

Onboard Optimisation of Engine Emissions and Consumption According to Diesel Fuel Quality

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ABSTRACT

In response to the demand to lower CO₂ emission, all engine developers face the challenge of drastically reducing fuel consumption. At the same time, they will need to meet future exhaust emission legislation by simultaneously employing internal measures and after treatment systems.

Additionally, they will have to deal with increasing fuel variability. As different properties can lead to very different behavior in engine operation, information onboard the vehicle providing the fuel composition would allow to adjust engine operating parameters accordingly, to make the most beneficial use of the available fuel quality. This will be obvious considering future diesel fuels blends, or the ever increasing amount of biodiesel content mixed into Diesel fuel, but could already be interesting considering existing fuel variability faced in Europe or America.

In this context, an innovative Fuel Quality Sensor technology [1] [2] has been developed: it provides detailed information about the molecular structure of the diesel fuel flowing to the engine as well as its biodiesel content.

In the context of the presented study, a matrix of 10 diesel fuels representative of real world fuel variability and including future trends in biodiesel introduction has been prepared, and systematically tested on a modern single cylinder engine, with a fully flexible engine parameters management.

First step was to test all fuels with basic Engine Control Unit (ECU) settings optimized for EN590 fuel, showing the impact of fuel variability on engine emissions and specific fuel consumption.

Second step was to investigate influence of several engine parameter (pilot and main injection, EGR rate, ...) in order to understand the ways to optimise ECU settings for each fuel blend.

The final step will be a compensating algorithm, enabling the engine to run different fuel qualities with optimized emissions, fuel consumption and running behavior, using information from the Fuel Quality Sensor.

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INTRODUCTION

Fuel quality must match climate constraints. During winter, Diesel engine must start up when the ambient temperature is -30°C in Scandinavia: to ensure cold start, the Diesel contains about 40% kerosene in cold countries. The Diesel does not contain any kerosene in south of Spain at the same period of the year. Such variability in kerosene content strongly impacts the fuel composition and its key properties.

This is one simple example showing that fuel variability is a real matter for engine developers, despite regulations tending to limit it.

The fuel quality obviously depends on geographical commercial specifications and on the level of sophistication

of the refining tools, and is rather important in emerging countries.

The [figure 1](#) shows that the Diesel quality in the US also presents a large variability [3]. Such variability is explained by the fact that US refining tools have been Gasoline oriented because of the local existing market demand.

Growing Fuel Variability

The [figure 2](#) displays the existing Diesel quality variability and the future variability, established with a worldwide database of more than 3000 fuel samples collected in 50 countries. The 3 axis are fuel molecular structure markers [1] of representative samples of the worldwide

