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Relationship between fuel properties and sensitivity analysis of non-aromatic and aromatic fuels used in a single cylinder heavy duty diesel engine

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ABSTRACT

Fuel properties are always considered as one of the main factors to diesel engines concerning performance and emission discussions. There are still challenges for researchers to identify the most correlating and non-correlating fuel properties and their effects on engine behavior. Statistical analyses have been applied in this study to derive the most un-correlating properties. In parallel, sensitivity analysis was performed for the fuel properties as well as to the emission and performance of the engine. On one hand, two different analyses were implemented; one with consideration of both, non-aromatic and aromatic fuels, and the other were performed separately for each individual fuel group. The results offer a different influence on each type of analysis. Finally, by considering both methods, most common correlating and non-correlating properties have been derived. In case of combustion phenomena some heterogeneous combustion were measured as base study and investigations were continued with a partly homogeneous combustion to see the effect of fuel homogenization and influence of each non-correlating properties. Separate DoE (Design of Experiment) tests have been implemented for each fuel and DoE models were developed and analyzed. Constraint points from the models and measurements have been studied in more detail and sensitivity analysis has been conducted concerning engine emissions versus fuel properties. Results display a correlation matrix of fuel properties based on Pearson method as well as sensitivities of each fuel properties to each engine emission and performance in partly homogeneous combustion. Finally, sensitivity analyses present criterions to find out the impact of each fuel and properties at each operating point and to verify the relationship between properties and engine outputs. Furthermore, it is resulted that at homogeneous combustion the highest influence of fuel properties exist in the part load and low speed area of the engine map. For the sensitivity analysis, the most independent fuel properties were applied. Results show good approaches for the NOx and PM emissions by using partly homogeneous combustion at the part load points. Besides, this analysis highlights the influence of the most independent properties to the NOx and PM emissions in different area of the engine map.

INTRODUCTION

Energy crises, new local emission legislations for ICE and global emission control are the main sources to force and encourage automotive industries and research centers to focus on further development of the ICE as well as assessment of new fuel compositions for future engines. These efforts are being performed in strong collaboration between the industry, research centers and universities, fuel refineries and fuel research laboratories to

investigate the dominating key fuel properties and later on the new characteristic fuel numbers on one side and the engine combustion strategies on the other side.

The necessity to reduce the emissions, pollutants as well as CO2 from ICE's leads since many years to the generalization of diesel engines, whose one of the advantage compared to spark ignition engines is the lowest level of these greenhouse gases, which contributes to the climatic effects. However, diesel engines produce higher NOx and particulate matter (PM) emissions that leads to expensive, difficult and complex exhaust gas after treatment systems. That is the driver for continuous research, heading towards alternative combustion modes, which allow a drastic reduction of engine-out emissions at favorable fuel efficiency. One way to achieve these objectives is since long time homogeneous charge compression ignition (HCCI) combustion. HCCI operation is based on burning a homogeneous mixture of air fuel and burned gas (internal or external EGR) with reduced combustion temperatures. Furthermore, theoretically the HCCI process eludes locally lean high temperature regions and rich low temperature regions, compared to the combustion process for conventional diesel engines, thereby reducing NOx and particulate matter formation. In this regards, the fuel composition and properties represent an extremely important rule in case of combustion control.

Besides, fuel research opens a vast area of potential improvement, since combustion behavior and the nature of the combustion products can be substantially influenced by the fuel composition. Technically speaking, for the ''Heavy Duty Diesel Engine'' the area of conventional combustion engine have been researched and studied intensively during the past decades and most high technology engines will be introduced to the market which achieve the current requirements like EU VI in Europe and US2010 and US2013 emission legislation in the US. However, still there are potentials to provide lower emission diesel engines considering homogeneous combustion together with more efficient diesel fuels. In this case, the key diesel fuel properties and fuel numbers have to be well known and characterized.

Figure 1 shows developments of the emission levels in the past years. Developments are happening now (2010) for the EU VI and US10 emission legislations which are not only requesting for beneficial combustion system design on the engine side but also demanding high investments on the exhaust aftertreatment system to reduce engine-out emissions further to the legislated levels.

