



HAL
open science

Knock management for dual fuel SI engines: RON evolution when mixing low RON base fuels with octane boosters

Nikola Rankovic, Guillaume Bourhis, Mélanie Loos, Roland Dauphin

► **To cite this version:**

Nikola Rankovic, Guillaume Bourhis, Mélanie Loos, Roland Dauphin. Knock management for dual fuel SI engines: RON evolution when mixing low RON base fuels with octane boosters. *Fuel*, 2015, 150, pp.41-47. 10.1016/j.fuel.2015.02.005 . hal-01143475

HAL Id: hal-01143475

<https://hal.science/hal-01143475>

Submitted on 17 Apr 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Knock management for dual fuel SI engines: RON evolution when mixing low RON base fuels with octane boosters

Nikola Rankovic ^{a,1}, Guillaume Bourhis ^b, Mélanie Loos ^c, Roland Dauphin ^b

^a *Aramco Fuel Research Center, 232 Avenue Napoléon Bonaparte, 92500 Rueil-Malmaison, France*

^b *IFP Energies nouvelles, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France; Institut Carnot IFPEN Transports Energie*

^c *IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize, France; Institut Carnot IFPEN Transports Energie*

Abstract

Most of the time, Spark Ignition (SI) engine performance is limited by knock phenomena (especially for turbocharged engines), which are linked to fuel resistance to auto-ignition, quantified by its octane number (Research Octane Number – RON and Motor Octane Number - MON). If high octane numbers are crucial for efficient high load operating points, they are less necessary at low load. Thus, if the octane number of the fuel could be tuned as any other engine setting parameter, the engine efficiency and CO₂ emissions could be improved, leading to an “Octane on Demand” concept, using for instance a dual fuel strategy. This requires understanding the behavior of dual fuel combustions with lower / higher octane fuels, and more particularly the evolution of RON when blending high RON fuels with low RON ones.

Developing an Octane on Demand concept requires to choose appropriate octane enhancers and understand their blending behavior. For this purpose, RON measurements were performed on a CFR engine using a wide range of mixtures of low-octane base fuels with various boosters capable of increasing the antiknock resistance of the blends. The chemical composition of booster streams was chosen to assess the potential of using alternative refinery products for improving fuel resistant auto-ignition properties when added to a whole-range naphtha and RON 91 gasoline. The study covers five octane boosters: ethanol, reformat, di-isobutylene, 2-butanol, and a mixture of butanols.

The experimental results show a non-linear behavior of RON values with respect to volumetric incorporation rates of octane boosters. In the cases when the booster is an alcohol (C2 or C4), linear by-mole blending rules can be applied with an acceptable prediction error. For boosters rich in olefins and aromatics, molar blending becomes less accurate. Ethanol shows the strongest boosting effect among all the octane boosters on the one hand, and on the other hand, the octane enhancing effect is stronger for the base fuel of lower starting RON value. Experimental results of the current study represent a comprehensive database for tailoring fuel RON properties aimed to explore combustion behavior of low-octane fuels enhanced through an addition of an external booster.

Keywords: CFR engine, Octane Booster, Blending Behavior, Research Octane Number, RON, Knock Management, Naphtha, Gasoline, Ethanol, Reformat, Di-isobutylene, Butanol

¹ Corresponding author. Tel: +31 88 262 21 32. Email address: nikola.rankovic@aramcooverseas.com

1. Introduction

The demand for transport fuels is increasing rapidly, mainly driven by the economic growth of the non-OECD countries. Most major energy players agree about the fact that the transport energy demand will grow higher for almost 40% until 2040 (e.g. in 2013 the US Energy Information Administration reference forecast featured an average 2010-2040 worldwide annual growth of 1.1% [1]). Even though alternatives to conventional fossil fuels exist today (e.g. biofuels, fuel cells, electric cars, etc.) and are likely to grow in the future, fossil energy is to remain the main powertrain enabler for the decades to come.

The projected growth in energy demand is however imbalanced throughout light, middle and heavy fuels [2-5]. It is primarily dictated by the ever growing commercial activities and impacts directly the demand in middle and heavy distillates (kerosene, gasoil, and marine fuels). The projected demand (Figure 1) of light fuel (gasoline) is to remain flat, since technological improvements (engine downsizing, hybridization, etc.) enable considerable fuel economies. From the supply side, the global refining infrastructure as of today is unable to meet the projected shift in demand without large-scale investments in hydrocracking units that lead to a substantial increase in associated CO₂ emissions [6]. This imbalance urges for less CO₂-intensive solutions for passenger transportation sector, among which is reducing the number of refinery processes required for producing fuels used in this sector. In addition, governments around the world are putting in place different legislation mechanisms to encourage car manufacturers to further decrease average fleet consumption and tailpipe GHG emission levels.

