

Using Ethanol's Double Octane Boosting Effect with Low RON Naphtha-Based Fuel for an Octane on Demand SI Engine

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ABSTRACT

The efficiency of spark ignition (SI) engines is usually limited by the occurrence of knock, which is linked to fuel octane number. If running the engine at its optimal efficiency requires a high octane number at high load, a lower octane number can be used at low load.

Saudi Aramco, along with its long-term partner IFP Energies nouvelles, has been developing a synergistic fuel engine system where the engine is fed by fuel with an octane number adjusted in real time, on an as needed basis, while running at its optimal efficiency.

Two major steps are identified to develop this "Octane on Demand" (OOD) concept:

- First, characterize the octane requirement needed to run the engine at its optimal efficiency over the entire map.
- Then, select the best dual fuel combination, including a base fuel and an octane booster to fit this concept.

For this purpose, the behavior of different octane boosters, including ethanol, reformat and a blend of butanol isomers (SuperButol™), are studied on a CFR engine when blended with a very low RON naphtha-based fuel (RON 71). It is shown that the fuel combination [naphtha; ethanol] offers the most promising boosting effect.

Dedicated tests on an up-to-date gasoline direct injection multicylinder engine reveal the opportunity to use a naphtha-based fuel of RON 71 over a significant area of the engine map. The advantage of using ethanol as an octane booster is then clearly demonstrated, linked both to its very high RON and its high latent heat of vaporization and favorable sensitivity. Finally, around two-thirds of the engine map can be run using a moderate ethanol rate within the range 0% to 40%, making this OOD concept compatible within the E10-E20 context. Finally, deeper analyses are also made to correlate the engine octane requirement with RON, MON, Octane Index, and heat of vaporization.

KEYWORDS: Octane on Demand, Research Octane Number, RON, Motor Octane Number, MON, Sensitivity, Latent Heat of Vaporization, Knock Management, Octane Index, Octane Requirement, Combustion Phasing, CA50, TRF, Naphtha, Ethanol

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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 that the transport energy demand will grow almost 40% by 2040 (e.g., in 2014, 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, 3, 4, 5]. This is primarily driven by the ever growing commercial sector of global aviation, the demand in middle and heavy distillates (kerosene, diesel, and

marine fuels). The projected demand (Figure 1) for gasoline is to remain fairly flat, since technological improvements (engine downsizing, hybridization, etc.) are expected to enable considerable fuel economies [3].

From the supply side, the global refining infrastructure, as of today, will find it increasingly difficult to meet the projected shift in demand towards middle and heavy distillates without large-scale investments in hydrocracking units that will lead to a substantial increase in associated CO₂ emissions [6]. This imbalance urges for less CO₂-intensive solutions for the passenger transportation sector to reduce the CO₂ footprint from well-to-tank and tank-to-wheel. In addition, governments around the world are putting in place different legislative mechanisms to encourage car manufacturers to further decrease average fleet consumption and tailpipe pollutants and GHG (Greenhouse Gas) emission levels.

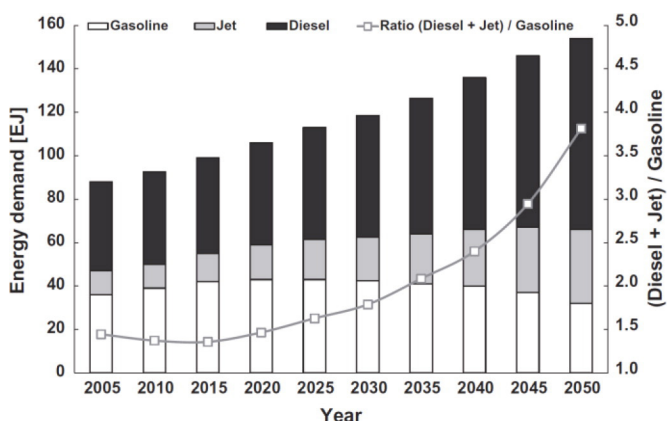


Figure 1. Projected gasoline, jet fuel, and diesel demand (left axis, (1 Exajoule = 10¹⁸ J), together with the ratio of middle-to-light distillates (right axis) from the World Energy Council Freeway Scenario 2050 [3]