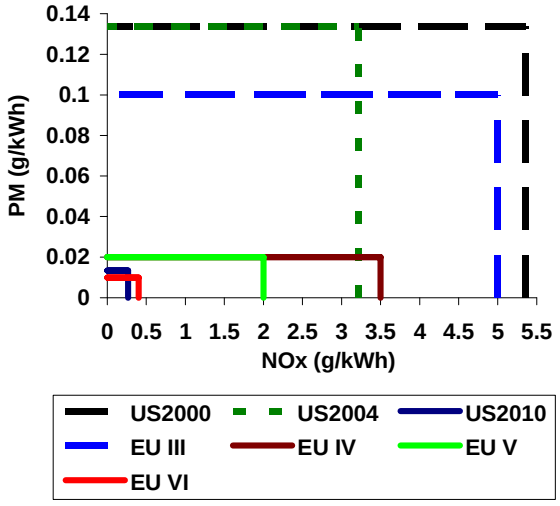


Figure 1 NOx- PM levels according to EU and US legislations

In this paper first the fuel matrix and the relevant properties will be explained. In the second part, relationship between fuel properties through statistical analysis will be presented and discussed. Later on DoE test results and finally with the help of sensitivity analysis, most important impact of independent fuel properties on NOx and PM emissions at different engine operation points will be presented. Deriving the most uncorrelated fuel properties would help to understand the impact of those properties on engine behavior irrelevant to the other properties which helps later on for fuel design.

SELECTED FUELS SPECIFICATION

Diesel fuel contains a large selection of hydrocarbons ranging from 10-22 carbon atoms per molecules. There are three major classes of molecules in diesel fuels: alkenes, cycloalkanes, and aromatics. Aromatics are known to increase oxides of nitrogen (NOx) emissions in conventional diesel combustion as they produce higher combustion temperatures **[1]**.

In total eleven types of different diesel, kerosene and naphthenic fuels were considered for this study. The idea of defining these fuels was to use different combination of aromatic fuels and paraffins, sorted with different cetane number to see the effect on partly homogeneous combustion. The different auto-ignition behavior is also a case of characterization of the different fuels. German Diesel fuel, which produces according to the EN590 diesel fuel standard, considered as the baseline fuel. These fuels have been chosen with a wide range of cetane numbers, considering also some aromatic and non-aromatic fuels. Figure 2 presents the main properties for these fuels. Three general types of different diesel fuels with diverse cetane number have been chosen as diesel fuels, two types of kerosene fuel, one fuel with aromatic content and the other non-aromatic fuel were also considered. Furthermore, two types of naphthenic fuel are selected and baseline diesel fuel based on EN590, as well as normal Heptane were included to generate a fuel matrix for this study. The fuels are divided to two main groups, namely ‘’Aromatic Fuels’’ and ‘’Non-Aromatic Fuels’’. In this paper, special nomenclature, namely AF1-6 and NAF1-3 have been used for Aromatic Fuel and Non-Aromatic Fuels respectively. Table 1 presents the main physical and chemical properties of the selected fuels and figure 2 shows distribution of the main properties for the fuel matrix. Besides, no cetane improver was applied to the fuels to get the higher cetane number.

FUEL PROPERTIES ANALYSIS

DISTILLATION

The distillation curve depends on the fuel chemical composition and, therefore, influences other properties such as viscosity, flash point, auto ignition temperature, cetane number and density. Lower Boiling points lead to faster evaporation and a faster mixture formation. It is clearly visible, that the reduced boiling temperatures results in a lower liquid penetration and a faster evaporation. In the engine, this will cause a faster mixture preparation **[2]**. Distillation curves for the selected fuels are illustrated in figure 3. Heptane has a constant boiling temperature and the baseline diesel has maximum T95, NAF2, 3 present the lowest boiling curve which is relevant to their naphthenic sources and the other aromatic and non aromatic fuels are in between. Slope of each curve has been defined to see the impact of sudden volatile behavior of such fuel like NAF1 with the kerosene sources. Slope is the temperature difference between T95 and T10.