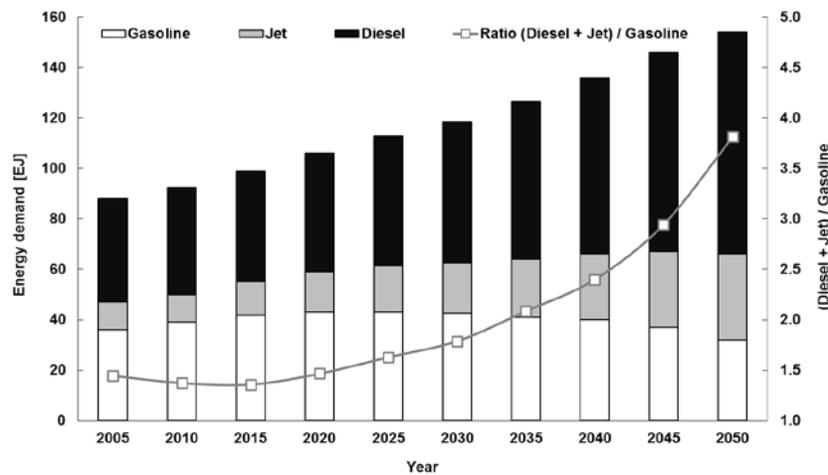


Figure 1: Projected gasoline, jet fuel, and diesel demand (left axis, exa Joules, 10^{18} J), together with the ratio of middle-to-light distillates (right axis) from the World Energy Council Freeway Scenario [3].

Motivated by the existing energy landscape and outlooks, and with the initiative to promote a responsible use of petroleum products in the transportation sector, Saudi Aramco pursues collaborative research

programs with IFP Energies nouvelles to develop and prove novel fuel/engine solutions, capable of challenging modern technological and environmental issues. One of the research initiatives uses naphtha-based fuels to power spark ignition (SI) engines, today operated on conventional gasoline. Naphtha is a generic term designating the fraction of crude oil boiling within the 30-180 °C range. It is composed of C5 to C11 hydrocarbons and has a low research octane number (RON) value, roughly within the 50-70 range. It is a refinery product that could potentially be beneficial for the automotive industry as an example of a less processed fuel. In effect, naphtha is only processed in the crude atmospheric distillation tower and undergoes light hydrodesulphurization, in contrast to premium commercial gasoline which is a blend of refined products from multiple process units (isomerization, reforming, FCC, alkylation, etc.).

Octane quality (which can be described by RON) of the fuel is crucial for avoiding knock phenomena. Without knock, the combustion phasing of a SI engine could be tuned in an optimal way, allowing the operations on high-load operating points to be more efficient; moreover, the engine compression ratio could be increased, improving thermodynamic efficiency on the whole range of engine speed and load. This is all the more true in case of turbocharged SI engine, but a high RON value becomes less necessary when the engine operates at low load. Based on this, unlocking fuel RON quality and adjusting it as any other engine operating parameter leads to what is known as the Octane on Demand concept. It is a dual fuel concept in which the engine operates on a low RON base fuel that is continuously boosted on as-needed basis through an addition of an external octane booster.

The present work is intended as the first block toward the Octane on Demand concept, aiming to understand antiknock properties, namely research octane number (RON) of blends of refinery naphtha and commercial gasoline used as base fuels and enhanced with octane boosters. We have conducted experimental measurements on a wide range of base fuel-booster mixtures in order to understand the way octane qualities increase with the addition of boosters. Previous literature work indicates that this evolution is strongly non-linear with respect to the volumetric incorporation rate of most common octane boosters (e.g. methanol and ethanol). Linear by-mole laws were suggested to help predicting the RON values of blends in a more direct way and might be very helpful for developing engine control strategies and accurately managing fuel RON quality in real driving conditions.

Ethanol has been widely accepted as an excellent octane vector (some examples of literature include the work by Stein et al., [7] and Wigg et al. [8]). Today, most conventional gasoline engines on the market (mainly US, Europe, and Brazil) are compatible with up to 10 vol. % of ethanol (E10) blended with gasoline. The advantage that ethanol has over any other alcohol is its position as the end-product of the biochemical process of sugar fermentation. This opens numerous possibilities for producing ethanol from renewable non-fossil feedstock and leads to a possible reduction of its overall CO₂ footprint (e.g. [9;10]). Previous work on blending ethanol to gasoline blendstocks shows an approximately linear relationship of RON with ethanol mole fractions [11]. However, more recent piece of work suggests introducing a scaling parameter (2nd-order dependence with respect to ethanol mole fraction) to yield more accurate prediction results [7;12]. The main concern of such approach is that the values of the mentioned scaling parameters have little or no physical meaning.

Reformat is the main product of catalytic reforming, a refinery process that transforms heavy naphtha (80-180 °C boiling range) into a pool rich in aromatics (mainly C7 to C10). The catalytic reforming process is the heart of RON and hydrogen production of most refineries, since the aromatic molecules

have extraordinary high RON values and the reactions that the naphtha feedstock undergoes to yield aromatics produce hydrogen-rich gas stream. In the present study, we assessed the properties of a generic reformat (97 m. % of aromatic molecules, C7 to C10) as a potential octane booster.

Most recently, higher alcohols (four or more carbon atoms) have received great attention from the relevant research groups as additives for commercial gasoline, improving key properties of fuel used in SI engines. In terms of energy content, RON and volatility (Reid vapor pressure – RVP) properties, as well as feedstock used for their manufacturing, butanol mixtures can entirely substitute MTBE additives used today. Butanols have the advantage of high neat RON values (98 for 1-butanol, 105 for 2-butanol and *iso*-butanol [13]) and of lowering gasoline vapor pressure, making it easy to meet RVP constrains of gasoline even without removing light-end molecules. In addition, incorporating C4 oxygenates produced from syngas or renewable sources could lead to substantial fossil energy savings and avoid significant amount of GHG emissions associated to gasoline [14]. Saudi Aramco has recently patented a process for simultaneous dimerizing and hydrating of a hydrocarbon stream rich in C4 olefin molecules (1-butene, *cis*- and *trans*-2-butene, and isobutene) mainly coming from a FCC or a thermal cracking unit [15;16]. After reacting over a dedicated acidic support, the product (SuperButol™) consists of variable proportions of butanols and di-isobutylenes (DIB), with 2-butanol being the major component. In the present study, we thus investigate, in addition to ethanol and reformat, boosters of potential interest for the automotive industry obtained through the mentioned process. DIB used in the present study represents a mixture of 2,4,4-trimethyl-1-pentene and 2,4,4-trimethyl-2-pentene (3.75:1 mass ratio). SuperButol™ booster is a mixture representative of the product obtained in the patented process (mainly butanol isomers, with minor quantities of DIB).

