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Revisiting diesel fuel formulation from Petroleum light and middle refinery streams based on optimized engine behavior

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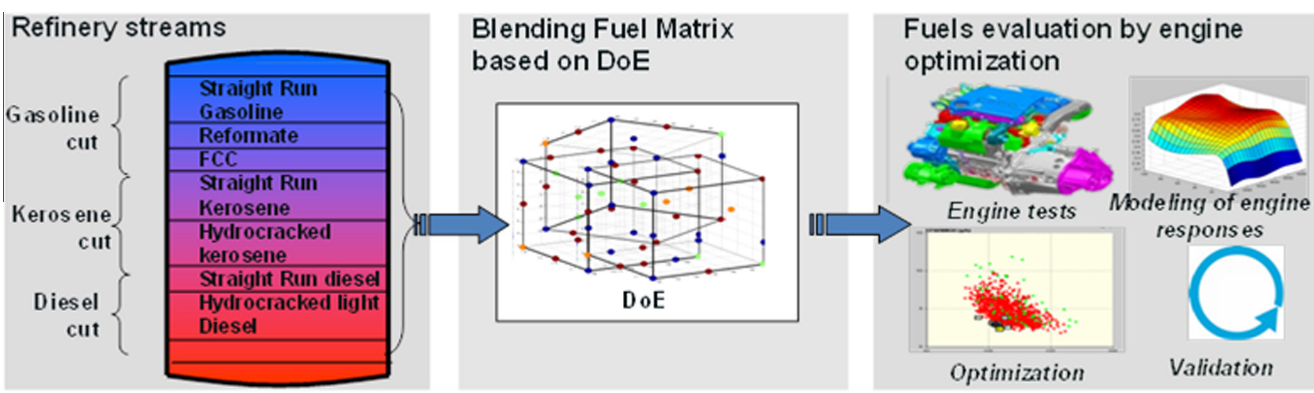
GRAPHICAL ABSTRACT



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ABSTRACT

The share of diesel fuel in European transport sector, which currently represents over 50% of total demand, is increasing, requiring massive imports of this product, while at the same time, gasoline fuels are today in surplus. In terms of air pollutant emissions, gasoline and kerosene streams have shown potential in achieving lower emissions in Compression Ignition (CI) engines, particularly nitrogen oxides (NOx) and particulates. A new fuel formulation approach through the use of light fractions within diesel technology could consequently address both questions of energy demand balance and reduction of diesel engines pollution footprint. In this study, a fuel formulation for a Diesel engine is optimized to achieve lower pollutants emissions and higher engine efficiency. The fuel matrix is based on seven refinery streams representative of gasoline (Hydrotreated Straight-Run Gasoline HSRG, Hydrotreated Fluid Catalytic Cracking HFCC and Reformate REF), kerosene (Hydrotreated Straight-Run Kerosene HSRK and Hydrocracked Kerosene HCKK) and diesel cuts (Hydrotreated Straight-Run Diesel HSRD and Hydrocracked Light Diesel HCKLD). A D-Optimal mixture design is applied to build, a 12-run, 7-factor fuel matrix and the fuels are thoroughly optimized on two engine conditions at light and mid-load representative of typical vehicle running conditions. The results show a high sensitivity and a good correlation of the engine efficiency and pollutants emissions with the volumetric contribution of each refinery stream to the fuel composition. The optimum fuel composition varies across the range of engine operating points. At light load for example, the addition of up to 50 vol% of gasoline streams (HSRG and HFCC) to diesel streams demonstrates a good potential to simultaneously reduce NOx and particulate emissions

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and an overall good engine performance. Reformate, a highly aromatic gasoline stream, did not offer an advantage at any of the tested conditions due to high particulate emissions. The two kerosene streams perform similarly to diesel streams in terms of engine efficiency and pollutants emissions. A compromise fuel, composed of 50 vol% HSRG and 50 vol% HSRD, is proposed that allowed halving NOx and particulate emissions and reducing the fuel consumption by 5 wt% compared to reference diesel HSRD. The optimized fuel represents an alternative for balancing diesel and gasoline demand and for pollutant emissions reduction.