Table 1 Selected fuel matrix and proper properties

Fuel Properties	unit	Aromatic Fuels						Non-Aromatic Fuels				Baseline
		AF1	AF2	AF3	AF4	AF5	AF6	NAF1	NAF2	NAF3	Heptane	
Molecular Formula	-	$C_{10.36}H_{20.65}O_{0.063}$	$C_{14.16}H_{25.53}O_{0.011}$	$C_{14.36}H_{28.03}O_{0.082}$	$C_{15.39}H_{29.51}O_{0.08}$	$C_{15.82}H_{30.53}O_{0.004}$	$C_{10.9}H_{19.9}$	$C_{11.02}H_{22.64}O_{0.016}$	$C_{8.39}H_{18.09}$	$C_{8.78}H_{18.61}$	C_7H_{16}	$C_{13.32}H_{24.52}O_{0.016}$
C- Distribution	-	C_7-C_{13}	C_9-C_{23}	C_{10}-C_{25}	C_{10}-C_{26}	C_{10}-C_{27}	C_7-C_{23}	C_7-C_{28}	C_7-C_{13}	C_7-C_{15}	C_7	C_9-C_{23}
St. AFR		14.61	14.47	14.56	14.52	14.65	14.50	14.80	14.97	14.92	15.14	14.51
Density @ 15°C	*kg/m³*	780.6	830.5	799.7	812.9	817.3	809.1	769.5	728.3	743.0	688.1	839.6
Viscosity @ 40°C	*mm²/s*	1.073	3.152	2.468	2.975	3.117	1.019	1.067	0.652	0.706	0.361	2.7
Cetane (CFR)	-	44.2	51.3	50.3	56.7	60.4	38.4	50.3	35.4	48.2	53	52.5
IBP	*°C*	158.7	148.4	192.2	205.7	229.8	153.3	150.2	87.0	92.2	95.4	169.1
T50	*°C*	176.7	274.2	244.0	272.1	275.0	172.2	165.1	116.5	127.1	95.4	266.9
T80	*°C*	187.7	304.3	289.3	296.8	296.6	194.0	172.8	135.2	146.5	95.4	311.2
T95	*°C*	209.7	352.3	317.6	323.6	321.6	257.0	308.3	149.8	161.5	95.4	348.5
Slope	*°C*	42.5	128.2	117.0	101.9	74.2	97.1	151.2	48.7	46.5	0.0	141.4
T95/T90	-	1.073	1.078	1.042	1.042	1.040	1.064	1.311	1.035	1.041	1.000	1.048
T95-T80	*°C*	22.0	48.0	28.3	26.8	25.0	63.0	135.5	14.6	15.0	0.0	37.3
LHV	*MJ/kg*	43.64	43.01	43.98	43.66	43.49	43.26	43.87	44.37	44.23	44.71	42.9
Energy Density	*MJ/l*	34.07	35.72	35.17	35.49	35.54	35.00	33.76	32.31	32.86	30.76	36.02
Mono Aromatics	*m %*	0.4	14.64	2.7	3.5	4.5	5.0	0.0	0.0	0.0	0.0	22.3
Di Aromatics	*m %*	0.0	1.48	0.1	0.0	0.1	13.2	0.0	0.0	0.0	0.0	3.9
Poly Aromatics	*m %*	0.0	1.59	0.1	0.0	0.1	0.1	0.0	0.0	0.0	0.0	4.5
Total Aromatic	*m %*	0.4	16.23	2.8	3.5	4.5	18.2	0.0	0.0	0.0	0.0	26.8
Mol mass	*g/mol*	146.3	196.0	202.1	215.9	220.8	151.1	155.4	119.0	124.2	99.0	185.0
C/H	-	5.98	6.61	6.11	6.21	6.17	6.54	5.80	5.53	5.62	5.20	6.45
ACN (Average Carbon Number)	-	10.31	13.86	14.29	15.28	15.63	10.65	10.96	8.36	8.73	6.93	13.07
Sulfur Content	*mg/kg*	<5	2	<5	<5	<5	<10	<10	<10	<10	0.8	7