Motivated by the existing energy landscape and outlooks, and with the desire to promote the responsible use of petroleum products in the transportation sector, Saudi Aramco is pursuing collaborative research programs with IFP Energies nouvelles to develop and prove novel fuel/engine solutions, capable of addressing modern technological and environmental challenges. One of the research initiatives explores the possible use of naphtha-based fuels to power spark ignition (SI) engines, today operated on conventional gasoline. Naphtha is a generic term describing the fraction of crude oil that boils in the 30-180°C range. It is composed of C5 to C11 hydrocarbons and has a low research octane number (RON), roughly within the 50-70 range. It is a refinery product that can potentially be beneficial for the automotive industry as an example of a less processed fuel, responsible for less CO₂ emissions during the refining process. In fact, naphtha is only processed in the crude atmospheric distillation tower and undergoes light hydrosulphurization, in contrast to premium commercial gasoline, which is a blend of refined products from multiple process units (isomerization, reforming, FCC, alkylation, etc.). Moreover, thanks to its higher hydrogen to carbon ratio, burning naphtha in engines produces less CO₂ per unit of energy injected compared to regular gasoline. The theoretical reduction (Figure 2) is between -4 to -7% CO₂ emissions for naphtha fuel compared to non-oxygenated regular gasoline depending on the

naphtha's composition and assuming the same engine efficiency. This engine-out CO₂ benefit can contribute towards meeting future legislation to limit CO₂ emissions.

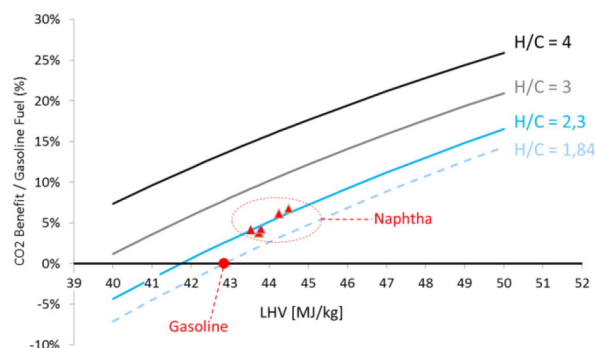


Figure 2. Theoretical CO₂ benefit (%) / gasoline fuel versus Lower Heating Value (LHV) (MJ/kg) and H to C ratio of fuel

The octane quality of a fuel, which can be described by RON, is crucial for avoiding engine knock: a higher RON reduces the likelihood of knock occurring. In the absence of knock, the combustion phasing of a SI engine can be set to deliver optimal efficiency. As a matter of fact, engines require a different RON at different operating conditions. At low engine loads, a lower RON fuel can be used without knock occurrence. Recent work by Kalghatgi et al. even suggests that the anti-knock quality of a fuel in modern SI engines also depends on its sensitivity (difference between RON and MON (Motor Octane Number) values) [7]. Based on this, varying fuel RON quality and adjusting it as any other engine operating parameter leads to what is known as the Octane on Demand (OOD) concept. It is a dual fuel system in which the engine operates on a more or less low RON base fuel that is continuously boosted on an as needed basis through the addition of an external octane booster [8, 9]. For such a concept, it is important to know the RON of the blended fuel depending on the quantity of fuel and booster in the mixture [10].

In a conventional combustion engine, a change of fuel properties, especially the RON, and its effects on engine response has been studied for several years [11, 12, 13, 14]. The increasing body of work in this area indicates that this is becoming an opportunity for car makers to further decrease average fleet fuel consumption and tailpipe GHG emission levels [8, 9, 15, 16]. Indeed, unlocking RON is a key parameter for enabling novel engine design. In fact, if higher RON is made available, higher compression ratios can be enabled, leading to better engine efficiency at low load with less knock limitation at higher load due to the increased knock resistance of the fuel. Today, high RON streams (> 105) are commonly obtained with ethanol blends or from refinery products rich in aromatic molecules, such as reformate.

In this context, Saudi Aramco, through its French subsidiary Aramco Fuel Research Centre Paris (AFRC) and its strategic partner IFP Energies nouvelles, has initiated a three-year research program to demonstrate the benefits of an OOD concept. This program is divided in several major steps, of which three significant ones have already been achieved:

