

PREDICTION OF OCTANE NUMBERS OF PETROLEUM FRACTIONS USING APPROACHES CORRELATIONS

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Abstract:

Octane number is an important characteristic of spark engine fuels such as gasoline and jet fuel or fractions that are used to produce these fuels (i.e., naphthas) and its represents antiknock characteristic of a fuel. It is that percentage of isooctane in a blend of isooctane and normal heptane that exactly matches the knock behavior of the gasoline. Two octane numbers are usually determined. The first is the research octane number RON and the second is the motor octane number MON. The main objective of this study is to predict the octane numbers (RON & MON) using various correlations methods for the petroleum fractions of light and heavy naphtha. The study was conducted on the petroleum fractions of both light and heavy naphtha for the blend of Messla and Sarir crude oils at Tobruk refinery. The main objective of the study is to highlighting on procedures for prediction of ON using approaches correlations. The results show that the estimation of RON by using RON values for pure hydrocarbons shows 73.93 with a deviation 2.43 from clear RON 71.50; while, estimation RON from the pseudocomponent method using predicted PNA composition is 74.12 with an error 2.62 from clear RON 71.50. RON from Nelson graphical correlations using K_w , T_b and total paraffins (x_p , x_{Ip}) and T_b

reported 73.98 and 73.90 with an errors 2.48 and 2.40 from clear RON 71.50 respectively. The calculated MON from actual reported RON shows $(MON)_{est.} = 67.55$ with an error 1.43 from the reported value 68.98; and from predicted RON shows $(MON)_{est.} = 69.56$ with an error -0.58, is in good agreement with the reported value 68.98. Consequently, the findings indicate that the approaches correlations can be applied to predict the octane numbers for petroleum fractions because of their consistency with the reported experimental data.

Keywords: crude oil, petroleum fractions, octane number, correlations.

الملخص

يُعد الرقم الأوكتاني أحد الخصائص الهامة لشرارة وقود المحرك كالجازولين ووقود الطائرات أو المشتقات المستخدمة في إنتاج هذا الوقود مثل النافثا، والذي يمثل نسبة الأيزوأوكتان في مزيج الأيزوأوكتان والهيبتان العادي. ويتم في العادة تحديد نوعين من الرقم الأوكتاني، الأول هو رقم أوكتان البحث *RON* والثاني رقم أوكتان المحرك *MON*. لقد أجريت هذه الدراسة على المشتقات النفطية لكل من النافثا الخفيفة والنافثا الثقيلة لمزيج خام حقلي مسلة والسرير بمصفاة طبرق. حيث يتمحور الهدف الرئيسي لهذه الدراسة حول تسليط الضوء على طرق التنبؤ للرقم الأوكتاني باستخدام نهج المضاهات. لقد أظهرت النتائج أن تقدير *RON* باستخدام قيم *RON* للهيدروكربونات النقية هو 73.93 بانحراف قدره 2.43 عن *RON* النظيف 71.50، بينما كان تقدير *RON* من طريقة المكونات المزيّفة باستخدام تنبؤ تركيب *PNA* هو 74.12 بخطأ قدره 2.62 عن *RON* النظيف 71.50. لقد كانت قيم *RON* من مضاهات نيلسون البيانية باستخدام معامل واتسون K_w ونقطة الغليان الحقيقي T_b والبارافينات الكلية (x_p, x_{Ip}) و T_b هي 73.98 و 73.90 بقيمة خطأ قدرها 2.48 و 2.40 عن *RON* النظيف 71.50 على التوالي. كما أن حساب *MON* من القيم الحقيقية لـ *RON* أظهرت أن $(MON)_{est.} = 67.55$ بخطأ قدره

1.43 عن القيمة المسجلة وهي 68.98 وعن قيمة تنبؤ RON $(MON)_{est.} = RON$ بخطأ قيمته -0.58، وهذا يتفق على نحو جيد مع القيم المسجلة وهي 68.98. وبناءً عليه تشير النتائج إلى أن استخدام نهج المضاهاة يتناغم مع البيانات التجريبية المسجلة.

الكلمات الدالة: النفط الخام، المشتقات النفطية، النافثا الخفيفة، النافثا الثقيلة، الرقم الأوكتاني، المضاهاة.

1. Introduction

Fluids produced from oil and gas wells generally constitute mixtures of crude oil, natural gas, and salt water. These mixtures are very difficult to handle, meter, or transport. In addition to the difficulty, it is also unsafe and uneconomical to ship or to transport these mixtures to refineries and gas plants for processing. Further, hydrocarbon shipping tankers, oil refineries, and gas plants require certain specifications for the fluids that each receive. Also, environmental constraints exist for the safe and acceptable handling of hydrocarbon fluids and disposal of produced salt water. It is therefore necessary to process the produced fluids in the field to yield products that meet the specifications set by the customer and are safe to handle [1].