1. Introduction

Energy and environmental concerns are driving several changes in the European transport sector, with increasing incentives towards alternative renewable energy sources and new refining processes. However, conventional fossil fuels remain the sector's major energy source. Conventional liquid fuels represented 95% of European demand in 2012 [1] and according to recent forecasts from the European Commission, are likely to remain dominant over the coming decades [2]. For transport applications, the share of diesel fuel represents over 50% of the European market (in comparison with gasoline and jet fuel, 32% and 14% respectively) and demand is rising [2]. The main drivers for such high demand are the high efficiency of diesel engines and recent improvements of after-treatment systems, noise and drivability. Conversely, light products like gasoline cuts, issuing from straight run distillation or Fluid Catalytic Cracking (FCC), a conversion process widely used in European refineries, are today in surplus. This has drawn much attention to their use as an alternative fuel in diesel engines to balance the energy demand and to meet future pollutant emissions legislation. To achieve pollutant targets for light duty diesel engines, several technological solutions are used to enhance the control of ignition timing and combustion rate [3] including variable compression ratio, adapted injection systems, improved piston geometry, increased exhaust gas recirculation (EGR) rates, and improved cooling or boosting capacity [4–7]. However, the physical and chemical characteristics of a fuel can have an important impact on mixture formation, ignition and heat release rate [8,9]. Higher volatility enhances the mixture formation during the ignition delay and a lower cetane number delays the ignition occurrence, mainly at low-to-mid loads [10]. Increasing fuel volatility in fuels of similar chemical composition has shown a soot reduction potential in CI engines for diesel and kerosene cuts due to the reduction of over-rich areas, and a moderate effect for gasoline cuts [11]. Increasing diesel volatility at equal cetane number [12] leads to a reduction of liquid film formation on cylinder walls, and thus, a reduction in smoke and enhanced fuel-conversion efficiency. The application of highly mixed combustion modes however presents the disadvantage of a load range limited by difficult combustion control at high load and an increase in HC and CO due to lower combustion efficiency [7]. Fuel wall impingement, the crevices, boundary layers, and fuel-lean regions formed during longer auto-ignition delay may constitute additional sources of HC and CO emissions [13–15].

2. Petroleum-based formulations for Diesel engines and impacts on pollutants

The use of gasoline or kerosene as alternatives to diesel fuel has been studied by several groups for their pollutants reducing potential. Han et al. [16] proved a simultaneous reduction of NOx and soot emissions using up to 40% gasoline with low EGR requirement compared to diesel fuel. CO and HC emissions were comparable to diesel engines at light loads, however increased at high loads [17]. Kerosene fuels are also attractive for their higher volatility and lower cetane number, generally between EU diesel and gasoline. Tested alone in compression ignition engines, kerosene presents lower NOx emissions than diesel at a similar soot level [18,19] and in mixture with diesel, it enhances the combustion efficiency [20]. The chemical effect of fuel formulation is difficult to separate from the physical effect, especially in complex engine configurations. Nevertheless, several general trends have been put forward in recent literature. Most usually, fuels containing high level of aromatics increase soot formation [10,21]. Diminishing the aromatic content generally correlates with particulate reduction for diesel, gasoline and kerosene distillation cuts [11]. Paraffinic saturated fuels have, in comparison, lower soot tendency regardless of their molecular structure [22,23]. Note however, the exception of fuels containing a high proportion of long-chain normal paraffins, which may lead to enhanced soot formation through increasing fuel ignitability and the creation of local rich areas [21]. Unsaturated hydrocarbons, namely, monoaromatics and short-chain olefins, can lead to over 2 and 5 folds higher NOx tendency respectively when compared to paraffinic saturated compounds [24]. Aromatic-rich fuels can have longer ignition delay times but can also form higher level of NOx towards the end of the combustion [25]. The safety question related to lighter fractions introduction in Diesel fuels has been recently addressed by Al-Abdullah et al. [26] where the flash points (FP) and volatilities of blends of a commercial diesel and a commercial gasoline were measured. According to their results, the flash point decreases as the concentration of gasoline is increased. For a mixture of 16 vol% of gasoline in diesel, FP reaches 40 °C. These results suggest that blends with high gasoline fractions should present very similar behavior compared with gasoline which has a FP of 45 °C.

3. Modeling approaches for fuel design

Optimizing a fuel's formulation for advanced combustion modes requires an accurate knowledge of the fuel's behavior over a wide range of engine operating conditions, both in steady state and transient modes. To better address these complex physical and chemical phenomena involved, statistical modeling approaches can represent powerful tools. Especially, Design of Experiments (DoE), refers to the process of planning, designing and analyzing the experiments. It involves the development of statistical relations between the response variables and the input factors and their interactions. In engine applications, DoE have been widely applied in engine optimization processes [27]. DoE has also been used to optimize fuel properties in terms of cetane number (CN), volatility and total aromatics content [28]. However, to our knowledge, few studies have used DoE to optimize the fuel formulation with regards to combustion behavior. In this study, we propose to evaluate a DoE approach to optimize fuel formulation for diesel engines based on existing refinery streams, to improve engine efficiency and reduce main pollutant emissions. Engine outputs were modeled as a function of the fuel composition and an optimum fuel is proposed.