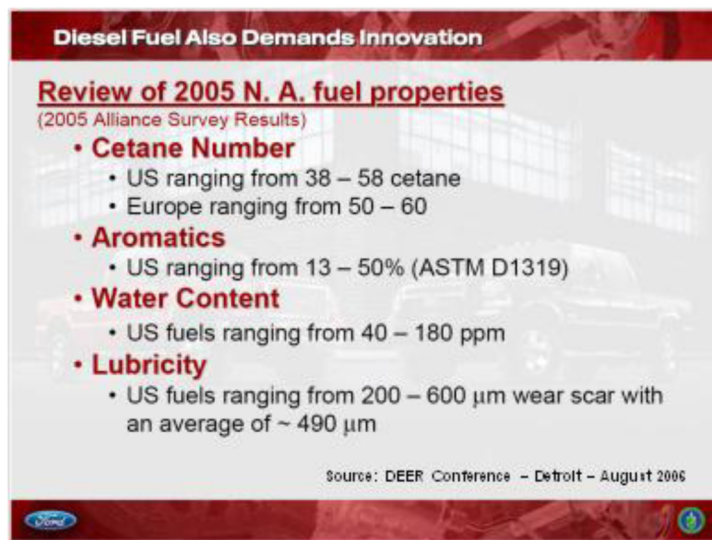


Figure 1. Diesel Fuel variability in US

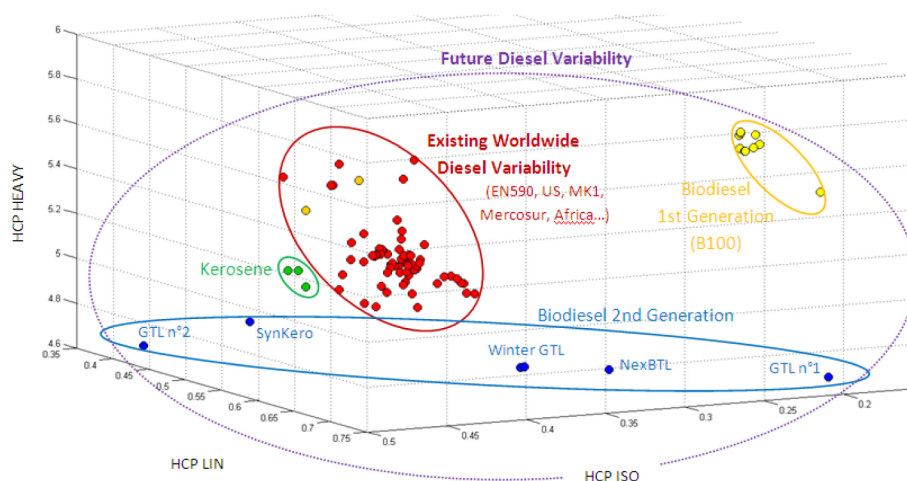


Figure 2. Existing and future Diesel quality variability

database, classifying the different samples according to their content in linear paraffin bonds (HCP LIN), isomeric bonds (HCP ISO) and to their heaviest fraction (HCP Heavy). These markers are described with more details in a further chapter of the present document. The “Balkanization” of fuel with the incorporation of first and second generation biodiesels (Methyl Esters based on Soja, Palm, Rapeseed,..., CTL, GTL and BTL) will exacerbate significantly the fuel variability:

- first generation biodiesels with their high density, long linear paraffin chains, and low quantity of isomeric bonds.
- second generation biodiesels much lighter, and with various possible ratios between isomeric and linear paraffin bonds.

The figure 3 shows that the first generation biodiesel itself presents huge quality variability since different sources (rapeseed, palm, sun flower, groundnut...) can be feedstock of several different processes [4]. The future generation of Biofuels (e.g. hydrogenation of vegetable oil) will also lead to a certain variability mainly of the carbon chain length.

Impact of Fuel Variability

For existing and future markets, including emerging countries, engine developers will have to deal with increasing fuel variability. Several studies have been performed to understand better the impact of the fuel on the engine performances.

Biofuels technologies today Resources - Technologies - Markets

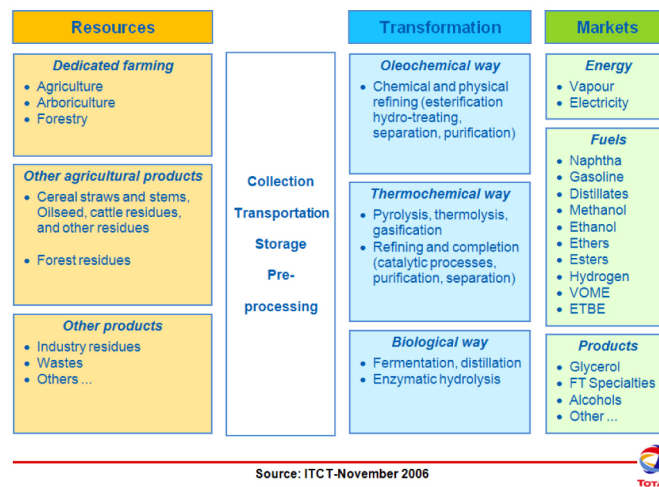


Figure 3. Biofuels quality variability

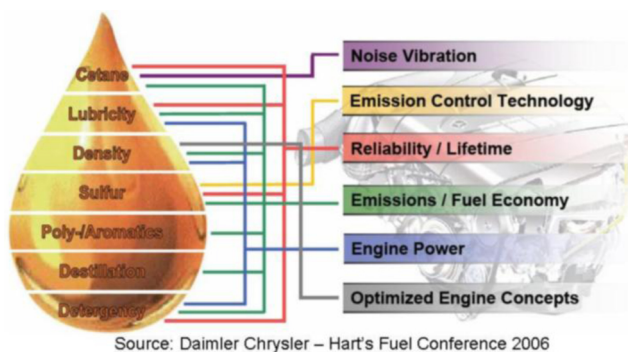


Figure 4. Overview of Key Diesel Properties and their Impacts

The figure 4 summarizes the main key properties of Diesel fuel and its impact on engine performances [5]. As a general understanding and according to the conclusion of most of the past studies, a single property cannot fully explain a specific engine related parameters. This is mainly explained by the fact that these conventional properties remain at the macroscopic level, whereas combustion phenomena require a much finer approach (molecular level).