The oil refinery in Tobruk city lies on the southern side of Tobruk Bay on the Mediterranean Sea coast (Figure 1) and has been designed with refinery capacity about 20,000 bb/day under atmospheric overhead distillate. The main products of refinery are the straight run LPG, light naphtha, heavy naphtha, kerosene and diesel.

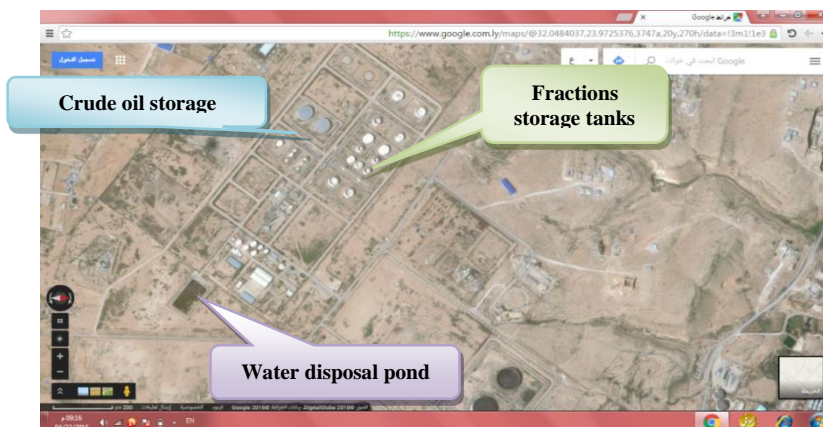
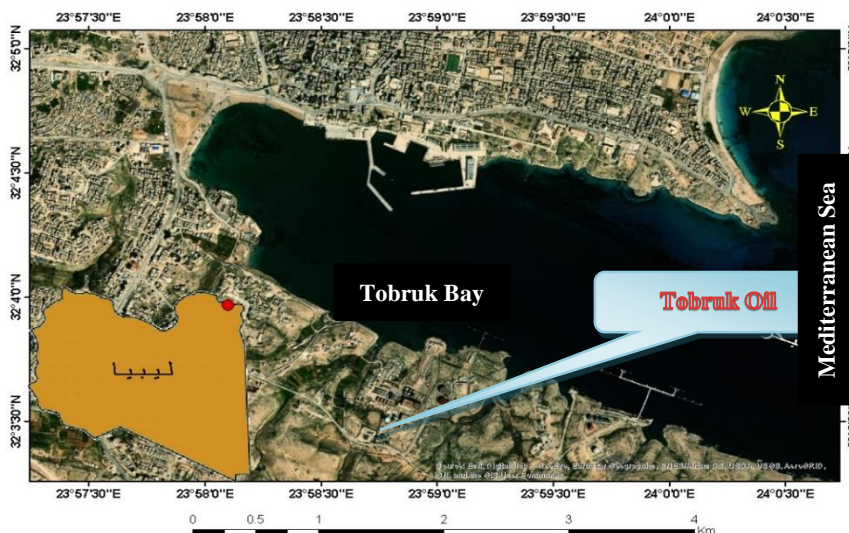


Fig. 1 Satellite image shows the location of Tobruk refinery

2. Materials and Methods

The octane number can be estimated by different techniques of experimental testing using the various ASTM methods and by applying correlations. This methodology was reported in this study.

Octane numbers are a measure of a gasoline's resistance to knock or detonation in a cylinder of a gasoline engine. The higher this

resistance is the higher will be the efficiency of the fuel to produce work. A relationship exists between the antiknock characteristic of the gasoline (octane number) and the compression ratio of the engine in which it is to be used. The higher the octane rating of the fuel then the higher the compression ratio of engine in which it can be used.

By definition, an octane number is that percentage of isooctane in a blend of isooctane and normal heptane that exactly matches the knock behavior of the gasoline. Thus, a 90 octane gasoline matches the knock characteristic of a blend containing 90% isooctane and 10% *n*-heptane. The knock characteristics are determined in the laboratory using a standard single cylinder test engine equipped with a super sensitive knock meter. The reference fuel (isooctane blend) is run and compared with a second run using the gasoline sample. Details of this method are given in the ASTM standards, Part 7 Petroleum products and Lubricants.

Two octane numbers are usually determined. The first is the research octane number (ON res or RON) and the second is the motor octane number (ON mm or MON). The same basic equipment is used to determine both octane numbers, but the engine speed for the motor method is much higher than that used to determine the research number. The actual octane number obtained in a commercial vehicle would be somewhere between these two. The significance of these two octane numbers is to evaluate the sensitivity of the gasoline to the severity of operating conditions in the engine. The research octane number is usually higher than the motor number by 6-12 points, the difference between them is termed the sensitivity of the gasoline.