2. Experimental techniques

Octane Number (ON) measurements are based on comparing knock occurrence of the studied fuel to the blend of reference molecules (n-heptane, with the ON value set to 0, and 2,2,4-trimethylpentane (also named iso-octane), set to 100). ON measurements were performed on a Cooperative Fuel Research (CFR) engine. The CFR engine is a single-cylinder, 611 cm³, four-stroke engine with a variable compression ratio, dynamically adjustable while operating from 4.0:1 to 18.0:1. Fueling of the engine is done through a carburetor with multiple float chambers so that the switch between the tested fuel and the reference one is instantaneous. Heaters control the temperature of inlet air and of the air/fuel mixture, while gauges monitor the engine operation and detect the occurrence of detonations. To perform Research Octane Number (RON) tests, the engine speed is set to 600 rpm, the inlet air temperature is adapted depending on the barometric pressure, and the ignition timing is fixed regardless the compression ratio [17]. The tested fuel RON is obtained when the occurrence of detonations is the same as with a blend of n-heptane and 2,2,4-trimethylpentane). RON value represents the volumetric percentage of 2,2,4-trimethylpentane.

By definition, the RON scale ranges from 0 to 100. Alternative methods for measuring values above this scale were proposed previously, but with less reliable reproducibility, often leading to multiple values available in the literature. In the present work, reference fuels for measuring RON above 100 were made

by adding tetraethyl lead to isooctane, as per ASTM D2699 instructions. The repeatability of the present RON measurements within the 90-100 scale is around 0.2.

Molecular composition of fuels used in the present study was assessed using gas chromatography according to ASTM D6733 derived methods. Compounds are separated according to their volatility on an apolar column (PONA, 50 m, 0.2 mm, 0.5 μm), quantified with a flame ionization detector, and identified through their retention indices. Operating conditions are adapted to the type of streams that are analyzed (naphtha, reformat or commercial gasoline) as well as the identification files used to assign a chromatographic peak to a defined compound. Molecular weights of the blendstocks were calculated directly from the GC results.

3. Results

RON of Base Fuels and Octane Boosters

To assess the potential of using refinery naphtha as a less processed transportation fuel, we herein investigate the behavior of a base fuel obtained through mixing a whole boiling range naphtha stream with non-oxygenated commercial gasoline (RON 91). The naphtha stream has the RON value of 53, and the tested blend was obtained by using the 56/44 vol. % naphtha to gasoline ratio. Its measured RON was 71. For creating a more complete image of the boosting properties and to be able to assess the impact of the base fuel to the RON values of blends, we also investigated the behavior of boosters added to pure non-oxygenated commercial gasoline.

Table 1: Base fuels and octane boosters used in the present study and their respective measured RON values.

Stream Name	Stream Composition	RON²
RON 71 Base Fuel	56/44 vol. % Refinery naphtha/commercial RON 91 gasoline	71
RON 91 Base Fuel	Commercial RON 91 gasoline	91
Ethanol	High purity ethanol, water content: 200 mg/kg	108
Reformat	Catalytic reforming unit product	111
DIB	2,4,4-trimethyl-1-pentene and 2,4,4-trimethyl-2-pentene (3.75:1 mass ratio)	104
2-butanol	Water content: 460 mg/kg	106
SuperButol™	Mixture of butanol isomers with a minor DIB fraction	107

Measured values for base fuels and octane boosters are reported in Table 1. RON value of pure ethanol (108) in the present work fits well within the range of values available in the literature (106 – 111) [18-21]. Concerning 2-butanol, its measured neat RON value of 106 corresponds well to the literature value of 105 [13]. RON value for DIB reported in previous work at Saudi Aramco is 101, and the present work reports a value of 104 (no detail was given about the exact composition in terms of 1- and 2- isomers used in the patent).

² Present work

RON 71 Base Fuel

Experimental results for blending octane boosters to the RON 71 base fuel are available in Table 2 and RON evolution as a function of booster volumetric incorporation rate is plotted in Figure 2. For almost all blends, the effect of incorporating the booster on volumetric base is non-linear, with the exception of reformat. It is worth noting that the slope of RON evolution decreases with the incorporation rate, proving the ‘boosting’ effect, and the advantage of using boosters at low concentrations.

Table 2: Experimental RON values for blending boosters with RON 71 base fuel.