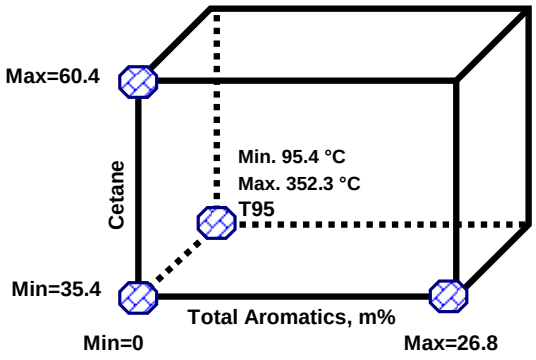


Figure 2 Distributions of Cetane, Aromatics and T95

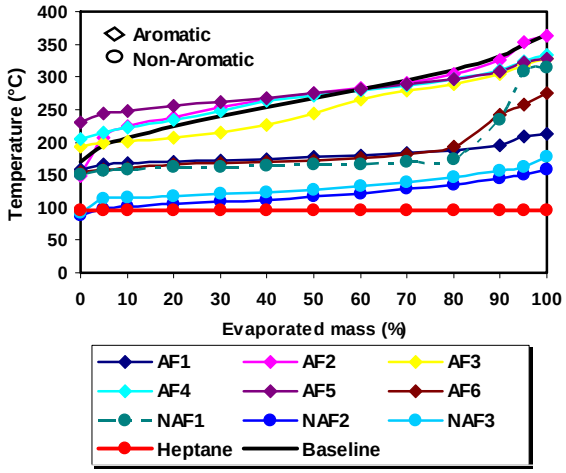


Figure 3 Boiling curves of different aromatic and non-aromatic fuels

Boiling curves of the aromatic fuels are in a higher range than non-aromatic ones. The reason is given by the higher average carbon content for aromatic fuels. Increasing of aromatic contents leads to have more complex fuel molecules instead of a certain straight chain molecules and causes higher boiling points. This can be explained by considering figure 4. However, there is an exception for AF6 fuel due to the lower cetane number, which causes a longer ignition delay. AF6 is a kerosene fuel and its boiling curve steeply increased at 80% evaporation.

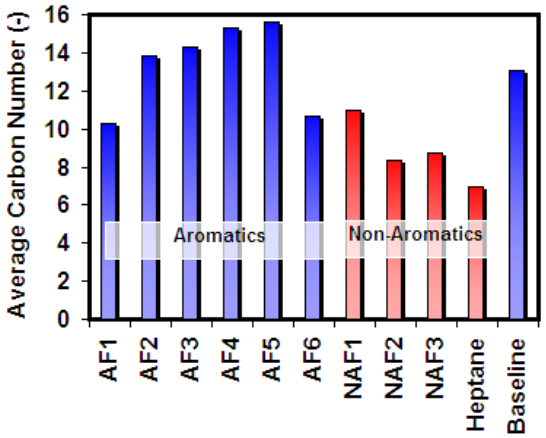


Figure 4 Average carbon number for all fuels

AROMATIC CONTENT

Figure 5 depicts the different aromatic contents of the selected fuels. As obvious, all selected fuels have lower aromatic contents compared to the baseline fuel. Aromatic hydrocarbons are HC compounds containing one or more “benzene-like” ring structures. They are distinguished from paraffin and naphthenic, the other major HC constituents of diesel fuel, which lack such structures. Aromatic hydrocarbons are denser; they have poorer self-ignition qualities, and produce more soot in burning. Ordinarily, “straight run” diesel fuel produced by simple distillation of crude oil is low in aromatic hydrocarbons. Catalytic cracking of residual oil to increase gasoline and diesel production, however,

results in increased aromatic content. There is also some evidence that more highly aromatic fuels have a greater tendency to form deposits on fuel injectors and other critical components **[3]**. Such deposits can interfere with proper fuel-air mixing, significantly increasing PM and HC emissions. Polycyclic aromatic hydrocarbons (PAH) are included in a high number of compounds present in the group of unregulated pollutants emitted from vehicles. Aromatic fuels have also more energy density since they are denser than the non-aromatic. Figure 5 illustrates these discussed effects.
By looking at figure 6, it is clear that the non-aromatic fuels feature lighter carbon structures and a comparably low density, in the other hand aromatic fuels have more average carbon number and denser. Furthermore, distribution of the mono, poly and total aromatic in the selected fuels is shown in figure 7.

