

An Investigation of High Load (Compression Ignition) Operation of the “Naphtha Engine” – a Combustion Strategy for Low Well-to-Wheel CO₂ Emissions

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ABSTRACT

A computational and experimental study has been carried out to assess the high load efficiency and emissions potential of a combustion system designed to operate on low octane gasoline (or naphtha). The “naphtha engine” concept utilizes spark ignition at low load, HCCI at intermediate load, and compression ignition at high load; this paper focuses on high load (compression ignition) operation. Experiments were carried out in a single cylinder diesel engine with compression ratio of 16 and a common rail injector/fuel delivery system. Three fuels were examined: a light naphtha (RON~59, CN~34), heavy naphtha (RON~66, CN~31), and heavy naphtha additized with cetane improver (CN~40). With single fuel injection near top dead center (TDC) (diesel-like combustion), excessive combustion noise is generated as the load increases. This noise limits the maximum power, in agreement with the CFD predictions. The noise-limited maximum power increases somewhat with the use of single pilot injection. Operation at peak loads comparable to conventional light duty diesel power levels requires a “split combustion” approach that utilizes a widely-separated pilot and main injection. The engine results show good performance and efficiency at low speeds across medium to high loads. High speed operation of split combustion is limited to engine speeds of < 2700 rpm due to insufficient ignitability of the naphthas even when cetane improver is added. While the large amount of premixed combustion at low and medium loads results in low NO_x and PM emissions, high (diesel-like) emissions are observed at high load with the split combustion

approach. Thus, while the approach yields promising peak load levels and high efficiency operation speed and emission considerations limit the utility of this approach at present and further research is required to improve its attractiveness.

INTRODUCTION

There is currently significant worldwide industry and governmental effort focused on reducing vehicle CO₂ emissions. CO₂ emissions associated with vehicle operation can be partitioned into two categories – those from the production and transport of the fuel, and those from combustion of the fuel on the vehicle. The CO₂ generated during production and transport of the fuel to the service station is referred to as the well-to-tank (WTT) CO₂ emissions. Correspondingly, the CO₂ generated during vehicle operation is denoted the tank-to-wheel (TTW) CO₂. Collectively, the sum of these is referred to as the well-to-wheel (WTW) emissions:

$$\text{WTW} = \text{TTW} + \text{WTT} \quad \text{eq. 1}$$

The various elements of the vehicle WTW emissions are shown in Figure 1. It is increasingly being recognized that it is the total, or WTW, CO₂ emissions that must be reduced in order to achieve overall CO₂ reductions. Thus, combustion strategies that achieve high vehicle efficiency (lower TTW) but require fuel that is more energy-intensive to produce (higher WTT) may not yield an overall WTW CO₂ reduction.

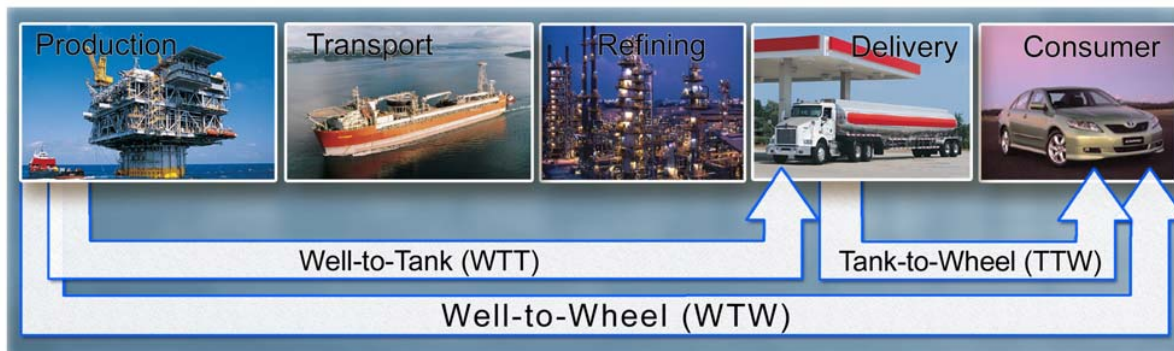


Figure 1: Schematic of processes involved in well-to-tank (WTT), tank-to-wheel (TTW), and well-to-wheel (WTW) emissions.