Octane number is an important characteristic of spark engine fuels such as gasoline and jet fuel or fractions that are used to produce these fuels (i.e., naphthas) and its represents antiknock characteristic of a fuel. Isooctane (2,2,4-trimethylpentane) has

octane number of 100 and n-heptane has octane number of 0 on both scales of RON and MON.

Octane number of their mixtures is determined by the vol.% of isooctane used. Isoparaffins and aromatics have high octane numbers while n-paraffins and olefins have low octane numbers. Therefore, octane number of gasoline depends on its molecular weight type composition especially the amount of isoparaffins.

RON of fuels is determined by ASTM D 908 and MON is measured by ASTM D 357 test methods. Generally there three kinds of gasolines: regular, intermediate, and premium with PON of 87, 90 and 93 respectively. Improving the octane number of fuel would result in reducing power loss of the engine, improving fuel economy, and a reduction in environmental pollutants and engine damage. For these reasons, octane number is one of the important properties related to the quality of gasolines. There are number of additives that can improve octane number of gasoline or jet fuels. These additives are tetra-ethyl lead (TEL), alcohols, and ethers such as ethanol, methyl-tetra-butyl ether (MTBE), ethyl-tertiary-butyl ether (ETBE), or tertiary-amyl methyl ether (TAME). For a fuel with octane number (ON) of 100, increase in the ON depends on the concentration of TEL added. The following correlations are developed based on the data provided by Speight [2].

$$TEL = -871.05 + 2507.81 \left(\frac{ON}{100}\right) - 2415.94 \left(\frac{ON}{100}\right)^2 + 779.12 \left(\frac{ON}{100}\right)^3 \quad [1]$$

$$ON = 100.35 + 11.06(TEL) - 3.406(TEL)^2 + 0.577(TEL)^3 - 0.038(TEL)^4 \quad [2]$$

where ON is the octane number and TEL is milliliter TEL added to one U.S. gallon of fuel. In these equations when clear octane number (without TEL) is 100, TEL concentration is zero. By subtracting the

calculated ON from 100, the increase in the octane number due to the addition of TEL can be estimated, which may be used to calculate the increase in ON of fuels with clear ON different from 100. Equation [1] is useful to calculate amount of TEL required for a certain amount for a certain ON while Equation [2] gives ON of a fuel after a certain amount of TEL is added [3].

Octane numbers of some oxygenates (alcohols and ethers) are published. Once these oxygenates are added to a fuel with volume fraction of x_{ox} the octane number of product blend is [4].

$$ON = x_{ox}(ON)_{ox} + (1 - x_{ox})(ON)_{clear} \quad [3]$$

where $(ON)_{clear}$ is the clear octane number (RON or MON) of a fuel and ON is the corresponding octane number of blend after addition of an additive. $(ON)_{ox}$ is the corresponding octane number of oxygenates, which can be taken as the average values for the range of RON and MON. Du Pont has introduced interaction parameters between two or three components for blending indexes of octane number which are presented in graphical forms [5]. Several other blending approaches are provided in the literature [6]. The simplest form of their tabulated blending indexes have been converted into the following analytical relations:

$$BI_{RON} = \begin{cases} 36.01 + 38.33x - 99.8x^2 + 341.3x^3 - 507.2x^4 + \\ 268.64x^5 & 11 \leq RON < 76 \\ -299.5 + 1272x - 1552.9x^2 + \\ 651x^3 & 76 \leq RON \leq 103 \\ 2206.3 - 4313.64x + \\ 2178.57x^2 & 103 \leq RON \leq 106 \\ x = RON/100 \end{cases} \quad [4]$$

where BI_{RON} is the blending index for RON and should be used together with Equation [4] to calculate RON of a blend. Equation [4] reproduce the tabulated values of RON blending indexes with AAD of .06%.

Estimation of octane number of a fuel from its bulk properties is challenging task, since ON very much depends on the chemical structure of components of the mixture. Figure 2 shows variation of RON with boiling point of pure hydrocarbons from different families. If PIONA composition of a fuel is known, RON of a fuel may be estimated from the pseudocomponent techniques in the following form.

$$RON = x_{NP}(RON)_{NP} + x_{IP}(RON)_{IP} + x_o(RON)_o + x_N(RON)_N + x_A(RON)_A \quad [5]$$

where x is the volume fraction of different hydrocarbon families i.e., n-paraffins (NP), isoparaffins (IP), olefins (O), naphthenes (N) and aromatics (A). $(RON)_{NP}$, $(RON)_{IP}$, $(RON)_o$, $(RON)_N$ and $(RON)_A$ are the values of RON of pseudocomponents from n-paraffins, isoparaffins, olefins, naphthenes and aromatics families whose boiling points are the same as the mid boiling point or the ASTM D 86 temperature at 50% point of the fraction and can be determined from Figure 2. Generally petroleum products are free of olefins and the main groups present in a petroleum products are n-paraffins, isoparaffins, naphthenes and aromatics. The role of isoparaffins on octane number is significant as they have ON values greater than n-paraffins. In addition different types of isoparaffins have different octane number at the same boiling point. As the number of branches in an iso-paraffin compound increases the octane number also increases. For this reason it would be more appropriate if $(RON)_{IP}$ in Equation [5] is an average value of octane numbers of various types of isoparaffins. For convenience and