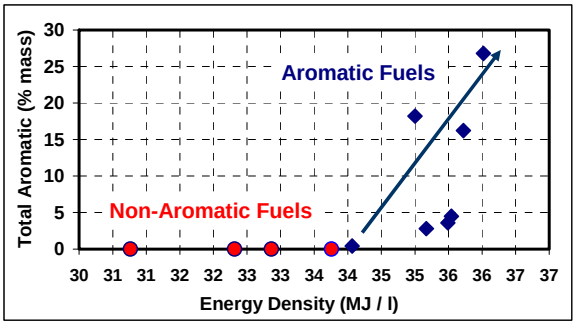


Figure 5 Total aromatic content vs. energy density

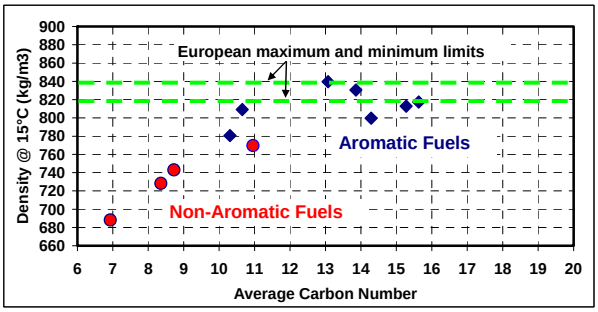


Figure 6 Density Vs average carbon number

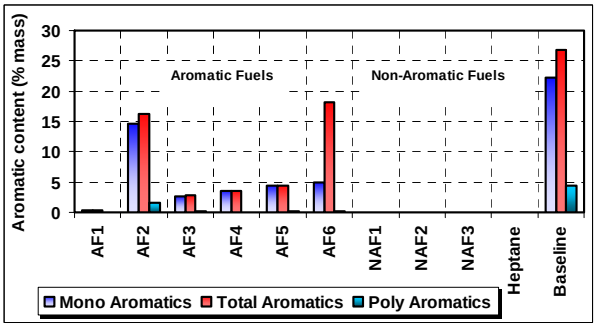


Figure 7 Aromatic content of the selected fuels

CETANE NUMBER

Selected fuels have a variety of cetane numbers with a minimum of 35.4 belongs to NAF2 (naphthenic fuel) and a maximum of 60.44 for AF5. As it's shown in figure 8, the higher

aromatic content does not lead to the lower cetane number as it's expected. The structure of the fuel molecule can be the reason of such behavior.

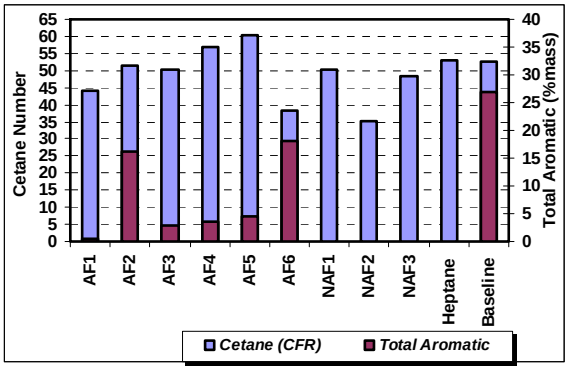


Figure 8 Cetane number and total aromatic content

DENSITY AND VISCOSITY

Fuel density represents an important fuel property with respect to volumetric fuel economy and maximum power. In general, the energy per unit volume increases with increasing density. Studies that decouple the effects of density from those of other fuel properties (e.g. aromatics) prove that it is also an important factor influencing regulated diesel emissions **[4]**. Figures 9, 10 show density and aromatic content and density-viscosity relations. Increasing aromatic content leads to higher density. Heptane is a very straight hydrocarbon, includes no aromatic content, without any branch in the molecular structure, and has the lowest density. Besides, naphthenic fuels (NAF2, 3) fuels have a low molar mass and a low average carbon number, thus low density. In summary, the density of fuels varied from 688 to 839 kg/m3, which mean an 18% variation. Viscosity in the other hand affects fuel spray atomization and fuel system lubrication. It also affects fuel system leakage. Kinematic viscosity affects the line pressure, leakage and friction of the plunger in the injection pumps. According to the European diesel fuel standard, EN590, viscosity of the standard diesel can be varied between 2.0 to 4.5 mm2/s. Elimination of the aromatic content from the fuel molecule leads to a dramatically drop-off of the viscosity afterwards.