- The first one deals with the understanding of the antiknock properties (RON) of a wide range of refinery streams using naphtha as base fuel mixed with various octane boosters (ethanol, reformat, a blend of butanol isomers, diisobutylene (DIB)) [10]. RON measurements of various mixtures covering large RON values from 71 to 111 highlights the promising octane boosting effect of blending RON 71 naphtha-based fuel with ethanol RON 108.
- The second one, performed on an engine test bench aims at understanding the anti-knock (or RON) requirements of a modern turbocharged GDI engine (1.6L from PSA Peugeot Citroen) [17]. Using surrogate Toluene Reference Fuels (TRF, Cf. section “*TRF Fuel matrix*”) with a wide range of RON from 71 to 111 demonstrates that low RON fuels (71 up to 91) can be used on a significant engine operating zone (low load) while maintaining the engine’s optimal efficiency (thanks to keeping optimal combustion phasing).
- The third one, which is the object of this paper, aims at understanding and quantifying the anti-knock (or RON) requirements for the same engine using blended “real fuels” composed by a base fuel and an octane booster fully premixed prior the injection and directly injected into the combustion chamber. For this purpose, similar experimental work, as previously performed with TRF [17], are conducted at the engine test bed. A wide range of RON values is assessed by varying the proportion of base fuels and octane booster in the mixture according to the result obtained on the previous CFR engine experiments [10]. By following a specific fuel matrix, different blends are then tested using:
 - As base fuel: Naphtha-based fuel RON 71, as a blend of pure naphtha RON 51 with Non-Oxygenate Gasoline (NOG) RON 91;
 - As Octane Boosters: Ethanol RON 108, a blend of butanol isomers RON 107 (Aramco patent [18, 19]) and reformat RON 111 (mainly composed of aromatics and directly derived from the refinery reforming unit process).

These results allow to compare the engine RON requirement using TRF and real fuels on the one hand and ultimately, to understand the differences in terms of knock limit by introducing parameters such as the heat of vaporization, the Sensitivity S (RON-MON), the Octane Index (OI) as well as the K factor (Cf. section “*MON and Sensitivity Analysis*”) [7, 20]. The results also point out the ‘double’ octane boosting effect of ethanol on a low RON base fuel and identify this fuel combination as highly valuable for the OOD concept.

FUEL MATRIX AND FUEL ANALYSES

As mentioned in the introduction, the present work quantifies the anti-knock requirements of a modern turbocharged GDI engine using blended “real fuels”, as previously done using TRF fuels [17]. Before describing the fuel matrix with the “real fuels”, it is interesting to briefly revisit the TRF fuel matrix. Indeed, the latter and its associated results on the multicylinder engine have contributed to the definition of the matrix of real fuels.

TRF Fuel Matrix

In this paper, TRF refers to a mixture of n-heptane and toluene whose RON is derived from a linear-by-mole blending rule [21].

The TRF fuel matrix (Table 1) is used to characterize the octane requirement of the engine when running at its optimal efficiency (optimal combustion phasing) [17].

Table 1. TRF fuel matrix

TRF	RON [-]	Molar n-heptane/toluene proportion [%]
#1	71	39.8 / 60.2
#2	85	28.2 / 71.8
#3	91	23.3 / 76.7
#4	97.5 (idem as regular E5)	17.7 / 82.3
#5	105	11.3 / 88.7
#6	111	6.1 / 93.9

This matrix is designed considering multiple criteria as detailed below:

- #1 - The lowest RON 71 corresponds to the naphtha-based fuel RON used for the OOD concept (56%vol. pure hydrotreated straight-run naphtha mixed with 44%vol. NOG RON 91);
- #2 - Intermediate RON 85 is a strategic value to quantify the reduction of antiknock properties for a low octane fuel, and to specifically address the question of antiknock property linearity with low RON;
- #3 - RON 91 corresponds to the exact RON of the NOG used in this study as regular gasoline;
- #4 - RON 97.5 is the average RON of commercial Unleaded 95-E5 fuel, compliant with the European standard EN 228;
- #5 - For RON above 97.5, the objective is to correlate the behavior of knock occurrence when using octane boosters. For this purpose, RON 105 is an intermediate and interesting value that can be roughly associated with the use of an octane booster such as the blend of butanol isomers (RON=107) or ethanol (RON=108);
- #6 - RON 111 perfectly matches with the RON of pure reformat.

Finally, the lowest RON (71) is hardly reported in the literature. Most of the time, this is the RON increase effect which is studied [8, 9, 11, 12, 14, 16]. In the present study both the RON increase and RON decrease is of interest. Compared to regular E5 gasoline (RON 97.5), the highest RON (111) corresponds to an increase of 13 pt RON and the lowest RON (71) corresponds to a decrease of 26 pt RON which is twice as much as the RON increase.

Real Fuel Matrix

This section refers to the design of the fuel matrix using real fuels, as illustrated in Figure 3. The RON of these fuels was measured on the CFR engine [10].