computer calculations, values of RON for these various homologous hydrocarbon groups have been correlated to normal boiling point, T_b in the following forms:

$$RON = a + bT + cT^2 + dT^3 + eT^4 \quad [6]$$

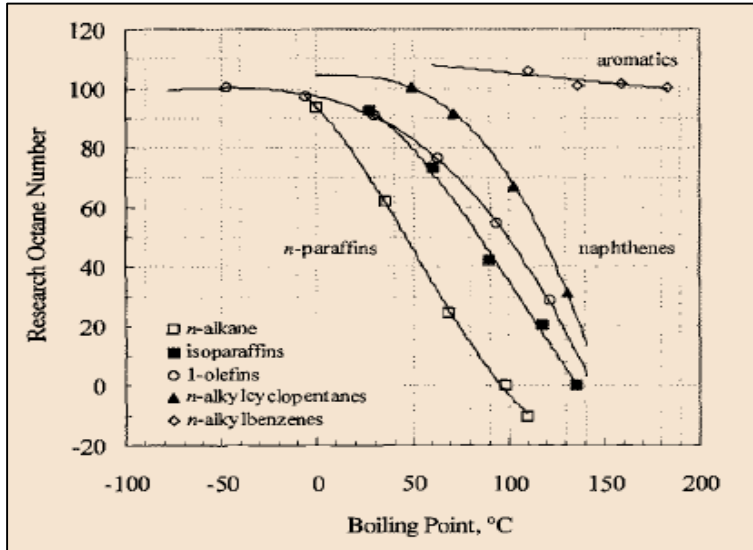


Fig. 2 Research octane number of different families of hydrocarbons [7]

Where RON is the clear research octane number and $T = (T_b - 273.15)/100$ in which T_b is the boiling point in kelvin. Based on the data taken from the API-TDB [8], the coefficients $a-e$ were determined and are given in Table 1 [9,10]. It should be noted that for isoparaffins the coefficients are given for four different groups of 2-methylpentanes, 3-methylpentanes, 2,2-dimethylpentanes and 2,3-dimethylpentanes. Octane numbers of various isoparaffins vary significantly and for this reason an average value of RON for these four different isoparaffinic groups is considered as the value of RON_{IP} for use in Equation [5].

Table 1 Coefficient for Equation (6) for estimation of RON [9,10]

Hydrocarbon family	a	b	c	d	E
n-Paraffins	92.809	-70.97	-53	20	10
isoparaffins					
2-Methyl-pentanes	95.927	-157.53	561	-600	200
3- Methyl-pentanes	92.069	57.63	-65	0	0
2,2- Dimethyl-pentanes	109.38	-38.83	-26	0	0
2,3- Dimethyl-pentanes	97.652	-20.8	58	-200	100
Naphthenes	-77.536	471.59	-418	100	0
Aromatics	145.668	-54.336	16.276	0	0

Nelson [7] gives graphical relation for estimation of RON of naphthas in terms of K_w characterization factor or paraffin content (wt%) and mid boiling point as given in Figure 3 and 4, respectively.

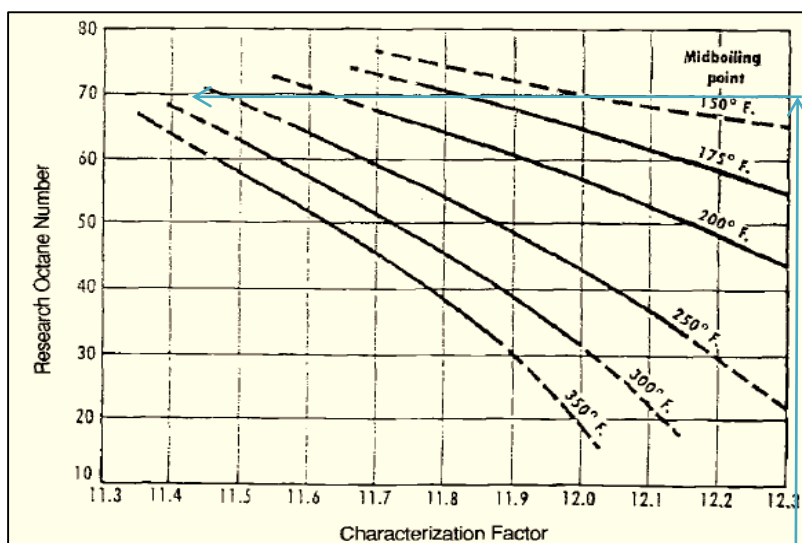


Fig. 3 Research octane number of naphthas [7]