With regard to gasoline engines, researchers have long recognized that a significant increase in efficiency can be realized by raising the compression ratio (CR). Similarly, turbocharged gasoline engines have increased power density and thus can be downsized, leading to improved fuel economy and decreased TTW emissions. However, the more severe conditions (higher temperature and pressure) of the end gas during the piston compression and flame expansion exacerbates engine knock. Consequently, if the octane rating of the fuel is insufficient, the engine operation must be modified to minimize knock, which reduces power and fuel economy.

While increasing the octane number of the fuel minimizes knock, the production of higher octane gasoline requires energy-intensive refinery processes, leading to a corresponding WTT debit. This is demonstrated schematically in Figure 2, which shows the changes in vehicle (TTW) efficiency and CO₂ emissions required to offset refinery (WTT) emissions and CO₂ changes associated with changing the octane number of part of the total gasoline pool.¹ The calculations are from a model (only briefly summarized here) based on a integrated European refinery/chemicals complex. The model incorporates linear programming calculations that identify the impact on energy and CO₂ emissions of gasoline research octane number (RON) changes on the entire material balance of a refining complex. The base case scenario assumes a gasoline pool consisting of 25% "98" RON and 75% "95" RON, yielding an average RON of 95.8. Alternative scenarios are based on a production strategy consisting of maintaining 50% of the fuel at the standard grade (25/75% Premium/Regular) and producing 50% of a new grade whose RON varies over the range 80-105. No oxygenates, amines, or metal containing additives are used, other fuel properties (vapor pressure, distillation curve, etc.) are unchanged.

¹ Although the WTT contributions include CO₂ due to shipping and transport, these contributions are small compared to those from the refinery and are constant, and thus are neglected in the present discussion.

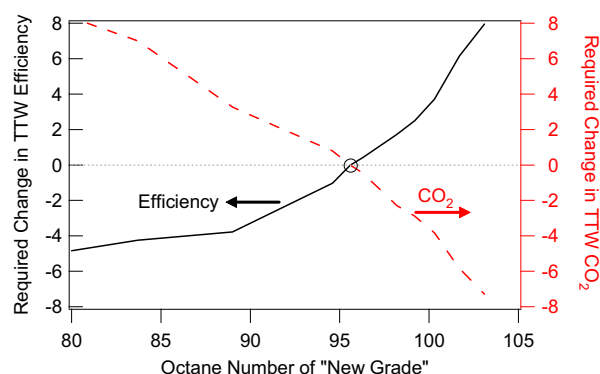


Figure 2: Vehicle tank-to-wheel (TTW) efficiency and CO₂ changes required to offset refinery efficiency and CO₂ changes associated with producing 50% of a different octane number fuel.

The model adjusts the average RON of the overall gasoline pool in steps away from the RON=95.8 base case and optimizes the refinery operation to accommodate this change. This includes modifying processes such as distillate (diesel, jet, kerosene, and heating oil) production, natural gas imports to balance refinery hydrogen needs, etc. The total energy content of the gasoline pool is kept constant. The base case and the alternative scenarios are chosen carefully so that they do not represent extreme conditions that would bias rationalization of the results. The output of the model is the energy change, relative to the base case, associated with producing the "new grade" of fuel, which can also be expressed as a CO₂ change.

The figure shows that increasing the octane number of the new grade requires large changes in TTW efficiency and corresponding large CO₂ reductions. For example, raising the octane number of the new grade from 95.6 (base case) to 103 requires the vehicles operating with this fuel to exhibit 7% lower CO₂ emissions – solely attributable to the increase in octane number – to offset the increased refinery CO₂ emissions.

It is important to note that the above results are specific to a single refinery/chemicals complex, and as such are not representative of the entire refining industry either in a geographical region or globally. However, the model captures the major trends and the general result that increasing the octane number of the new grade (and hence, the entire gasoline pool) leads to a large CO₂ increase that requires significant improvements in vehicle efficiency to offset these refinery increases, and even larger gains to justify on a WTW basis.

A key element of the above analysis is the change in octane number for the *entire* pool that results from changes in the octane number for the special grade. However, other scenarios can be considered that keep the overall pool octane number unchanged but change the split (octane difference and relative volume) between regular and premium gasoline. This change is readily achieved in a modern refinery through changes in blending strategies, as market gasoline is blended from numerous diverse streams that have markedly different properties (composition and octane numbers). The reblending could be carried out to change only the ON while maintaining key properties such as vapor pressure, distillation characteristics, etc.