The design of the fuel matrix, including the selection of fuel baselines and octane boosters is made:

1. to ensure a consistency between their respective RON and the octane requirement map made with TRF on the multicylinder engine [17].
2. to meet specific objectives while respecting a few constraints, as detailed below.

Base fuel - One base fuel is considered:

- Naphtha-based fuel RON 71

Octane Boosters - Three octane boosters are considered:

- Ethanol (RON 108) is a well-known and widely used octane booster. Today, ethanol is present on the market (mainly US, Europe and Brazil) and can be used directly as a neat fuel E100 or blended with gasoline in significant proportion (E22, E85) for flex-fuel engine applications. Currently, most conventional gasoline engines are compliant with European Unleaded 95-E10 (EN 228) fuel, which contains up to 10%vol. ethanol blended with gasoline. Ethanol allows a natural CO₂ benefit in a combustion process because of its favorable H/C ratio; but its low Lower Heating Value (LHV) leads to higher volumetric fuel consumption compared to fossil fuels. Moreover, ethanol is a renewable energy source produced by a biochemical process and hence allows reducing CO₂ and avoiding additional governmental taxes in Europe when blended with gasoline.
- SuperButol™ (RON 107) is an octane booster, which is produced thanks to a recent Saudi Aramco patented process [18, 19] by simultaneously dimerizing and hydrating a hydrocarbon stream rich in C4 olefin molecules. In terms of composition, this butanol blend consists of variable proportions of butanols and DIB, with 2-butanol being the major component. Butanol isomers allow obtaining high RON [22], increasing energy content (LHV) compared to ethanol and decreasing CO₂ emission during the combustion process compared to fossil fuels due to a higher H/C ratio.
- Reformate (RON 111) 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 in most refineries, since the aromatic molecules have extraordinary high RON and the reactions that the naphtha feedstock undergoes to yield aromatics produce a hydrogen-rich gas stream. In the present study, a generic reformate has been used with 97 %m. of aromatic molecules (C7 to C10). Compared to ethanol and the blend of butanol isomers, reformate has the highest RON, density and LHV, but the worst H/C ratio in terms of CO₂ emission during the combustion process and no alcohol or oxygen compounds.

Objectives guiding the fuel matrix design:

- Demonstrate the feasibility of running a multicylinder engine at its maximum efficiency (as far as possible) using a low RON fuel (RON 71) as a single fuel or blended with an octane booster (ethanol, butanol blend, reformate);
- Get a clear comparison of differences regarding engine RON requirement when using TRF and real fuels and thereby understand the differences in terms of knock limit;
- Demonstrate the benefits of an OOD concept using premixed fuels before moving forward with a dedicated dual fuel injection system (see next step of the project as reported in the conclusion);
- Use the volumetric proportion of base fuel and octane booster previously defined by the CFR engine tests [10], to match each RON target;

Finally, this matrix is composed of eight fuels:

- One fuel is a 100% base fuel:
 - ① Naphtha-based fuel - RON 71
- Four fuels result from blending naphtha-based fuel RON 71 with:
 - ② 43.2%vol. of the blend of butanol isomers - RON 91
 - ③ 24.3%vol. of ethanol - RON 91
 - ④ 42.3%vol. of reformate - RON 91
 - ⑤ 36.9%vol. of ethanol - RON 97.5
- Three fuels are 100% octane booster:
 - ⑥ Blend of butanol isomers - RON 107
 - ⑦ Ethanol - RON 108
 - ⑧ Reformate - RON 111

Base Fuel		RON Target	
Naphtha			
Octane Booster	① 100%		71
	Butanol blend 43.2% ②		91
	Ethanol 24.3% ③		
	Reformate 42.3% ④		
	Ethanol 36.9% ⑤		97.5
	Butanol blend ⑥ 100%		107 - 111
	Ethanol ⑦ 100%		
	Reformate ⑧ 100%		

Figure 3. Real fuel matrix including eight combinations with their respective RON target and volumetric rate [%] of octane booster or base fuel

MON AND SENSITIVITY ANALYSIS

The comparison of the engine octane appetite using TRF and real fuels is based on the RON requirement. However, work described in the literature [14, 20, 23, 24, 25] shows that in the context of an up-to-date turbocharged SI engine, the anti-knock quality of the fuel can also be represented by the Octane Index (OI), meaning that the higher the OI, the better the knock resistance:

$$OI = RON - KS \quad (1)$$

$$S = RON - MON \quad (2)$$

S is known as the fuel Sensitivity and is usually positive.