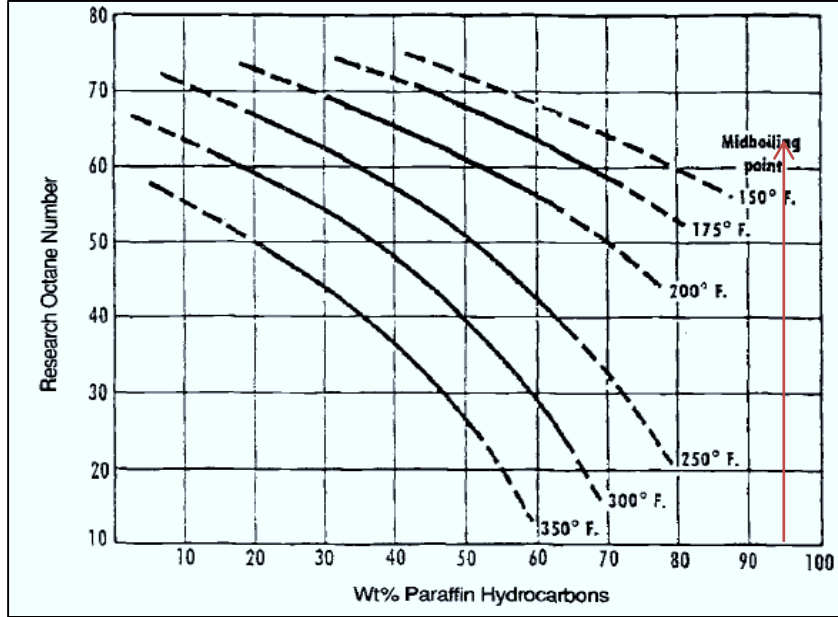


Fig. 4 Research octane number versus paraffin content [7]

As mentioned earlier if amount of paraffins in wt% is not available, vol.% may be used instead of wt% if necessary. Once RON is determined, Mon can be calculated from the following relation proposed by Jenkins [11]:

$$MON = 22.5 + 0.83RON - 20.0 SG - 0.12(\%O) + 0.50(TML) + 0.20(TEL) \quad [7]$$

where SG is the specific gravity, TML and TEL are the concentrations of tetra methyl lead and tetra ethyl lead in ml/UK gallon, and %O is the volume% of olefins in the gasoline.

3. Results and Discussion

This study was conducted on the naphtha fractions of distilled blend of Messla and Sarir crude oils at Tobruk refinery. Table 2 presented the products of distillation crude oils.

Table 2 Distillation of blend crude oils

Products	Light naphtha	Heavy naphtha	Kerosene	Diesel	Residue
True boiling point, TBP (°C)	95	160	255	325	402
Fractional distillation ratio	15.4	31.5	22.9	18.8	11.02

On the other hand, the TBP of petroleum fractions according to ASTM are reported in Table 3. while Table 4 gives the characterizations of naphtha [12].

Table 3 True boiling point of petroleum fractions, ASTM method [12]

True boiling point, TBP (°C)	Light naphtha	Heavy naphtha	Kerosene	Jet fuel	Diesel
IBP	32	79	112	87	200
5% vol.	53	137	166	162	211
10% vol.	63	138	169	163	221
20% vol.	68	141	171	165	232
30% vol.	75	142	175	166	242
40% vol.	81	144	176	169	252
50% vol.	87	146	179	170	264
60% vol.	95	148	180	173	278
70% vol.	102	149	183	175	291
80% vol.	108	152	185	178	307
90% vol.	116	155	189	183	326
95% vol.	121	158	192	188	340
FBP	130	172	202	195	347

IBP = initial boiling point

FBP = final boiling point

3.1 Research Octane Number Estimation (RON) for Light Naphtha

To estimation and prediction of octane numbers for naphtha fractions, the calculation procedure has been carried out based on the following steps:

1. Calculation RON from the pseudocomponents using experimental composition

Boiling point range 32°C - 130°C for light naphtha.

For this fraction: $T_b = (32 + 130)/2 = 81^\circ\text{C} = 354 \text{ K}$

Sp. G. average value = $(0.7152 + 0.7161)/2 = 0.7156$

Clear RON = 71.50 MON = 68.98

$x_p = 40.48$, $x_{Ip} = 35.90$, $x_N = 20.05$, $x_A = 3.57$

Table 4 Naphtha characterizations [12]