A device onboard the vehicle providing pertinent information on fuel molecular structure would allow to adjust engine operating parameters accordingly. This could lead to the most beneficial use of the available fuel quality, giving lowest possible engine emissions and lowest brake specific fuel consumption.

This will be obvious considering future diesel fuel blends, or the ever increasing amount of biodiesel content mixed into Diesel fuel.

Different solutions are under development to be able to provide information on fuel quality onboard the vehicles in near future.

The present study focuses on the existing fuel variability faced in Europe or America, and on the interest to already consider it on short term applications, particularly in the case of Heavy Duty transport, where trucks covering large distances are likely to face Diesel fuels of which quality can vary significantly.

APPROACH TO HANDLE FUEL VARIABILITY

Today, no industrial solution is available to provide complete information about fuel variability.

Some solutions are developed to provide limited information on one physical fuel characteristics:

- Acoustic based devices (resonance tube, tuning fork [6]...) providing an information correlated to density and viscosity of the fuel
- Physical sensing devices based on conductivity, inductance or capacitance to try to provide information on Ethanol content in Gasoline fuels [7-8], or biodiesel in Diesel fuels. This information is moreover reliable in a very limited range of fuel:
 - Presence of water or methanol in alcohol-gasoline mixtures will affect measurement validity of Ethanol content [9-10]
 - Dielectric constant of the base diesel can vary significantly, affecting measurement validity of biodiesel content
- Sensorless computational approach ("Soft sensor") based on use of existing engine sensor (lambda probe, cylinder pressure sensor...) and specific close-loop strategies to

estimate the rate of alcohol in Gasoline [11] or the rate of biodiesel in Diesel [12].

An optical sensor based on Near Infra Red (NIR) technology determining molecular structure information about the fuel should provide a complete picture of its structure and consequently about its behaviour when used in an engine.

A sensor based on Nuclear Magnetic Resonance (NMR) technology could also be a powerful tool to handle a similar approach, but obvious cost and technical constraints do not make it a good candidate for Automotive Onboard applications.

INTRODUCTION TO NEAR INFRARED SPECTROSCOPY

The NIR spectroscopy is an analytical technique based on the absorption of the electromagnetic radiations contained in the near infrared region between 780 and 2500 nm [13].

Theory of Vibrational Spectroscopy

When the molecules are in their fundamental vibrational energy levels, atoms which are involved in atomic bonds move along the axis of the bond at a frequency defined by the strength of the bond and the mass of bonded atoms. Amplitudes of these vibrations will increase if some energy is transferred to the molecule. This energy can be transferred from a photon from a light source at a given wavelength. NIR theory is based on the fact that part of the radiation energy can be absorbed by the molecule at a given frequency (i.e. wavelength).

This is only possible if the energy supplied is exactly the same that is needed between two vibrational levels and then can produce excitation to a higher vibrational energy level.

The match of radiation energy with the energy difference between two vibrational levels causes a selective response of the molecular system to the incident radiation. It means that in a given wavelength range, some frequencies will be absorbed; others (that do not match any of the energy differences possible for that molecule) will not be absorbed while some will be partially absorbed.

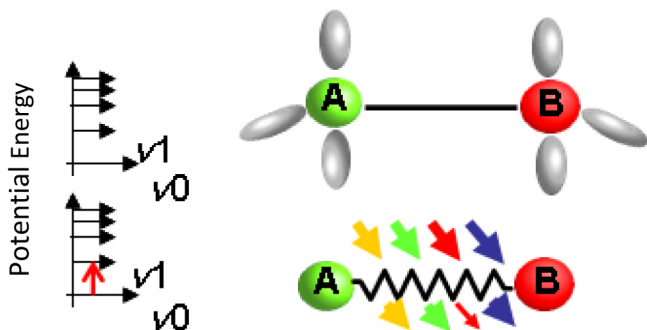


Figure 5. Vibrational spectroscopy mechanism

Since the molecular structure of most compounds is very complex, the final spectrum is the result of many overlapping “peaks and valleys”, whereas there are many fundamentals and well identified peaks in the mid and far infrared regions [14].