The K value is an engine condition dependent weighting factor. It has recently been shown [20, 25], that:

- At part load, K is often positive. As a result, for a given RON a high OI needs a low S value, meaning that the higher the MON, the better the knock resistance.
- At full load, K can be negative. Consequently, for a given RON a high OI requires a high S value, meaning that a lower MON allows a better knock resistance.

In this context, MON values of TRF and real fuels are also determined to further analyze the engine results considering the fuel OI requirement and not only the basic RON need.

MON, Sensitivity and Latent Heat of Vaporization (Lv) of TRF

As previously done for RON, the MON values of TRF are assessed using a linear-by-mole blending rule [21], for latent heat of vaporization assessment linear mass blending rule is used. The results are presented in Table 2. It can be seen that the growth of the sensitivity is linear when increasing RON (Figure 4). These results are fully consistent with the literature [26]. It can also be observed that latent heat of vaporization of all TRF remains in the same range (only 10% between the lowest and the highest value; a much bigger spread is seen with the real fuels).

Table 2. RON, MON, and sensitivity values and latent heat of vaporization for different blends using TRF

TRF	RON [-]	MON [-]	Sensitivity [-]	Lv [kJ/kg]
#1	71	63	8	366
#2	85	76	9	376
#3	91	81	10	381
#4	97.5	86.5	10	386
#5	105	93	12	391
#6	111	99	12	396

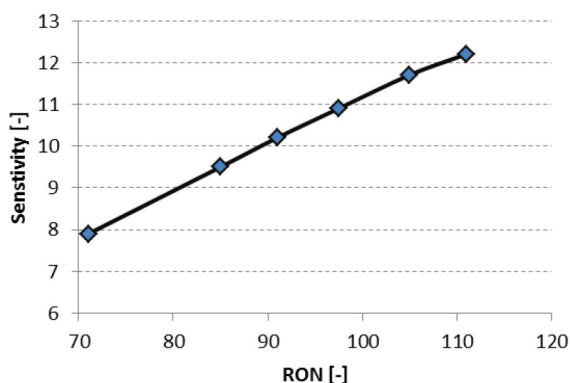


Figure 4. Evolution of Sensitivity of TRF versus RON

MON, Sensitivity and Latent Heat of Vaporization of Real Fuels

Experimental Techniques for MON Measurements

With real fuels, the MON is measured on a CFR engine. To perform MON measurements, the engine speed is set to 900 rpm, and the inlet mixture temperature is regulated at 149 °C [27]. These engine speed and inlet temperature levels are the main differences with regards to RON measurement [28] where they are set respectively at 600 rpm and ambient temperature. As a consequence, experimental conditions are much more severe with regards to auto-ignition during MON measurement than during RON measurement.

The tested fuel MON is obtained when the occurrence of detonations is the same as with a blend of n-heptane and 2,2,4-trimethylpentane (iso-octane). The MON value represents the volumetric percentage of iso-octane in MON CFR engine conditions.

Synthesis of RON, MON, sensitivity and Lv for real fuels

Table 3 gives a synthesis of the different measurements performed to characterize the real fuels. Latent heat of vaporization is assessed by using linear mass blending rule.

Table 3. RON, MON, sensitivity and Lv for real

Real fuels	Blend	RON [-]	MON [-]	Sensitivity [-]	Lv [kJ/kg]
#1	Naphtha	71	69	2	274
#2	Naphtha (56.8%v.) + Butanol blend (43.2%v.)	91	84	7	367
#3	Naphtha (75.7%v.) + Ethanol (24.3%v.)	91	82	9	421
#4	Naphtha(57.7%v.) + Reformate (42.3%v.)	91	81	10	284
#5	Naphtha (63.1%v.) + Ethanol (36.9%v.)	97.5	85.0	12.5	497
#6	Butanol blend	107	95	12	479
#7	Reformate	111	102	9	296
#8	Ethanol	108	90	18	854
-	Regular E5	97.5	87	10.5	289

Analysis of Blending Behavior for RON, MON and Sensitivity

Figure 5, Figure 6 and Figure 7, respectively, display the response of RON and MON, the sensitivity, and the deviation of RON and MON from linear trends, as a function of octane booster volumetric incorporation rate, when blended with naphtha-based fuel.

From these figures, it may be noted the following and interesting results:

- Ethanol delivers the strongest octane boosting effect for both RON and MON whereas reformate and the blend of butanol isomers have the lowest ones, despite the higher RON of pure