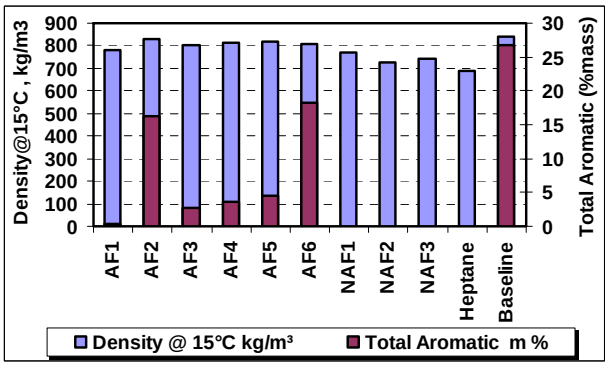


Figure 9 Density and total aromatic content

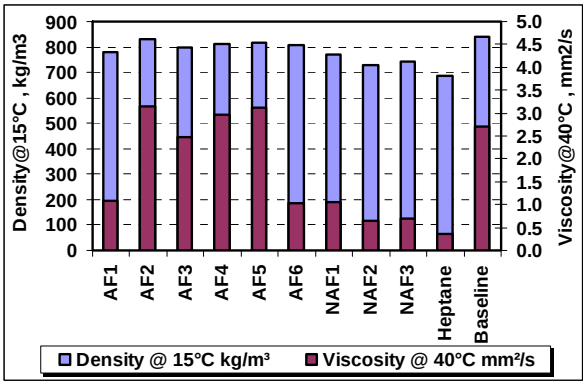


Figure 10 Density and viscosity

VOLATILITY, EVAPORATION SLOPE, MOL MASS

The volatility of a fuel determines the mixture formation in the combustion chamber, and thus the course of the combustion process. With the latest engine generations featuring low compression ratios and late injection timing, the boiling characteristics of fuels becomes more important for ignition and combustion behavior **[5]**. It describes the temperature at which 95% of the fuel is evaporated. Slope is the difference between T95 and T10 as it is described in figure 11.
On the other hand molar mass of the selected fuels are presented in figure 12. Relatively big differences can be seen in molar mass of the aromatic and non-aromatic fuels. Non-aromatic fuels are quite lighter in comparison with aromatic ones. Under consideration of such wide and distributed properties, it is mandatory to use a certain analysis to determine the independent and correlating fuel properties to be used for further investigations. In this case, sensitivity analysis for the fuel properties has been implemented.

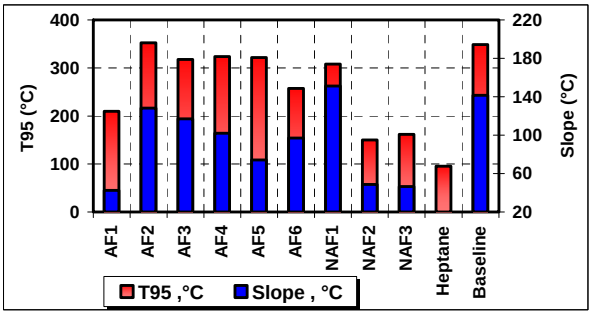


Figure 11 T95 and slope

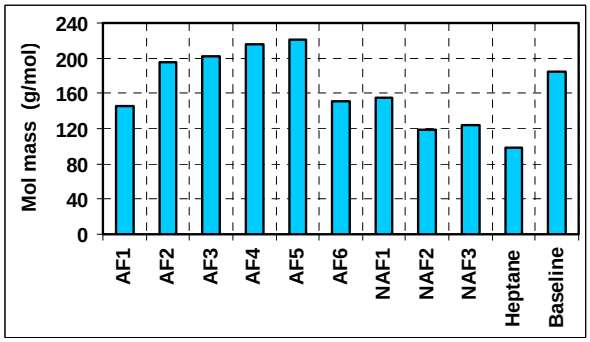


Figure 12 molar mass

SENSITIVITY ANALYSIS

Sensitivity analysis is a technique to determine how different values of an independent variable will affect a particular dependent variable under a given set of assumptions. Sensitivity analysis is very useful when attempting to determine the impact the actual outcome of a particular variable will have if it differs from what was previously assumed (in our case, what we considered for the base line fuel properties). Terms such as influence, importance, ranking by importance and dominance are all related to sensitivity analysis **[6]**. First, calculation of change from the base for some properties will illustrate the importance of the sensitivity analysis. Figures 13-14 present an example of some fuel properties. They show a wide range of changes corresponding to the baseline fuel in molar mass as well as in aromatic content and cetane number.