However, the NIR spectra are much richer than the Infra Red (IR) spectra because they result from various polyatomic vibrations of molecules whereas IR spectroscopy involves mainly diatomic vibrations [15].

In addition this technology involves a short spectrum collection time (from msec to sec) and is a non destructive method. These advantages have lead to a wide range of industrial applications for this analytical technique since the 90's and the access at low cost to powerful microcomputers and advanced statistical and mathematical tools. The NIR technology is now considered as a proven, mature and successful application particularly in chemical, petrochemical, food-processing, aeronautical and space industries.

The NIR spectrum is considered as the fuel DNA or the fuel fingerprint and is the first link in a complex data treatment process to extract valuable information from the NIR spectrum called Chemometrics.

The NIR method relies on the spectra-structure correlations existing between a measured spectral response caused by overtones and combination of the fundamental vibrations occurring at infrared frequencies. Qualitative and quantitative methods typically require the application of multivariate calibration algorithms and statistical computation (to predict the chemical and physical properties of an unknown sample from its NIR spectrum). Because changes in the NIR spectrum are proportional to changes in the concentration of chemical components, NIR spectrum is also highly correlated with the physical characteristics of samples.

NIR Spectrum Acquisition

A light source emits at different wavelengths through the fuel sample. The molecules contained in the fuel absorb part of the energy at specific wavelengths. The remaining energy is received on a NIR detector. By comparing - for each wavelength - the emitted Energy to transmitted one, we can deduce the energy absorbed by the molecule and build the NIR absorbency spectrum of the fuel.

For organic molecules containing C-C, C-H, O-H bonds, the fundamental vibrations occur in medium infrared regions which is commonly known as IR (2500 to 25000 nm) while overtones and combinations are measured in the near infrared area. Near-infrared spectra are primarily the result of overtones and combinations bands [16].

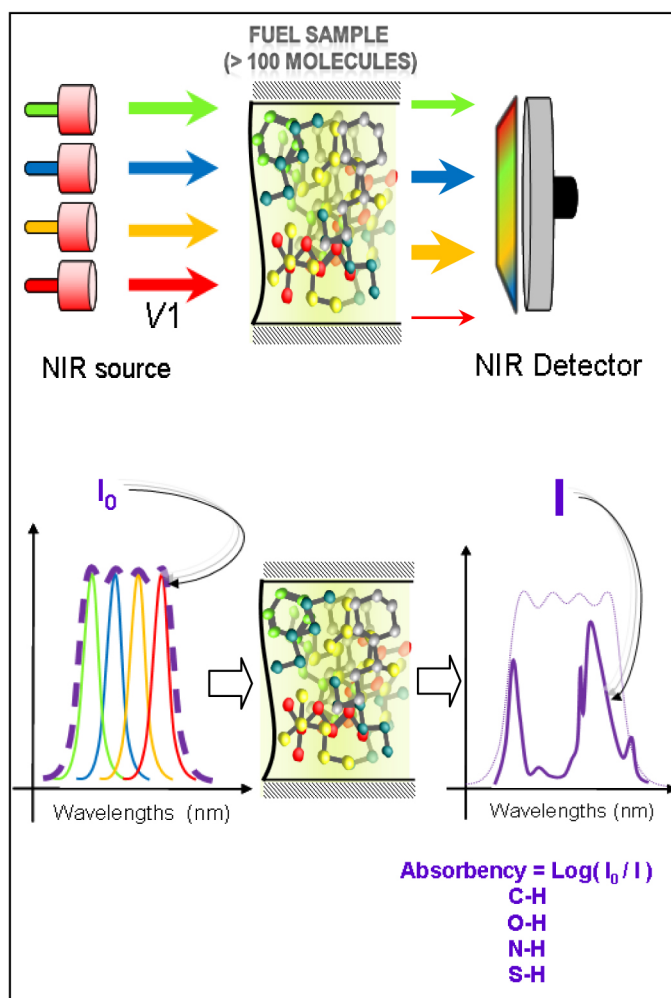


Figure 6. NIR spectrum acquisition scheme

Table 1 shows the relative intensities of C-H stretch bands for infrared and the various NIR overtone and combination regions. It gives a great deal of flexibility for path length selection and information content. For example, the closer one approached the fundamental region the more detailed is the vibrational information.