S/N	Parameters	Method	Minimum value	Maximum value	Average	Unit
1	Specific gravity @15.6/15.6°C	ASTM D1298	0.7152	0.7161	0.7156	----
2	Rid vapour pressure @37.8°C	ASTM D323	6.4	7.5	6.8	Psi
3	Total sulphur content	ASTM D5453	2.25	2.25	2.250	Ppm
4	Aniline point	ASTM D611	60	60.0	60.0	°C
5	Mercaptan	UOP 163	1>	1>	1>	Ppm
6	H ₂ S content	UOP 163	1>	1>	1>	Ppm
7	Paraffins content	IP 382	76.38	62.48	59.43	Vol. %
8	Naphthenes content	IP 382	20.05	33.95	27.00	Vol. %
9	Aromatic content	IP 382	3.57	3.57	3.57	Vol. %
10	Initial boiling point	ASTM D86	32.0	37.0	35.8	°C
11	Distillation recovery at 10%	ASTM D86	56.0	72.0	64.5	°C

12	Distillation recovery at 50%	ASTM D86	101.0	112.0	105.8	°C
13	Distillation recovery at 90%	ASTM D86	142.0	152.0	146.8	°C
14	Final boiling point	ASTM D86	130.0	175.0	166.8	°C

Estimation RON from Equation [5] using RON values for pure hydrocarbons calculated from Equation [6] and Table 1 with $T_b = 354$ K. Results of calculations are:

$$(RON)_{NP} = 50.13$$

$$(RON)_{IP} = (75.15 + 86.90 + 74.16 + 69.66)/4 = 76.47$$

$$(RON)_{NP} = 54.01$$

$$(RON)_A = 61.08$$

Clear octane number can be determined as:

$$RON = 0.4048*50.13 + 0.3590*76.47 + 0.2005*54.01 + 0.357*61.08 = 73.93$$

In comparison with the reported value of 71.50 the error is $73.93 - 71.50 = 2.43$.

2. Estimation RON from the pseudocomponent method using predicted PNA composition

To predict paraffins, naphthenes and aromatics (PNA), molecular weight must be determined from Equation [8] [13-15]:

$$M = 1.6607 \times 10^{-4} T_b^{2.1962} SG^{-1.064} = 85.12 \quad [8]$$

Since $M < 200$ Equations [9] and [10] and 3.72 to predict the composition:

$$x_p = 3.7387 - 4.0829 SG + 0.014772M \quad [9]$$

$$x_N = 1.5027 + 2.10152 Sg - 0.2388M \quad [10]$$

$$x_A = 1 - (x_P + x_N) \quad [11]$$

The predicted composition for P(%), N(%) and A(%) is 84.14%, 10.15% and 5.71% respectively. In this case RON = 74.12, and the error in calculation of RON is $74.12 - 71.50 = 2.62$

3. Determination RON from Nelson correlation using K_w and T_b

RON can be estimated by using Nelson correlation in Figure 3 through boiling point and characterization factor which can be obtained from Equation [12]:

$$K_w = \frac{(1.8T_b)^{1/3}}{SG} \quad [12]$$
$$= \frac{1.8 \times 354}{0.71} = 12.09$$

Using the K_w value which is calculated as $K_w = 12.09$ and the mid boiling point (140°F) outside the range of curves in Figure 3, accurate reading is not possible, but from the values of K_w it is obvious that the RON can be obtained from Figure 3.33 is above 70 about 73.98.

4. Determination RON from Nelson correlation using total paraffins

In this case RON can be determined using Nelson correlation in Figure 4 through total paraffins ($x_p = 40.48$, $x_{Ip} = 35.90$) and boiling point:

$$\text{Total paraffins} = 40.48 + 35.90 = 76.38\%$$

Also, the mid boiling point (140°F) outside the range of curves in Figure 4, accurate reading is not possible, but from the values of

total paraffins it is obvious that the RON can be obtained from Figure 4 is above 70 about 73.90.

3.2 Motor Octane Number Estimation (MON) for Light Naphtha

1. Calculation MON from actual reported RON

Equation [7] was applied to calculate MON with RON = 71.50, and specific gravity (SG) = 0.7156, and TML = 0%, TEL = 0%.

The estimated value is $(MON)_{est.} = 67.55$, which is in deviation with the reported value of 68.98 with error of $68.98 - 67.55 = +1.43$.

2. Calculation MON from predicted RON (part No. 6.1.2.1)

Equation [7] was applied to calculate MON with RON = 73.93, and specific gravity (SG) = 0.7156.

The estimated value is $(MON)_{est.} = 69.56$, which is in good agreement with the reported value of 68.98 with error of $68.98 - 69.56 = -0.58$.

3. Errors calculations and deviation between estimated and reported values

- For Equation [5] gives an error 2.43 when experimental PIONA composition is used.
- The predicted composition for P(%), N(%) and A(%). In this case the error in calculation of RON is 2.62.
- The estimated value with RON = 71.50, and specific gravity (SG) = 0.7156, is $(MON)_{est.} = 67.55$, which is in deviation with the reported value of 68.98 with error of 1.43.
- Calculation MON with RON = 73.93, and specific gravity (SG) = 0.7156, is in good agreement with the reported value of 68.98 with error -0.58.

