J. King Saud Univ., Vol. 9, *Eng. Sci.* (2), pp 311-318 (A.H. 1417/1997)

TECHNICAL NOTE

Correlation Between the Octane Number of Motor Gasoline and Its Boiling Range

Hassan Al-haj Ibrahim and Mourhaf Al-Kassmi
Department of Chemical Engineering
Al-Baath University, P.O. Box 77, Homs, Syria

(Received 24 February 1996; accepted for publication 28 September 1996)

Abstract. A significant correlation was found between the research octane number of unleaded motor gasoline and its 90% boiling point using a computer-run regression analysis of data from European and Syrian Sources. A correlation equation was derived with a correlation factor of 0.43 and an average error of 1.9%.

Introduction

The octane number is the most important single performance indicator of motor gasoline. It is a measure of both fuel quality and the maximum compression ratio that can be used in internal combustion engines without the occurrence of knocking. Increasing the compression ratio tends to improve the engine efficiency, but it also increases the knocking tendency of the engine, i.e. it increases the octane number requirement of the automobile.

There are two standard laboratory procedures for the measurement of octane numbers, viz. the research and motor methods. Actual performance, however, is not always indicated by the octane number as measured by these two methods. For this reason the so-called Road Octane Number is sometimes used for better approximation to actual fuel performance. There is no standard laboratory test for the measurement of Road Octane Numbers but two procedures for its measurement have been developed in the U.S.A. These procedures involve the use of particular fuels in special automobile makes. A number of correlations were also developed between the octane number as measured by the two laboratory procedures and the Road Octane Number, but these correlations have been of limited value and application. The laboratory measurement of the octane number, on the other hand, is neither quick nor easy, and besides it requires a standard engine. This standard engine may not be always available, particularly in mobile or small laboratories.

With the above considerations in mind, the search for a simpler and quicker procedure for the evaluation of the anti-knock quality of motor gasoline can be rewarding and beneficial. This will be particularly so if a method can be found for calculating an octane index from a knowledge of basic easy-to-measure gasoline properties such as density and boiling range. Octane index is used here to refer to the calculated octane quality in contradistinction to the (measured) research or motor octane number.

The boiling range in particular has a dramatic effect on the measured octane number. Significant correlation between these two properties is to be expected which would make it possible to calculate an octane index that may better describe the performance quality of gasoline.

Octane number as a function of boiling range

The octane number decreases in general with increasing boiling range [1,2]. This effect is, however, different for different types of fuel. It is more pronounced for straight-run gasoline [2]. This is probably due to greater variation in the composition of straight-run gasolines as compared to reformate or racked gasoline.

Increasing the mid-boiling point tends to decrease octane quality [2,3]. Increasing the mid-boiling point from 40^{o}C to 180^{o}C is accompanied with a decrease in the motor octane number. The magnitude of this decrease depends on the type of fuel. It ranges between 42 for straight-run gasoline to 6 for catalytically cracked gasoline [2].

Effects of the initial boiling point (IBP) is significant because light compounds in gasoline (C_4 hydrocarbons) have high blending octane values and increasing the IBP can substantially reduce octane quality.

Similar effects are observed if 90% boiling point or final boiling point is changed, because even though the higher boiling fraction of gasoline is relatively high in aromatic content the total gasoline fraction is low in octane due to the diluting effect of a high paraffin content. Hence, a reduction in the final boiling point can result in higher overall gasoline octane [2].

Increasing the 90% boiling point seems to decrease the octane number in most cases with the exception of the catalytically-reformed naphtha where a slight increase in the octane number is observed. The octane number of the catalytically-cracked naphtha, on the other hand, is not greatly affected by the 90% boiling point. The different relative amounts of aromatics and paraffins in the naphtha fractions is the most likely explanation for this anomaly.

A close study of the relationship between the octane number and boiling range indicates that for higher octane numbers and lower boiling temperatures (50%, 90% etc.) the correlation tends to be more significant. The change in octane number ranges from 5 for gasolines of $40^{o}C$ mid boiling point to 41 for gasolines of $180^{o}C$. Similarly the change in octane number ranges from 19 for gasolines of $140^{o}C$ (90% boiling point) to 41 for gasolines of $200^{o}C$ [2,3].

Method of Study and Results

To ascertain the relationship and correlation between the octane number and the boiling range, data were collected from the Octel Co. [4] and the Homs Oil Refinery (HOR) in Syria (platforming unit) as well as from other sources including the Banias Oil Refinery in Syria. A total of 1142 value points were used in the analysis. Regression Analysis of these data (using the least squares method) was carried out using a specially-prepared computer program [5,6]. The boiling points considered in this analysis were the 10%, 50% and 90% boiling points as measured by the test method ASTM D86 (measured to the nearest $1^{o}C$). In each case correlation factors and average errors were computed for the best correlations.

These optimum correlations did not however lead to simple easy-to-apply equations. For this reason straight-line correlations assuming linear relationships were included for comparison purposes.

Three runs were tried for each boiling temperature. The octel data were used for the first run. Data from HOR-Platforming unit were tried next, and finally both Octel and HOR data as well as data from other sources were used. The results obtained are given in Tables 1-3.