	<i>Octane booster incorporation rate (vol. %)</i>							
	0	10	20	30	40	60	80	100
Ethanol	71	81	88	94	99	104	107	108
Reformat	71	-	81	-	91	98	104	111
DIB	71	-	83	-	94	99	102	104
2-Butanol	71	-	81	-	91	99	104	106
SuperButol™	71	-	80	-	89	98	103	107

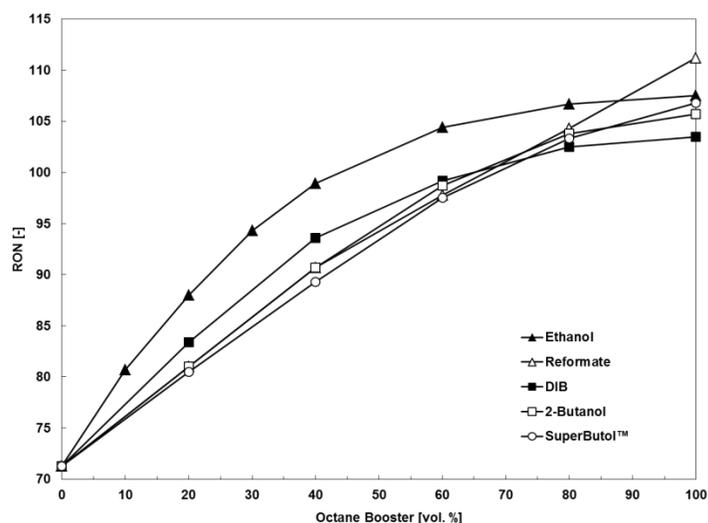


Figure 2: RON measurements for RON 71 base fuel blends with octane boosters, plotted as a function of the booster volumetric incorporation rate. DIB = di-isobutylene, SuperButol™ = mixture of butanol isomers and DIB.

RON 91 Base Fuel

For the case of incorporating boosters to the RON 91 base non-oxygenated gasoline, experimental measurements confirm a similar non-linear behavior. Data are available in Table 3 and the plots are illustrated in Figure 3. It is interesting to note that, for both base fuels, reformat, 2-butanol, and DIB

have a similar behavior for the incorporation values below 60 vol. % when RON evolution is expressed on the volumetric incorporation basis. This phenomenon suggests that, at this concentration, 2-butanol has an antiknock behavior similar to the aromatic molecules of the reformat pool, in spite of radical differences in their respective chemical structures.

Table 3: Experimental RON values for blending boosters with RON 91 base fuel.

	<i>Octane booster incorporation rate (vol. %)</i>						
	<i>0</i>	<i>10</i>	<i>20</i>	<i>40</i>	<i>60</i>	<i>80</i>	<i>100</i>
Ethanol	91	95	99	103	105	108	108
Reformat	91	-	95	99	102	106	111
DIB	91	93	96	99	102	103	104
2-Butanol	91	-	95	98	102	104	106
SuperButol™	91	-	94	98	102	104	107

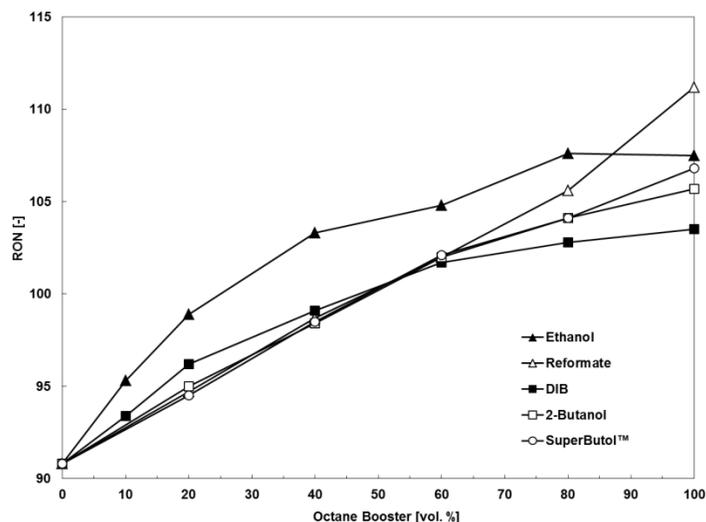


Figure 3: RON measurements for RON 91 base fuel with octane boosters, plotted as a function of the booster volumetric incorporation rate.

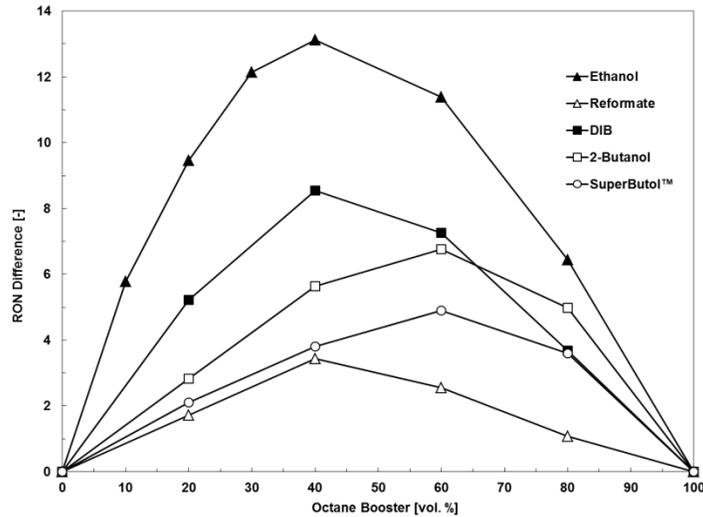
Octane booster vs RON: Summary

These results show an interesting potential for the use of naphtha based fuels, in spite of their low RON values. Indeed, our measurements show that, starting with a RON of 71, an addition of 30 vol. % of ethanol is enough to roughly reach the same anti-knock properties as a commercial RON 95 unleaded gasoline. In addition, the RON value reached with 60 vol. % of ethanol is roughly the same whether using a RON 71 or a RON 91 base fuel. This shows alternative ways to obtain octane number by using less processed fuels and adapted blending properties.

