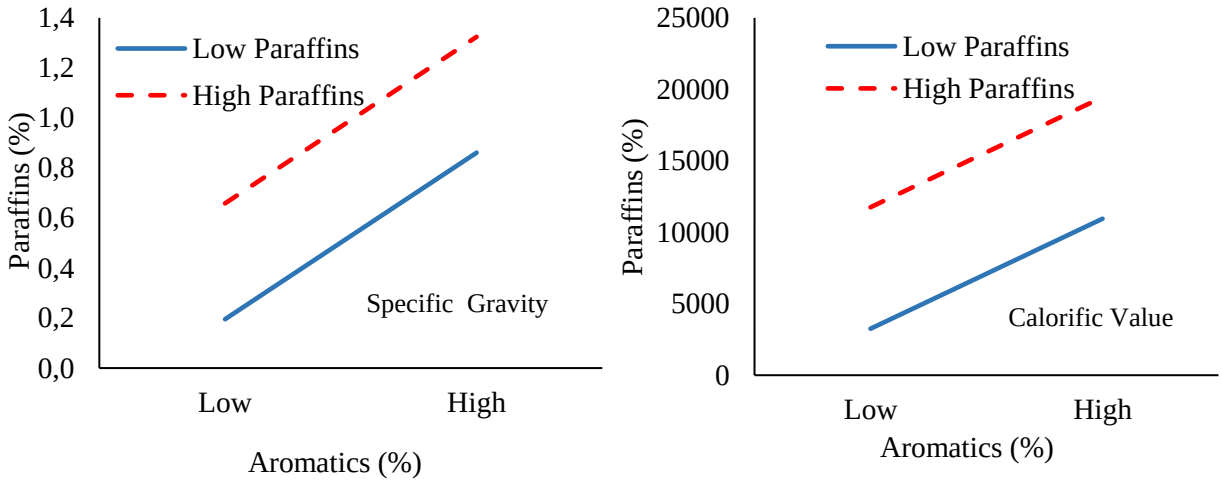


Figure 4-b. *Effect on fuel specific gravity and calorific value*

The carbon-to-hydrogen (C/H) ratios of the aromatic compounds are higher than those of naphthenes, which are higher than those of paraffins. The C/H ratio of crude oil increases with weight (specific gravity). Aromatics have a heating value of 5.4 MJ/kg, while paraffins have the highest [32].

This helps explain the results shown in Figure 4-b where both properties show almost similar trends with change in paraffins and aromatics with higher effect for paraffins on calorific value compared with aromatics. The use of higher specific gravity fuel would improve the fuel consumption of the vehicle. Moreover, increasing the specific gravity of the fuel would result in increasing the boiling point and ON for the fuel. On the other hand, increasing the aromatics percentage has an adverse effect on the fuel's calorific value, which is an undesired effect.

An indicator of how volatile petroleum products like gasoline, diesel, and others is the Reid Vapor Pressure (RVP), which is shown in Figure 4-c below. It can be referred to as the pressure exerted on the fuel at a temperature of 37.8 °C (100 °F) by the vapor of the liquid and any dissolved gases or moisture. It is typically measured using the test method ASTM-D-323, which originated in 1930 and has undergone numerous revisions. (the latest version is ASTM D323-15a).

One such problem faced in summer is the vapor lock caused by excessive fuel evaporation, while, in winter, difficulty in starting the vehicle due to low fuel evaporation is another problem. Thus, manipulating the RVP seasonally accurately to maintain gasoline engine reliability. Another disadvantage of using high-aromatics crude oil is the sulfur content (shown below in the figures) of the fuel. High aromatics resulted in the high sulfur content of the fuel.

Sulfur is the third most common element in crude oil and must be removed due to its corrosiveness, unbearable odor and harmful combination with sulfur dioxide (SO_2) and hydrogen sulfide (H_2S). Traditionally, excess sulfur is removed from crude oil during refining process, as sulfur oxides emitted to the atmosphere when oil is burned are the major pollutants.