Table 5 is summarizing the applicable equations for determination the octane numbers.

3.3 Heavy Naphtha

To determine the octane numbers for the fraction of heavy naphtha, the same procedure of previous steps have been applied but with different parameters. The calculation results for both light and heavy naphtha are summarized and reported in Table 6.

Table 5 The applicable equations for determination the octane numbers

S/N	Equation	Reference
1	$TEL = -871.05 + 2507.81 \left(\frac{ON}{100}\right) - 2415.94 \left(\frac{ON}{100}\right)^2 + 779.12 \left(\frac{ON}{100}\right)^3$	[2]
2	$ON = 100.35 + 11.06(TEL) - 3.406(TEL)^2 + 0.577(TEL)^3 - 0.038(TEL)^4$	[2]
3	$ON = x_{ox}(ON)_{ox} + (1 - x_{ox})(ON)_{clear}$	[4]
4	$BI_{RON} =$ $36.01 + 38.33x - 99.8x^2 + 341.3x^3 - 507.2x^4 + 268.64x^5$ $RON < 76$ $-299.5 + 1272x - 1552.9x^2 + 651x^3$ $RON \leq 103$ $2206.3 - 4313.64x + 2178.57x^2$ $103 \leq RON \leq 106$ $x = RON/100$	[5,6]
5	$RON = x_{NP}(RON)_{NP} + x_{IP}(RON)_{IP} + x_o(RON)_o + x_N(RON)_N + x_A(RON)_A$	[5,6]
6	$RON = a + bT + cT^2 + dT^3 + eT^4$	[8]
	$MON = 22.5 + 0.83RON - 20.0 SG - 0.12(\%O) + 0.50(TML) + 0.20(TEL)$	[11]
7	$M = 1.6607 \times 10^{-4} T_b^{2.1962} SG^{-1.064}$	[13]
8	$x_p = 3.7387 - 4.0829 SG + 0.014772M$	[13]
9	$x_N = 1.5027 + 2.10152 SG - 0.2388M$	[13]
10	$x_A = 1 - (x_p + x_N)$	[13]
11	$K_w = \frac{(1.8T_b)^{1/3}}{SG}$	[7]

Table 6 Results of octane numbers calculations for both light and heavy naphtha

Parameters	Results	Deviation
1. Light naphtha	$(RON)_{NP} = 50.13$ $(RON)_{IP} = (75.15 + 86.90 + 74.16 + 69.66)/4 = 76.47$ $(RON)_{NP} = 54.01$ $(RON)_A = 61.08$	
Boiling point range 32°C - 130°C for light naphtha. For this fraction: $T_b = (32 + 130)/2 = 81°C = 354$ K Sp. G. average value = $(0.7152 + 0.7161)/2 = 0.7156$ Clear RON = 71.50 MON = 68.98 $x_p = 40.48$, $x_{Ip} = 35.90$ $x_N = 20.05$, $x_A = 3.57$	Clear octane number: $RON = 73.93$	+2.43
	Predicted octane number: $RON = 74.12$	+2.62
	RON from Nelson K_w value correlation: $RON = 73.98$	+2.48
	RON from Nelson correlation: with Total paraffins= 76.38% $RON = 73.90$	+2.40
	MON from actual reported $RON = 67.55$	+1.43
	MON from predicted $RON = 69.56$	-0.58
	2. Heavy naphtha	$(RON)_{NP} = 48.16$ $(RON)_{IP} = (72.10 + 81.80 + 69.11 + 62.06)/4 = 71.26$ $(RON)_{NP} = 51.02$ $(RON)_A = 60.40$
Boiling point range 37°C - 175°C for heavy naphtha. For this fraction: $T_b = (37 + 175)/2 = 106°C = 379$ K	Clear octane number: $RON = 68.15$	+0.75
	Predicted octane number:	+2.37

Sp. G. average value = $(0.752 + 0.781)/2 = 0.767$ Clear RON = 67.40 MON = 61.98 $x_p = 38.16$, $x_{Ip} = 24.32$ $x_N = 33.95$, $x_A = 3.57$	$RON = 69.77$	
	RON from Nelson K_w value correlation: $RON = 69.88$	+2.48
	RON from Nelson correlation: with Total paraffins= 76.38% $RON = 69.52$	+2.12
	MON from actual reported $RON = 64.05$	-1.14
	MON from predicted RON $= 62.60$	-0.2.03

On the other hand, Figures 5 & 6 bar charts depict the predicted RON and MON for petroleum fractions and the from reported values respectively. The obtained results display more or less some variance, without much difference between the expected values and the reported ones.