Table 1. Relative intensities of C-H stretch bands in IR/NIR regions

Band	region (nm)	Relative Intensity	Pathlength (mm)
Fund. (n)	3380-3510	100	0.01
Combination	2000-2500	10	0.05
1st over. (2n)	1700-1900	1	1 to 2
2nd over.(3n)	1100-1200	0.1	10 to 20
3rd over. (4n)	800-1000	0.01	50 to 100
4th over. (5n)	690-780	0.005	100

Figure 7 presents the application of the theory of the vibrational spectroscopy; a molecule's vibration has a fundamental frequency which is associated with a series of overtones and combinations.

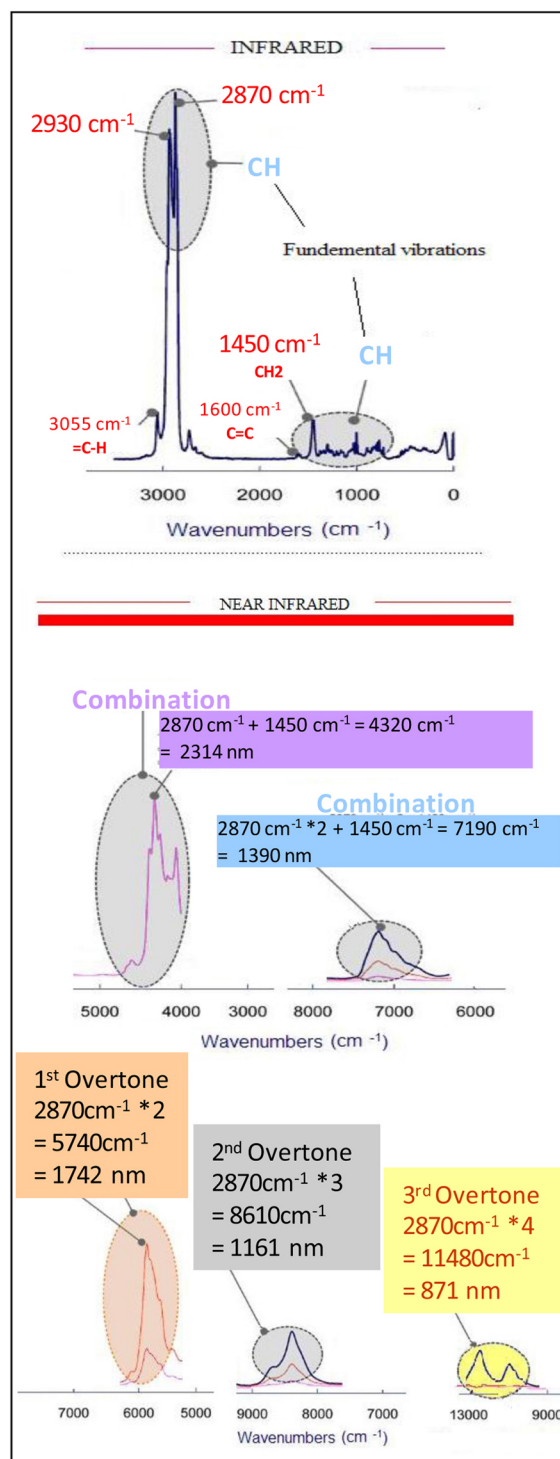


Figure 7. Fundamental vibrations in IR and associated Near Infrared vibrations (combinations & overtones) viewed in absorbency mode.

Table 2. HCP's meaning

HCP	Meaning : Impact on the engine based on
HCP Aro	Number of weighted Aromatic carbon-carbon bonds
HCP Lin	Number of weighted Linear saturated carbon-carbon bonds
HCP Naph	Number of weighted Cyclanics saturated carbon-carbon bonds
HCP Iso	Number of weighted Iso-Paraffins saturated carbon-carbon bonds
HCP Ether	Number of weighted carbon-oxygen bonds from ethers
HCP water	Number of O-H bond coming from water
HCP OL	Number of O-H bond coming from alcohol
HCP Olef	Number of weighted Olefins carbon-carbon bonds
HCP Sat	Number of weighted saturated carbon-carbon bonds
HCP Light	Number of carbon-carbon bonds having a small carbon chain
HCP Medium	Average number of carbon
HCP Heavy	Based on H/C rate or length of C-C chain

The combination bands area is the most sensitive and contains the richest information. But in the other hand, such area requires precision optical system that can hardly be transposed to the automotive market.