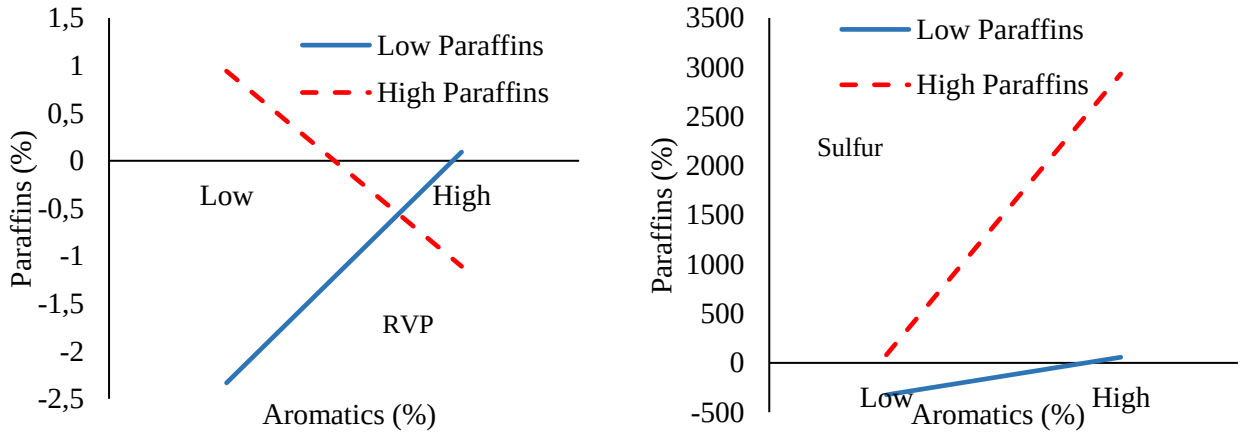


Figure 4-c. *Effect on fuel's Reid vapor pressure and sulphur content*

Aromatics increase the RVP of fuel at low levels of paraffins, while Paraffins decrease it. Similar findings is reported in [32]. Hence, it is expected that in summer, low percentages of Aromatics should be added, while in winter, Aromatics are desired. This is highly undesired as it increases the SO_2 levels in the exhaust with all its harmful effects on the environment (e.g., acid rain) and automotive parts (e.g., corrosion). Another undesired effect of the presence of sulfur is that it decreases the effectiveness of the catalytic converters as well as oxygen sensors in the exhaust.

Several factors affect the boiling point (shown below in Figures 4-d) for complex systems such as hydrocarbons. carbon number, molecular size, and the type of hydrocarbons (aliphatic, naphthenic, or aromatic) are an example of such factors affecting the boiling point of petroleum products.

Generally, it is noticed that boiling points tend to decrease with the increase of both Aromatics and Paraffins. Further noticed that the percentage of H_2O in the products also increase with both Aromatics and Paraffins. This has an undesired effect on fuel combustion properties as well as storage.