The Results obtained with the 10% boiling points indicate clearly that the correlation with octane number is not significant in general. The maximum correlation factor obtained was 0.35 for HOR-platformate with an average error of 2.0%.

With mid-boiling points the correlations obtained were siginficant but the results were different for different fuels. (Table 2). Again, platformate data gave the best results with a correlation factor of 0.60 and an average error of 1.6%.

The correlation results obtained were most significant with the 90% boiling points. The optimum correlation equation obtained was:

Table 1. Optimum and straight-line correlation between Research Octane Number and 10% boiling point

Source of data	No. of points	Range RON	Range $t_{10\%}$	Straight-line correlation Equation	R	Average error %	Best correlation Equation	R	Average error %
Octel	689	90-100	30-72	$RON=9554794+0.013237.\ t_{10\%}$	0.04	1.42	$RON=95.7544+132.54\cdot10^{-4}\cdot t^2_{10\%}$ $-467.465\cdot10^{-4}\cdot\ t^3_{10\%}-t^2_{10\%}$ $-9.282\cdot10^{-4}\cdot t^5_{10\%}-t^4_{10\%}$	0.06	1.40
Platformate (HOR)	623	85-100	75-96	$RON=105.7676-0.110112\cdot t_{10\%}$	0.13	2.16	$RON=-105.5712+4.95183\cdot t_{10\%}$ $-0.0302591\cdot t^2_{10\%}$	0.35	2.0
Octel, HOR and others	1142	85-100	30-96	$RON=95.03481+0.01881\cdot t_{10\%}$	0.14	1.82	$RON=0.990613\cdot(100-t_{10\%})$ $+0.885573\cdot\ t^2_{10\%}-t_{10\%}$ $+9.734\cdot10^{-4}\cdot\ t^4_{10\%}-t^3_{10\%}$	0.16	1.81

RON = Research Octane Number; $t_{10\%}$ = 10% Boiling point ^{0}C; R = Correlation Factor

Table 2. Optimum and straight-line correlation between Research Octane Number and Mid boiling point

Source of data	No. of points	Range RON	Range $t_{50\%}$	Straight-line correlation Equation	R	Average error %	Best correlation Equation	R	Average error %
Octel	687	90-100	60-120	$RON=94.225+0.019661\cdot t_{50\%}$	0.10	1.41	$RON=51.0514+0.516615\cdot t_{50\%}$ $-5.0387\cdot10^{-4}\cdot t^2_{50\%}$ $+4616554\cdot t^{-3}_{50\%}-6.017\cdot10^{-8}\cdot t^4_{50\%}$	0.13	1.40
Platformate (HOR)	630	85-100	115-135	$RON=31.0621+0.53542\cdot t_{50\%}$	0.58	1.61	$RON=0.00997\cdot(t^2_{50\%}-1000)$ $-0.00067\cdot e\sqrt{t_{50\%}}$	0.60	1.55
Octel, HOR and other	1264	85-100	60-140	$RON=91.4633+0.0437\cdot t_{50\%}$	0.23	1.85	$RON=1.9554+2.39191\cdot t_{50\%})$ $-175.3\ 10^{-4}\cdot t^2_{50\%}$ $+131912\cdot t^{-3}_{50\%}+2.8519\cdot10^{-7}\cdot t^4_{50\%}$	0.30	1.79

RON = Research Octane Number; $t_{10\%}$ = 10% Boiling point ^{0} C; R = Correlation Factor

Table 3. Optimum and straight-line correlation between Research Octane Number and 90% boiling point

Source of data	No. of points	Range RON	Range $T_{90\%}$	Straight-line correlation Equation	R	Average error %	Best correlation Equation	R	Average error %
Octel	685	90-100	138-185	$RON=105.0136+0.054139 \cdot t_{90\%}$	0.24	1.42	$RON=40.7452+15817.96 \cdot t^{-1}_{90\%}$ $-1128941 \cdot t^{2}_{90\%}$ $+3.71 \cdot 10^{-5} \cdot t^{4}_{90\%} - t^{3}_{90\%}$	0.25	1.40
Platformate (HOR)	620	85-100	150-168	$RON=43.66904+0.336175 \cdot t_{90\%}$	0.40	1.90	$RON=188.8976+6098.561 \cdot 10^{-4} \cdot t_{90\%}$ $-4.9035 \cdot 10^{-3} \cdot t^{2}_{90\%}$ $-259804.1 \cdot 10^{3} \cdot t^{-3}_{90\%}$	0.42	1.80
Octel, HOR and other	1236	85-100	138-185	$RON=101.9753-0.036322 \cdot t_{90\%}$	0.10	2.00	$RON=179.5415-0.136428 \cdot t_{90\%}$ $-1.3072 \cdot 10^{-3} \cdot t^{2}_{90\%}$ $-113222.4 \cdot 10^{3} \cdot t^{3}_{90\%}$	0.43	1.90

RON = Research Octane Number; $t_{90\%}$ = 10% Boiling point °C; R = Correlation factor

Table 4. Comparison between measured and calculated values of research octane numbers of Syrian unleaded gasolines