The current work evolved from consideration of a strategy to provide high octane fuel for high compression ratio, turbocharged gasoline engines that does not yield a WTT CO₂ debit. The strategy relies on reblending a *fraction* of the gasoline to yield a very high octane number premium fuel. However, in order to maintain the octane number of the overall pool, a (potentially much) lower ON stream would have to be produced. While such a low ON fuel would not provide high efficiency in a conventional spark ignition (SI) engine due to knocking, alternative combustion strategies could be identified that would permit high (diesel-like) efficiency with a low ON gasoline.

The present paper investigates the operability, efficiency, and emissions potential of a combustion system based on diesel engine hardware but adapted to operate on low octane gasoline. The system employs either compression or spark ignition to achieve satisfactory operation over the engine's entire load/speed range. Initial tests have been carried out with naphtha refinery streams, which are representative of low ON streams produced in refineries. The combustion strategy is referred to hereafter as the "naphtha engine," and the operating strategy is outlined in the following section.

OVERVIEW OF COMBUSTION STRATEGY

Adapting a diesel engine to run on naphtha while meeting stringent efficiency and emissions targets requires accommodating the large differences between naphtha and commercial diesel fuel. Two of the most significant differences are the higher volatility and lower ignitability of naphtha vs. commercial diesel fuels. A

schematic of a combustion strategy that takes advantage of these properties is shown in Figure 3. Homogeneous charge compression ignition (HCCI) is utilized in the intermediate load range, where high efficiency and low emissions is possible. The strategy employs HCCI over as wide an operating range as possible. However, previous HCCI studies [1,2] suggest that compression ignition of naphtha at low load might be difficult to achieve due to insufficient ignitability. Thus spark ignition (SI) is utilized for conditions such as cold start and idling/low load range where knock-free operation is possible even with low octane number fuels. The peak operating load for HCCI is also well below the engine's peak torque curve, and thus HCCI is also not well-suited for high load operation. In the current approach, a variation of conventional (diesel-like) compression ignition denoted "split combustion" (described below) is used at the highest loads.

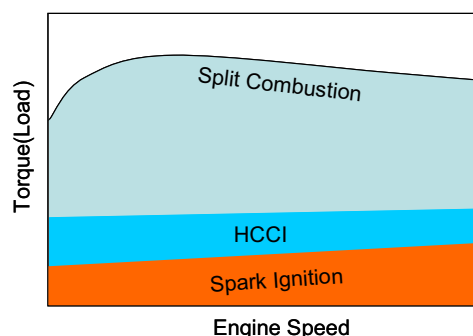


Figure 3: Combustion strategy of naphtha engine.

This hybrid approach has elements similar to those described in earlier gasoline- and diesel-based multifuel capability studies [3, 4]. More recently, Kitano et al. have investigated the effect of fuel properties on HCCI [1]. Over the years, numerous studies have been reported on the effects of low cetane number (CN) fuels similar to naphtha on diesel engine performance and emissions [5-10]. In most cases the use of low cetane fuels results in a decrease in engine performance (e.g., high pressure rise rates, increased maximum cylinder pressure) and high emissions levels. Cold starting can be particularly problematic with low CN fuels as operation of diesel engines at this temperature extreme usually results in hard starting and excessive white smoke emissions, which may lead to extremely high rates of pressure rise, and possible engine damage [11-15]. While the concept shown in Figure 3 has the potential to solve these problems with low CN fuels by taking advantage of fuel property of naphtha, several specific questions need to be addressed:

1. What is the load at which SI operation switches to HCCI?
2. What is the upper load limit of HCCI combustion?

- How will naphtha affect the performance of compression ignition under diffusion combustion conditions?
- How does engine performance compare to the conventional diesel fuel case?
- What is the maximum engine load and speed possible with naphtha compression ignition?

In this paper, a computational and experimental study has been carried out to address these questions and the overall feasibility of compression ignition operation of the naphtha engine. The present paper addresses operation over the entire load/speed range computationally, while experiments are only presented at high load conditions.