4. Discussions

RON Boosting: Deviations from Linearity

Differences between the measured points and those obtained by linear regression between base fuel and neat booster RON values are plotted in Figure 4 for both base fuels. The shape of curves suggests that the boosting effect reaches its maximum at roughly 50 vol. % of incorporated booster. Ethanol exhibits the strongest boosting effect, whilst reformat has the lowest one, in spite of its high neat RON value. Boosters respect the same order of deviation when incorporated in both base fuels, although the deviations for the RON 91-reformat blends actually appear to be slightly negative. The overall amplitude of deviations is greater for the RON 71 base fuel, indicating more octane boosting compared to the RON 91 base.



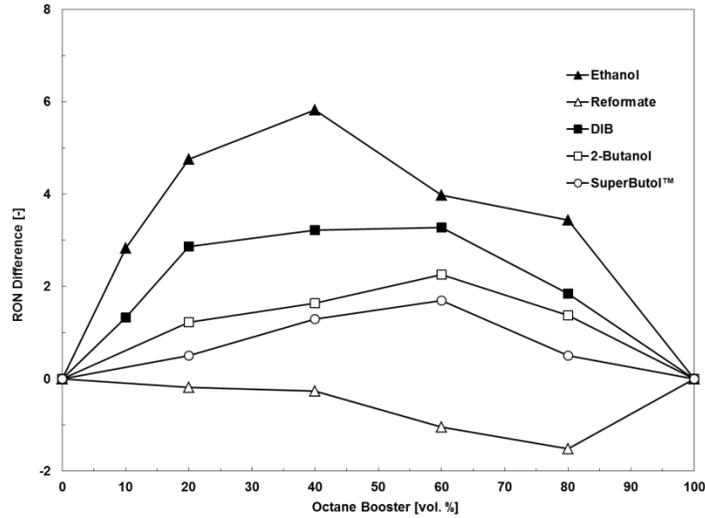


Figure 4: Deviation from linear RON evolution for different octane boosters incorporated on a volumetric basis to RON 71 base fuel (upper panel) and 91 base fuel (lower panel). Hypothetical linearity is calculated between the base fuel RON and neat booster RON values.

Boosting Effect and Blending Octane Number (BON)

A great aspect of the boosting effect is observed through a significant increase in RON values of blends when a small amount of booster is added to the base gasoline. As the first attempt to understand and linearize the evolution of RON as a function of booster volumetric proportion, and particularly so for the case of alcohols blended with base gasoline, the principle of Blending Octane Number (BON) has often been used in previous studies (e.g. [11;12]). RON value of the blend is expressed linearly as a function of base fuel RON (RON_{bf}), and booster BON (BON_i). C_{bf} and C_i represent volumetric fractions (vol. %) of base fuel and booster, respectively.

$$RON_{blend} = RON_{bf}C_{bf} + BON_iC_i$$

Eq. 1

Although very useful for linear extrapolations of RON values at low incorporation rates, the notion of BON has a major drawback, which is the variation of the BON value with the concentration of the booster. Moreover, in the relevant literature, the BON value extrapolated from low incorporation rates has often been mistakenly reported as the neat RON value of the booster [22]. Plots of BON (Figure 5) show a significant evolution of this value with the quantity of incorporated booster, especially for the case of ethanol-gasoline mixtures. This suggests that the boosting effect of ethanol on base gasoline is greater than for any other tested stream. It is interesting to notice higher BON values – thus a stronger boosting effect – for ethanol incorporated to the 71 RON base fuel, compared to the 91 RON base. This finding is particularly encouraging for the use of low octane naphtha-based streams mixed with ethanol.