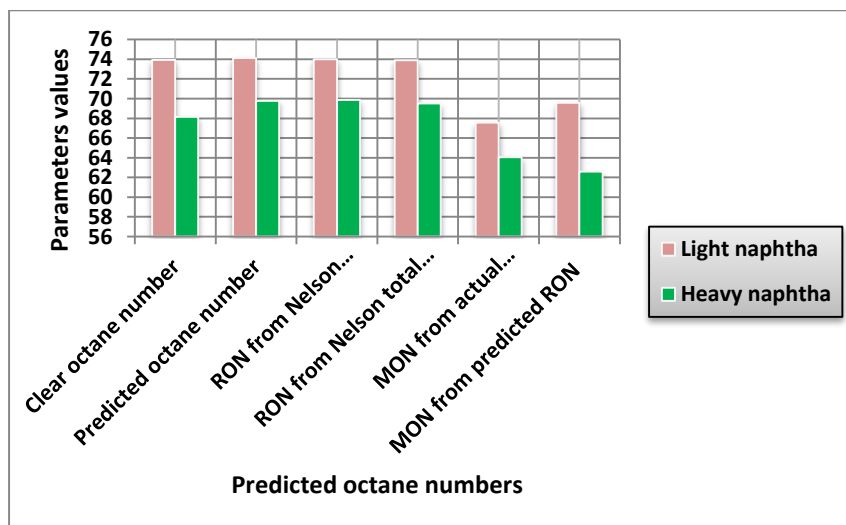


Fig. 5 Predicted RON and MON for petroleum fractions

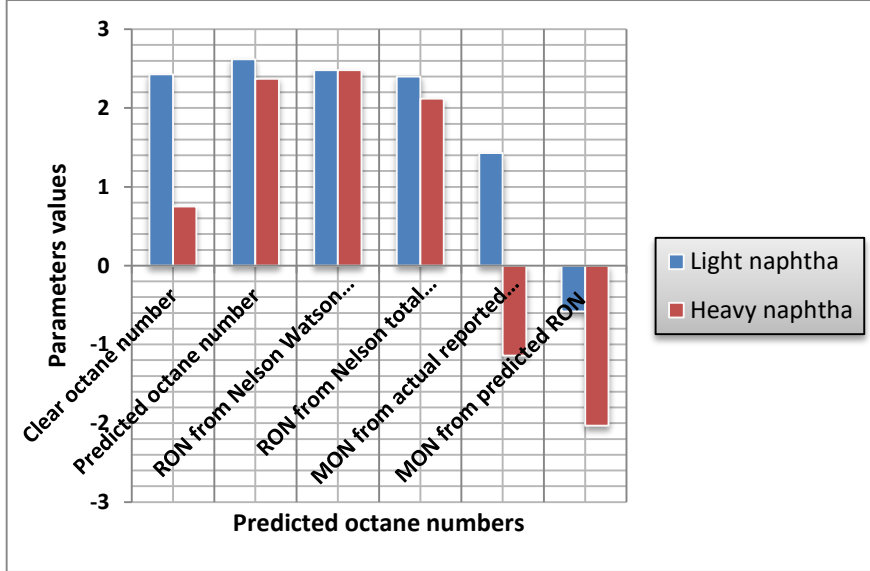


Fig. 6 Predicted RON and MON deviation from reported values

4. Conclusion

Based on the previous findings that obtained from petroleum fractions of both light and heavy naphthas, the following conclusion can be drawn

1. The study highlights on the various procedures for estimation octane numbers for petroleum fractions representing by light and heavy naphthas using the correlations.
2. Estimation RON from using RON values for pure hydrocarbons shows 73.93 with a deviation 2.43 from clear RON 71.50.
3. Estimation RON from the pseudocomponent method using predicted PNA composition is 74.12 with an error 2.62 from clear RON 71.50.

4. RON from Nelson graphical correlations using K_w , T_b and total paraffins (x_p , x_{Ip}) and T_b reported 73.98 and 73.90 with an errors 2.48 and 2.40 from clear RON 71.50 respectively.
5. The calculated MON from actual reported RON shows $(MON)_{est.} = 67.55$ with an error 1.43 from the reported value 68.98.
6. The calculated MON from predicted RON shows $(MON)_{est.} = 69.56$ with an error -0.58, is in good agreement with the reported value 68.98.
7. Errors calculations and deviation between estimated and reported values are:
 - a. For experimental PIONA composition is used gives an error 2.43.
 - b. The predicted composition for P(%), N(%) and A(%). In this case the error in calculation of RON is 2.62.
 - c. The estimated value with RON = 71.50, and specific gravity (SG) = 0.7156, is $(MON)_{est.} = 67.55$, which is in deviation with the reported value of 68.98 with error of +1.43.
 - d. Calculation MON with RON = 73.93, and specific gravity (SG) = 0.7156, is in good agreement with the reported value of 68.98 with error -0.58.
8. Generally, it could be say that the approaches correlations can be applied to predict the octane numbers for petroleum fractions.

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