FUEL PROPERTIES

Two refinery naphtha streams have been used in the engine tests described herein. The fuel properties are listed in Table 1. The fuels include both a light and heavy naphtha stream, which differ in both volatility and composition. The light naphtha has a Reid vapor pressure (RVP) of 12.4 psi, which is substantially higher than the market fuel specification (~ 8 psi), while the heavy naphtha RVP is markedly lower (2.4 psi). The ON of both fuels are comparable, with the heavy naphtha slightly lower (RON ~ 59 vs. 66). The composition of the light naphtha is mostly paraffinic with low aromatics, as the volatility range only just encompasses the C₇ and higher hydrocarbon range representative of the aromatics in market gasolines. Conversely, the heavy naphtha contains 17.4% aromatics, which is on the low end of market fuels which typically contain 20-35% aromatics. The light naphtha also includes substantially higher sulfur levels than the heavy naphtha, although this effect should be negligible in the present studies.

Table 1: Properties for the two naphtha streams and diesel fuel used in the engine tests.

		Light Naphtha	Heavy Naphtha	Diesel
RVP	psi	12.4	2.4	-
T10	deg. C	108.7	194.2	206.0
T50	deg. C	131.1	254.1	264.0
T90	deg. C	167.1	334.6	337.0
RON		66.3	59.2	-
MON		65.2	60.2	-
Derived CN		34.3	31.2	52.7
Aromatics	%v/v	1.4	17.4	18.4
Olefins	%v/v	3.3	0.7	-
Benzene	%v/v	1.0	1.2	-
Sulfur	ppm	179.0	0.0	8.0
H/C	mol/mol	2.29	1.94	1.892
Density	g/ml	0.6579	0.7607	0.8319
Higher Heating Value	MJ/kg	47.9	46.2	
Lower Heating Value	MJ/kg	44.5	43.2	42.9

The naphtha results have been compared to those of a diesel fuel whose properties are also shown in Table 1. The diesel fuel has a boiling range commensurate with market diesel fuel and a cetane number (CN) of 52.7,

which is comparable to Japanese and European diesel but higher than typical USA market diesel fuel.

3D-CFD CALCULATIONS

Three dimensional computational fluid dynamic (3D-CFD) simulations have been carried out to investigate the effects of CN and volatility on diesel-like combustion. Improvements in the spray [16], combustion and turbulence models of the original KIVA2 code were required to adequately model combustion in diesel engines. These improvements, summarized in Table 2, include revised models for droplet break-up and atomization, multi-step auto-ignition, and laminar-turbulent combustion. The Shell model [17] is used to model ignition until the gas temperature exceeds 1000K, after which the Laminar-Turbulence Characteristic Time Combustion (LTCTC) model [18] is used. The Shell model constants are tuned to agree with HCCI experimental data for various PRF fuels, where the CN was varied by changing the blending ratio of n-heptane and iso-octane. The model fuel properties used in the calculations are listed in Table 3. N-Dodecane and n-octane were used as vaporization surrogates for the low volatility fuel (diesel) and high volatility fuel (naphtha), respectively. Thus, diesel fuel is physically modeled by n-dodecane with the Shell constants tuned to match CN=52, and naphtha is modeled by n-octane physical properties with CN=30. Additionally, "virtual" low cetane diesel and high cetane naphtha fuels are modeled by n-dodecane with CN=30 and n-octane with CN=52, respectively, to distinguish CN and volatility effects.

Table 2: Sub-model used in KIVA2.

Drop breakup and atomization	Surface-wave-growth[15]
Ignition	Shell multi-step model[16]
Combustion	Laminar-turbulence char time model[17]
Turbulence	RNG k-ε [17]

Table 3: Fuel properties used in KIVA2.

	Diesel	Naphtha	Low CN diesel	High CN Naphtha
Cetane Number	52	30	30	52
Surrogate Fuel (Boiling Point °C)	n-C12 (214)	n-C8 (128)	n-C12 (214)	n-C8 (128)

The engine geometry and operating conditions utilized in the simulations are listed in Table 4. Although the nozzle geometry in the calculations differs from the configuration used experimentally (see Table 5), the geometries are sufficiently similar to predict qualitative trends. The operating conditions are representative of conventional diesel engine geometry at low speed and medium load. Figure 4 shows the heat release rate for