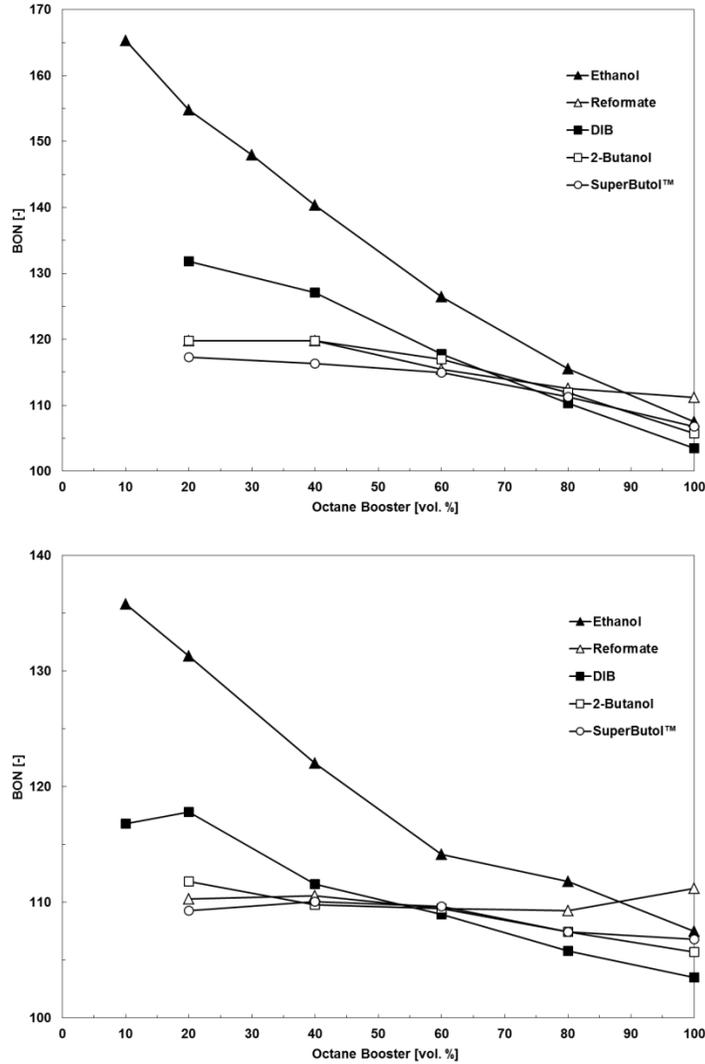


Figure 5: Blending octane (BON) values plotted vs. volumetric content of each octane booster. Upper panel: RON 71 base, lower panel: RON 91 base fuel.

Molar Octane Blending

As suggested in previous studies, [11;12;23] molar incorporation rates allow predicting RON values of alcohol-gasoline blends (methanol and ethanol) in a linear fashion (Eq. 2).

$$RON_{blend} = \sum_{i=1}^N x_i RON_i$$

Eq. 2

Such linear laws are easier to incorporate within system models dedicated to control and used for predicting the required booster quantity at different engine operating points. We have explored this linear

by-mole approach for all octane boosters, in order to understand the boundaries of its validity. Starting from the volumetric incorporation rate C (vol. %), molar fraction (x) of each octane booster i can be expressed as follows

$$x_i = \frac{\rho_i C_i}{M_i} \times \left(\frac{\rho_{bf}(100 - C_i)}{M_{bf}} + \frac{\rho_i C_i}{M_i} \right)^{-1}$$

Eq. 3

With ρ denoting density of booster i or base fuel bf (kg/m^3), and M its molecular weight (g/mol). Density and molecular weight data used in the calculations are available in Table 4. The example illustrated in Figure 6 shows the correlation between two values for the case of RON 91 base fuel and different boosters.

Table 4: Data used for converting volumetric to molar fractions. For base fuels and reformat molecular weight data were obtained from the GC analysis.

Compound	Density (kg/m^3)	Molecular Weight (g/mol)
Base fuel RON 71	0.738	99.3
Base fuel RON 91	0.745	94.1
Ethanol	0.794	46.1
Reformat	0.867	103.6
DIB	0.721	112.2
2-Butanol	0.811	74.1
SuperButol™	0.802	75.3

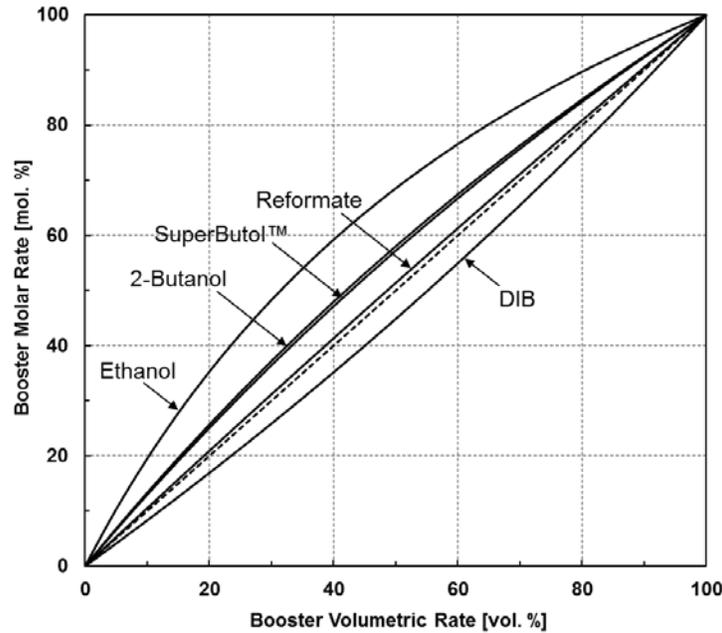


Figure 6: Molar vs. volumetric incorporation rates for different octane boosters and the base RON 91 fuel. For reference, dashed line represents a one-body state.

By observing the shape of the volumetric-molar dependence, it can be intuited that DIB will exhibit different behavior from the other boosters. When RON values of different blends are calculated using Eq. 2 and Eq. 3, the linear by-mole model gives satisfactory results for alcohol-based boosters (ethanol, 2-butanol, and SuperButol™), but also for reformat. The prediction error associated to DIB, however, is more significant, and the linear model does not seem appropriate for this case. Figure 7 illustrates the comparison between experimental and calculated RON results for the two base fuels. It is worth noting that, due to uncertainty of the measure, values above 105 RON were not considered for this comparison. According to Anderson et al., [11] high isoparaffin content of the base gasoline (above 50 vol. %) will lead to erroneous prediction of RON values calculated on the molar bases. Speculated chemical interactions between ethanol and isoparaffin molecules could be the cause of the deviation. In the present study, both base fuels had similar isoparaffin content (Table 5), thus leading to similar pattern in associated RON prediction errors. We could claim that, due to its branched iso-olefin structure, DIB is the only booster requiring a polynomial fit of RON vs. its molar content. However, with the existing knowledge on hydrocarbon interactions and their effect on RON, it is hard to clearly state the reason for this particular behavior.