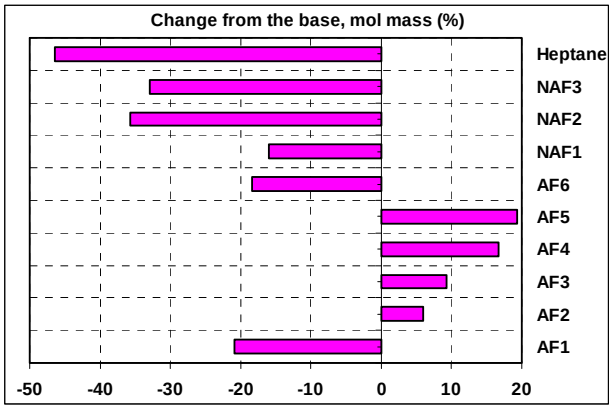


Figure 13 molar mass changes to the baseline

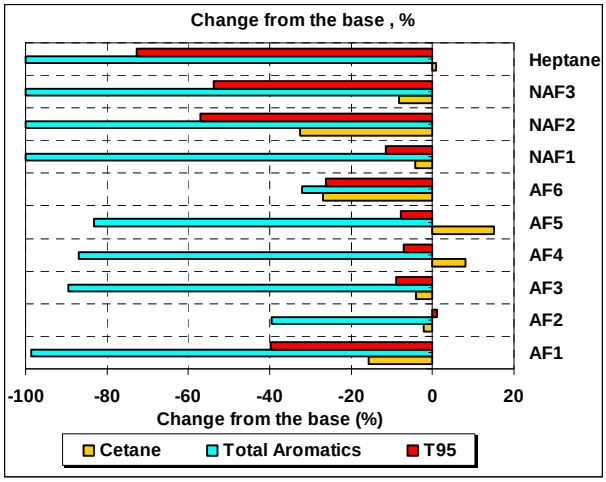


Figure 14 Aromatics and Cetane changes

Change from the base will give a picture of the variation inside the matrix to the baseline values. Wide changes for the molar mass can be explained based on the different fuel sources and structure and for the aromatic content, change of 100% represents of no aromatic content in these fuels. Significant changes in these diagrams show a complexity and importance of the analysis.

SENSITIVITY AND SENSITIVITY INDEX

To examine the relative importance of different fuel properties on engine output a normalized sensitivity function as described in equation 1 is used, where “y” is the variable and “x” denotes for the base point state.

A sensitivity index also delivers information about the relative sensitivity of the data to different parameters of the defined matrix. This measure indicates the relative importance of an individual input variable.

$$S_y^x = E_{x,y} = \lim_{\Delta y \longrightarrow 0} \frac{\frac{\Delta x}{x}}{\frac{\Delta y}{y}} = \frac{\partial x \times y}{\partial y \times x} \quad (1)$$

Sensitivity index can be illustrated by equation 2.

$$SI = (X_{max} - X_{min}) / X_{max} \quad (2)$$

Greater sensitivity index, indicates more dependency of the outputs to changes in that parameter. Sensitivity index is one of the key parameters to describe the importance of the properties. The main important properties of the used fuels are shown in figure 15. A high value of sensitivity index signals an important variable and vice versa. This figure shows aromatics, distillation, viscosity, molar mass and cetane number play main role in the fuel matrix. The AFRst, density and energy density seems to have less importance.