The first and second overtones present strong advantages but involve specific detectors or light sources not in line with the automotive market cost constraints.

The third overtone covering the wavelengths between 800 nm and 1000 nm has been selected to design and built an innovating, miniaturized, robust and low cost spectrometer for the demanding automotive market. This spectral area is compliant with the use of basic silicon detectors and light emitting diodes (LED). On the other hand, the information extraction from the third overtone is much more difficult than from the other NIR regions.

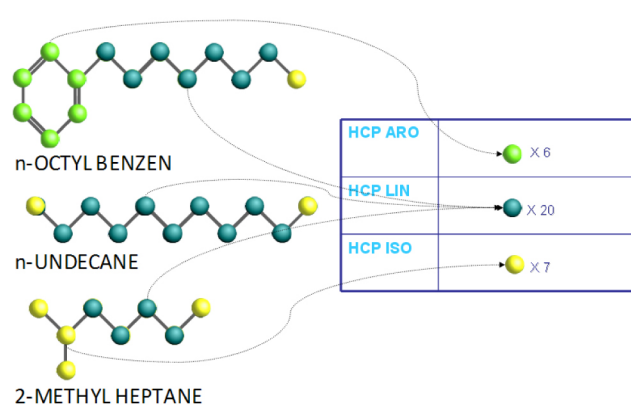
FROM THE NIR SPECTRUM TO ENGINE PARAMETERS OPTIMIZATION

NIR and Fuel Molecular Information

Since the injection, combustion and after treatment systems are affected by the fine chemistry of the fuel, the proposed solution consists in monitoring the number and weight of the different chemical bonds to give a detailed description of the fuel. Such level of detail is given by the HydroCarbon Profiling (HCP) approach [1].

Figure 8 shows an example of how it is possible to easily calculate HCP values from a hydrocarbon fuel made of three different molecules. The molecular information contained in the NIR spectrum is extracted and turned into a set of HCP values using advanced mathematics and deep understanding of fuels.

The absorbance of the fuel NIR spectrum is measured in the zones having the considered wavelengths. The values of absorbance measured for each selected wavelength are introduced into a mathematical/chemistry model which has been previously calibrated on a reference database, according to the known Chemiometrics rules so as to supply information to calculate the molecular structures of the fuel.

**Figure 8. HCP calculation Concept**

HCP are dimensionless and therefore cannot be compared to weight or volume percentage. The HCP approach is linked to the chemical bonds weighted by thermodynamic parameters such as combustion enthalpy and the bond dissociation energy. This approach also considers the impact of a type of component in the fuel mixture; the same kind of molecule having a different behavior depending on the blending recipe of the fuel. The [table 2](#) gives the meaning of different HCP.

HCP offer a way of separating and counting fuel components and their impact on combustion in more detail.

Limitation of Classical Approach

Products contained in the fuel are traditionally classified in different families:

- Saturated hydrocarbons (called linear paraffins, iso-paraffins and Naphtenics)
- Unsaturated hydrocarbons (called olefins and aromatics)
- Oxygenates (such as water, ethers, esters, alcohols...)

The product composition of a fuel is usually determined by means of gas chromatography using a standard method

[17] which consists in separating (Linear) Paraffins, Iso-paraffins, Aromatics, Napthenics, Olefins and Oxygenates.

Some others methods [18-19] were specifically defined in the last decade and became worldwide standards to cope with new formulation of Gasoline products with oxygenate base stocks such as alcohols and ethers.

The standard gas chromatography (GC) method classifies the benzene in the aromatic family, but this method also classifies e.g. the Isopropyl benzene (Cumene) and normal-propyl benzene as members of the Aromatic family.