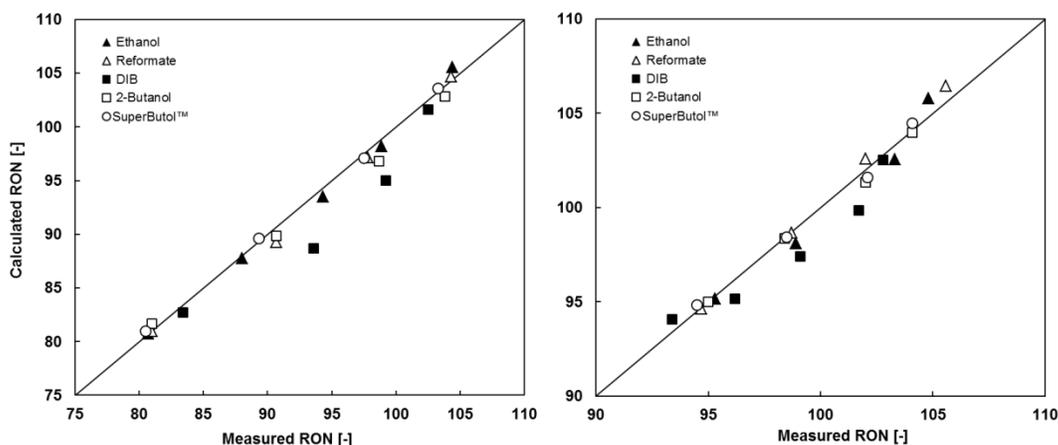


Figure 7: Calculated RON values vs. experimental results, using linear by-mole approach. Left panel: 71 RON base fuel, right panel: 91 RON base.

Table 5: PIONA analyses (m. %) of the base fuels.

Compound	RON 71	RON 91
n-paraffins	15.4	7.7
Isoparaffins	39.2	38.4
Naphtenes	22.0	15.0
Aromatics	21.3	34.1
Olefins	2.1	4.7
Oxygenates	below 0.1	0.1

To quantify the performance of the linear by-mole blending rule for each base fuel-booster combination, a global assessment of the model prediction was performed. The associated error (ϵ) over N experimental points was calculated using Eq. 4 and depicted in Figure 8. To better illustrate the advantage of using linear by-mole over linear volumetric laws, prediction errors are given side-by-side for both of these approaches. From interpreting the results in Figure 8, it can be easily concluded that the linear by-mole approach has a significant advantage for calculating RON values of alcohol-based boosters, offering a more confident estimation than the volumetric one. However, the linear by-mole approach offers no improvement for the prediction of RON for the olefin-based octane booster. Globally, the linear by-mole law predicts better the experimental results obtained when using the 91 RON base. A possible explanation for this finding could simply be the fact that the boosting effect is lesser for the higher base RON, so the model covers less values, automatically leading to more precise estimations.

$$\epsilon = \sqrt{\frac{1}{N} \sum_{i=1}^N (RON_{exp,i} - RON_{calc,i})^2}$$

Eq. 4

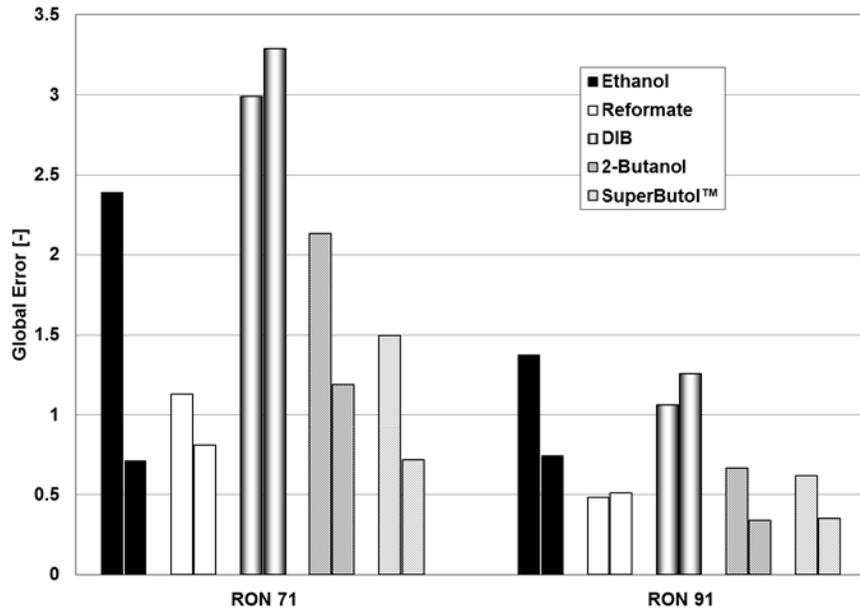


Figure 8: Global error (ϵ) for RON prediction using linear volumetric (bars to the left) and linear by-mole (bars to the right) approaches, calculated for each booster-base fuel combination.

Conclusions

The present study is a first step toward elucidating the Octane on Demand concept, in which a spark ignition (SI) engine is operated using fuel with adjustable octane quality. For this purpose, two low octane base fuels (71 and 91 RON for this study) were blended with five streams of high neat RON and the behavior of blends was analyzed and reported. High-RON streams (also called Octane Boosters) chosen for this study were ethanol, refinery reformat, a mixture of di-isobutylenes (DIB), 2-butanol, and a mixture of butanols (patented Saudi Aramco stream, SuperButol™). Experimental results showed a strongly non-linear behavior of blend RON with respect to the volumetric incorporation rate of boosters, especially with ethanol and DIB as octane boosters. The boosting effect reaches its maximum at roughly 50 vol. % of incorporated booster. Moreover, octane enhancement was stronger when boosters were incorporated to the lower RON base fuel.