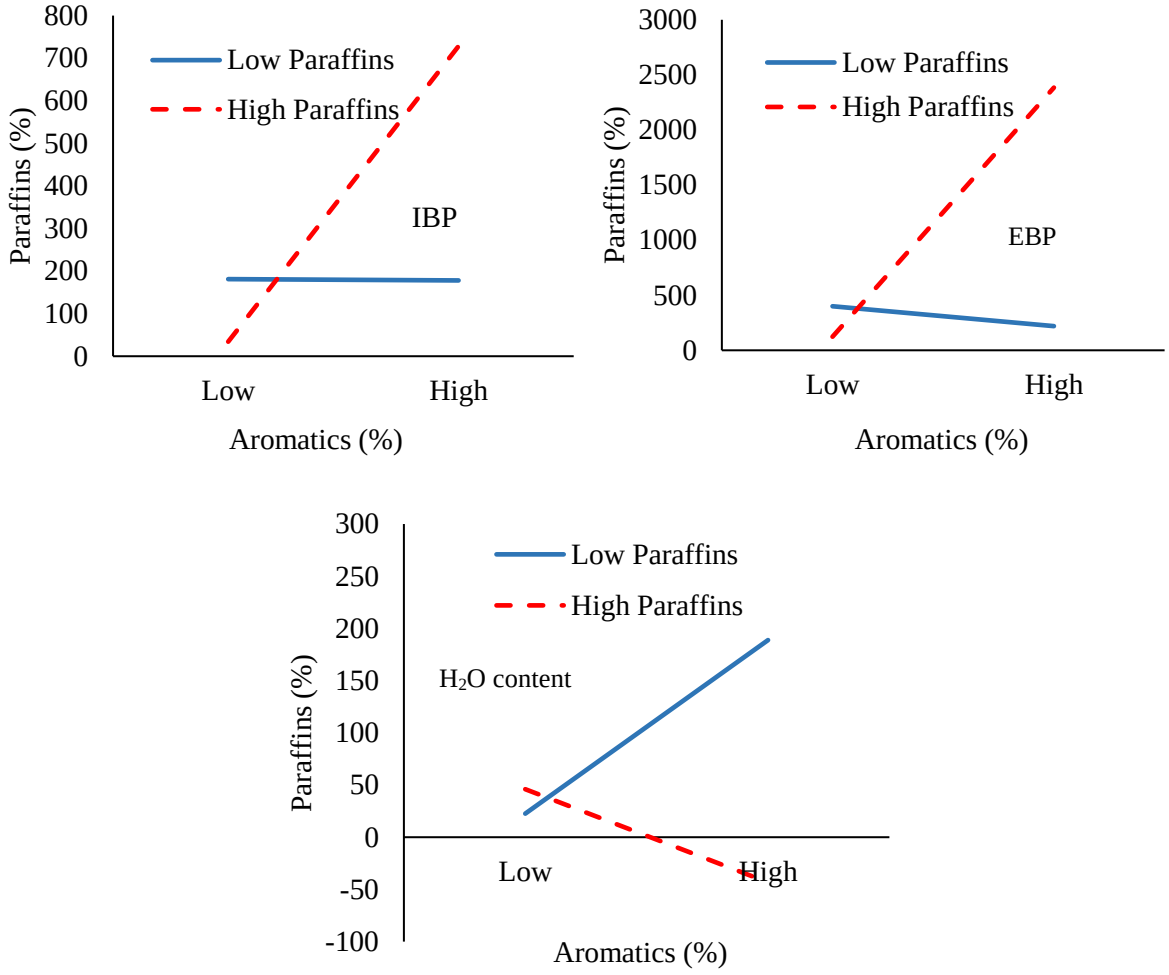


***Figure 4-d**. Effect on boiling points and water content*

Finally, based on the above, since Aromatics and Paraffins have a greater effect on fuel behavior in practical applications, optimization was done to improve the Octane number, specific gravity, calorific value, and minimum water and sulfur contents. The results are presented in Table 7. The best percentages for this purpose were found to be 97% Aromatics and 3% Paraffins.

***Table 7.** The result of the optimization study*

Parameter	Lowest (% vol)	Highest (% vol)	Optimum value (%)
Aromatics	0	100	96.9561
Paraffins	0	100	2.8126

5. SUMMARY AND CONCLUSION

To conclude the findings of this research, modeling the effect of Aromatics and Paraffins on distillate's properties was conducted using experimental data collected from different refineries in Iraq. ANN and DOE techniques were used.

The effect of both Aromats and Paraffins on product quality (e.g. MON, RON, …) differs considerably. Whereas Aromatics are used for increasing the octane number of the products and lowering its boiling point

limits, it is unfavorable for the calorific value and sulfur content of the products.

Aromatics have a stronger effect on the octane number at low concentrations of paraffin, while, for specific gravity and calorific value they have similar effects.

Regarding boiling points and sulfur contents, aromatics have almost no effect at lower levels of paraffin. Optimization based on RON, RVP, H_2O, and sulfur content showed that the best percentage of aromatics should not exceed 97%.

CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

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