90% boiling pt. oC	Measured	Calculated	Diff. (%)	Av. diff. (%)
142	93.05	94.3	0.9	
143	97.0	94.6	2.5	
144	96.8	94.9	2.0	
144	85.3	94.9	11.3	1.6
146	86.0	95.4	10.9	
147	98.0	95.6	2.4	
149	96.3	95.4	0.4	
150	96.3	96.1	0.2	
151	97.8	96.3	1.5	
152	91.1	96.4	5.8	
152	97.8	96.4	1.4	
152	97.5	96.4	1.1	
152	98.0	96.4	1.6	
153	97.5	96.5	1.0	1.7
153	99.0	96.5	2.5	
153	98.2	96.5	1.7	
154	99.3	96.5	1.7	
155	98.0	96.6	1.4	
156	87.5	96.6	10.4	
156	97.8	96.6	1.2	
157	97.0	96.6	0.4	
157	98.0	96.6	1.4	
158	99.1	96.6	2.5	
160	96.3	96.6	0.3	
161	96.3	96.6	0.3	
162	97.5	96.5	1.0	
162	96.8	96.5	0.3	2.0
164	90.0	96.3	7.0	
165	93.4	96.2	3.0	
166	96.0	96.1	0.1	
168	98.0	95.8	3.9	
171	93.7	95.3	1.7	
176	91.4	94.3	3.2	
177	93.0	94.0	5.9	
179	88.0	93.5	1.1	3.4
183	90.4	92.3	2.1	
185	87.4	91.7	4.9	
186	97.0	91.4	5.8	
186	89.0	91.3	2.6	

$$RON = 179.5415 - 0.136428\,(x) - 1.3072 \times 10^{-3}(x^{2}) - 113{,}222.4 \times 10^{3}(x^{-3})$$

Where x is the 90% boiling point (in ^{o}C) and RON the research octane number. The correlation factor obtained with this equation was 0.43 and the average error 1.9%. The straight-line correlation, on the other hand, was not signifcant.

This optimum equation can be used with acceptable accuracy for the estimation of the octane index of commercial unleaded gasolines. As a check on this equation, the octane index of different samples of Syrian unleaded gasolines as well as specially-prepared naphtha blends was calculated and the calculated values were then compared with the measured values using the research method. The results are given in Table 4.

As can be seen from this Table, the difference beween the measured and calculated octane numbers, can be as high as 11.3%. However, for most specimens (56%) the difference was less than 2%.

Neglecting odd values, where the difference is greater than 10%, the average error is 1.6% for 90% boiling points less than 150^{o}C and this increases to 3.5% for temperatures greater than 170^{o}C. This is in general agreement with the observation made earlier in this paper.

Conclusions

In conclusion it is apparent that the 90% boiling point for low boiling gasolines (90% boiling point > 168°C) can be used for the estimation of an octane index that may not vary by more than 2% (for 61% of fuels evaluated) from the measured research octane number. This is particularly apparent where fuel samples of smilar source and/or mode of manufacture are used in the analysis such as reformates or cracked naphthas. The precision of the calculated octane index will however be dependent on the precision of the distillation temperature determinations which enter into the calculation.

References

[1] Magee, J.S., Wallace, D.N. and Blazek, W.L. "FCC Feed Composition Affects Catalyst Octane Performance." *Oil and Gas Journal*, Aug. 4 (1980), 63-67.

[2] Nelson, W.L. *Petroleum Refinary Engineering*. New York: McGraw-Hill Book Co., 1958.

[3] Nelson, W.L. "What is the Octane Number of Straight-Run Gasoline?" *Oil and Gas Journal*, May 29 (1978), 81.

[4] European Gasoline Survey (1988-1993), The Associated octel Company ltd., London, U.K.

[5] Hurlburt, H.Z. "Curve Fitting by Computer." *Hydrocarbon Processing*, 59, No. 8 (1980), 107-110.

[6] Miller, A.R. *Basic Programs for Scientists and Engineers*. SyBex Inc., 1981.

دراسة الارتباط بين عدد الأكتان لبنزين السيارات ومجال غليانه

حسان الحاج ابراهيم و محمد مرهف القاسمي

قسم الهندسة الكيميائية ، جامعة البعث ، ص.ب ٧٧ ، حمص ، سورية

(استُلم في ٢٤/٢/١٩٩٦م ؛ وقُبل للنشر في ٢٨/٩/١٩٩٦م)

ملخص البحث. تبين من دراسة العلاقة بين عدد الأكتان المقاس بطريقة البحث لبنزين السيارات غير المُرَصَّص ودرجة غليان ٩٠٪ له وجود ارتباط مُعْتَمَد بينهما. وقد أجريت هذه الدراسة باستعمال برنامج نُفِّذ على الحاسوب واستعملت في الدراسة معطيات أوربيّة وسوريّة. ومن هذه الدراسة أمكن التوصل إلى معادلة يمكن الاستفادة منها في حساب دليل الأكتان وكان عامل الارتباط ٠,٤٣ ونسبة الخطأ الوسطى ١,٩٪.