As a result, an interesting potential for the use of naphtha based fuels has been demonstrated, in spite of their low RON values: starting with a RON of 71, an addition of 30 vol. % of ethanol is sufficient to reach the same anti-knock properties as a commercial RON 95 unleaded gasoline. This shows an alternative way to obtain high octane number by using less processed fuels and adapted blending properties. Moreover, this confirms one of the benefits of the Octane on Demand concept, where relatively high RON values can be obtained by using a relatively low amount of octane booster at mid and high load, while low RON fuels could be used at low load. This approach needs to be confirmed by knowing the octane requirement of an SI engine, which will be done in a subsequent study.

Since linear evolution laws are highly appreciated for any further application in developing system models for the dual fuel engine, the present paper attempted to predict the evolution of RON values of blends using linear by-mole laws, and assesses the boundaries of such approach.

The continuation of this work will make use of the experimental results for creating a comprehensive base for design of fuel matrix with desired octane properties. In a later development stage, optimized fuel formulations will undergo additional MON studies, and these measurements will help to validate and extend the linear by-mole approach studied within.

Acknowledgements

The authors would like to acknowledge collaborators from IFP Energies nouvelles, Aramco Fuel Research Center in Paris, and Saudi Aramco Fuel Technology Team in Dhahran for their fruitful inputs while performing the work.

References

- [1] US Energy Information Administration. International Energy Outlook. 2013. DOE/EIA-0484(2013).
- [2] ExxonMobil. The Outlook for Energy: A view to 2040. 2014.
- [3] World Energy Council London. Global Transport Scenarios 2050. 2011.
- [4] BP. Energy Outlook 2035. 2014.
- [5] International Energy Agency. World Energy Outlook 2011. 2011.
- [6] Lantz F, Saint-Antonin V, Gruson J-F, Suwala W. The OURSE model: Simulating the World Refining Sector to 2030. 2012.
- [7] Stein RA, Polovina D, Roth K, Foster M, Lyneskey M, Whiting T, et al. Effect of Heat of Vaporization, Chemical Octane, and Sensitivity on Knock Limit for Ethanol - Gasoline Blends. SAE International Journal of Fuels and Lubricants 2012;5:823-43.
- [8] Wigg EE, Lunt RS. Methanol as a Gasoline Extender-Fuel Economy, Emissions, and High Temperature Driveability. SAE Technical Paper Series 1974;1974-02-01.
- [9] JEC - Joint Research Centre-EUCAR-CONCAWE collaboration. Well-to-Wheels Report, Version 4.a. 2014.
- [10] Directive 2009/28/EC of the European Parliament and of the Council on the promotion and use of energy from renewable sources and amending and subsequently repealing Directives 2001/77/EC and 2003/30/EC, 2009.
- [11] Anderson JE, Kramer U, Mueller SA, Wallington TJ. Octane Numbers of Ethanol and Methanol Gasoline Blends Estimated from Molar Concentrations. Energy & Fuels 2010;24:6576-85.
- [12] Anderson JE, Leone TG, Shelby MH, Wallington TJ, Bizub JJ, Foster M, et al. Octane Numbers of Ethanol-Gasoline Blends: Measurements and Novel Estimation Method from Molar Composition. SAE International 2012;2012-01-1274.
- [13] Christensen E, Yanowitz J, Ratcliff M, McCormick RL. Renewable Oxygenate Blending Effects on Gasoline Properties. Energy & Fuels 2011;25:4723-33.
- [14] Wu M, Wang M, Liu J, Huo H. Assessment of Potential Life-Cycle Energy and Greenhouse Gas Emission Effects from Using Corn-Based Butanol as a Transportation Fuel. Biotechnology Progress 2008;24(6):1204-14.
- [15] Xu W, Mohammad TA, Shaik KM, Harale A. Method for Contemporaneously Dimerizing and Hydrating a Feed Having Butene.US2013/0104449 A1. 2013.
- [16] Xu W, Al-SHahrani FM, Bourane A, Ralf Vogel S. Process for the Hydration of Mixed Butenes to Produce Mixed Alcohols.US2014/0039226 A1. 2014.

- [17] Standard Test Method for Research Octane Number of Spark-Ignition Engine Fuel. 2008, ASTM D2699-08.
- [18] Heywood JB. Internal Combustion Engine Fundamentals. New York: 1988.
- [19] Wagner TO, Gray DS, Zarah BY, Kozinski AA. Practicity of Alcohols as Motor Fuels. SAE Technical Paper Series 1979;1979-02-01.
- [20] Ghosh P, Hickey KJ, Jaffe SB. Development of a Detailed Gasoline Composition-Based Octane Model. Ind Eng Chem Res 2006;45:337-45.
- [21] Van Basshuysen R, Schafer F. Modern Engine Technology: from A to Z. Warrendale, PA: SAE International; 2007.
- [22] Yates A, Bell A, Swarts A. Insights relating to the autoignition characteristics of alcohol fuels. Fuel 2010;89:83-93.
- [23] Knop V, Loos M, Pera C, Jeuland N. A linear by mole blending rule for octane numbers of n-heptane / iso-octane / toluene mixtures. Fuel 2014;115:666-73.