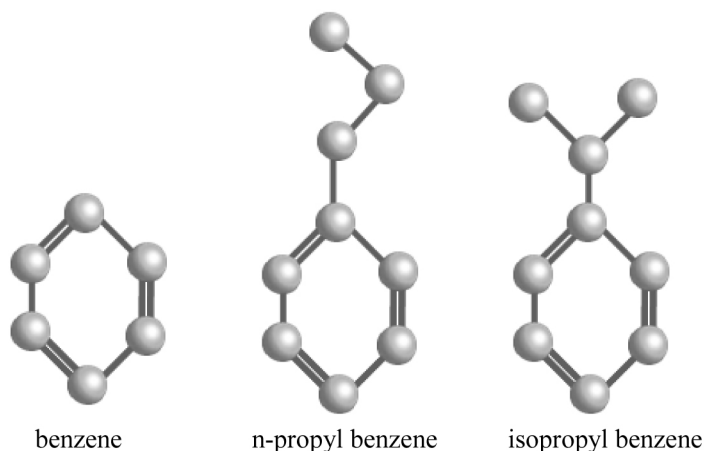


Figure 9. Molecular structure arrangement of benzene, n-propyl benzene and isopropyl benzene

However, as shown in [Figure 9](#), those molecules combine two chemical aspects: the aromatic and the Iso-paraffin for the cumene (isopropyl benzene); the aromatic and linear paraffin for the n-propyl benzene. This dual aspect inside one molecule impacts combustion. For instance, the self ignition delay of those three components, that are classified inside the same Aromatic family by the standard GC method, are significantly different:

- Benzene: ~12msec
- Iso Propyl Benzene: ~8msec
- N Propyl Benzene: ~7msec

The behavior of those components during the combustion is different. So the common and standard classification method does not provide sufficient information to understand combustion in details.

[Figure 10](#) illustrates the difference between the HCP and standard PIONA approaches.

While the standard GC approach classifies n-butyl benzene in the aromatic family, the HCP approach highlights both the aromatic and the linear characteristics of this compound. The different reactions (radical's formation) during the combustion process are accounted for by weighting the HCP with thermodynamic parameters. [20]

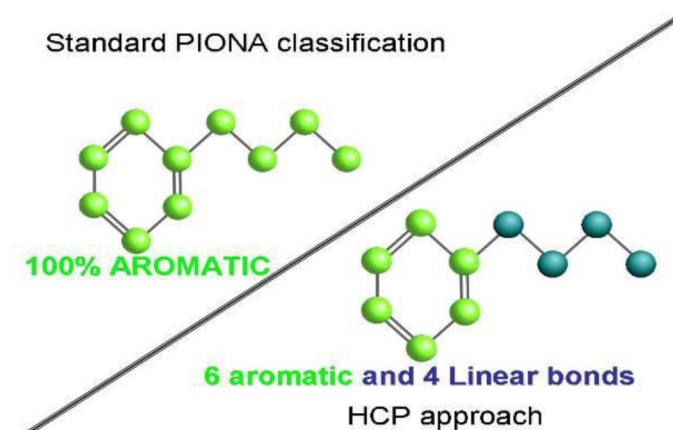


Fig. 10. Classification difference between Standard and HCP approaches

HCP Validation

From this new set of data, it becomes possible to select different combination of HCP to understand fuel molecular structure variation:

HCP linearity

In the following example, HCP trends are used to compare 4 mixtures between n-hexadecane and n-heptane blended at 60%, 65%, 70% and 75%. In HCP SAT and HCP LIN plot including gasoline and diesel world wide area, the four mixtures are represented by a red cross as proposed [figure 11](#).

All of the samples are gathered in the same “small” area with a value of HCP_SAT set at 1 (i.e. 100%) which mean that the products do not contain any unsaturated bonds.

One of the advantages of the molecular approach is the linearity of a component mixture making it easier to compare fuels together. [Figure 12](#) describes this accuracy using HCP_ISO and HCP_LIGHT.

[Figure 13](#) shows a representation of the 4 blends in HCP_LIN and HCP_LIGHT graph with a zoom in the diesel database including synthetic fuels boxes. It provides a clear alignment of the ramp with a lowest value of HCP_LIN and HCP_LIGHT for the 75% n-heptane blend (HCP_LIGHT is minimum with C4 molecules).

According to fuel quality and formulation, linear correlations can be observed between emission reduction and the HydroCarbon Profilers values.