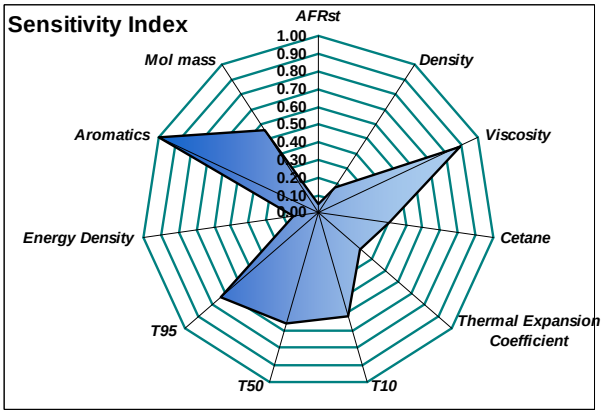


Figure 15 Sensitivity index for fuel properties

RELATIONSHIP BETWEEN FUEL PROPERTIES

Are there any correlations between diesel fuel properties? This highlights the main question, going to be answered using a certain methodology.
There exist many research efforts in different scientific areas to answer this question with different logics. Some of the researchers tried to create some correlations between diesel fuel properties and they proposed some correlations and equations **[7,8,9].** Other sources mentioned that some of fuel properties are somehow independent from each other. Researchers at refineries concluded, that depending on the feedstock, properties are changing and at refinery a certain diesel fuel considering utilization of the additives and some chemical processes can be produced.
Nevertheless, it is obvious, that some of certain properties like density and viscosity are not independent from each other.
Correlation between some of the diesel properties investigated by many researchers for example D. Karonis et al. **[10]** concluded that density, viscosity, aromatic and aniline point are quite dependant to each other with some correlations and constant values.
Testing these correlations illustrates a quite fit prediction to the standard and normal fuels, but as long as the diesel-like fuels, naphthenic and kerosene fuels showed up, correlations

are diverged and could not be used anymore. Figure 16 shows the implementation of the mentioned correlations to the current fuel properties to predict viscosity. It seems that a good prediction shown for baseline diesel and most of aromatic fuels, but for some kerosene and naphthenic fuels very diverse predictions are resulted.
Thus, an accurate study should be taken into account for each fuel matrix based on the significant fuel classification.

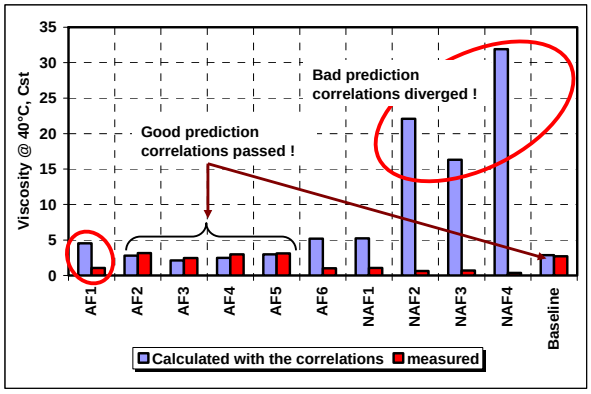


Figure 16 Prediction of viscosity using certain correlation

STATISTICAL ANALYSIS

For the current investigation first regression analysis has been considered as an initial step and to make sure that the inter-correlation of the properties are scientifically considered, work has been continued with Principal Component Analysis in different methodologies.

REGRESSION ANALYSIS

Regression analysis is the statistical technique that identifies the relationship between two or more quantitative variables: a dependent variable, whose value is to be predicted, and an independent or explanatory variable (or variables), about which knowledge is available. This technique is able to find the equation that represents the relationship between the variables **[11].** As it is shown in table 2, a normal regression analysis has been performed for some fuel properties to derive the most related properties as well as the independent ones. The highlighted numbers are mainly the most independent fuel properties.
In regression analysis, different variables have appropriate relation with the others. Mainly R^2 is the magnitude of effect, which is the model variation divided to total variation and it is the proportion of variance. The higher R^2 means the more dependency of the associated variables. In case of the current fuel properties, a linear regression analysis has been executed for the defined properties and the results, e.g. the magnitude of effect (R^2) inserted to the table 2 for comparison. The lower R^2 means the lower dependency between the two properties and vice versa.
Although regression analysis table shows some estimation for the correlating and non-correlating properties, but restriction of the regression analysis has to be considered in this stage to avoid any false interpretation. Regression analysis is likely to reach the conclusion that there is a strong link between two variables or there is not, whereas the influence of other, more important variables might not be estimated. This could provide errors for later studies.

Table 2 Correlation matrix of the normal regression analysis for the main fuel properties

Regression Analysis	Density	Viscosity	Cetane No.	Cetan Index	T10	T50	T90	T95	Energy Density	Mono Aromatics	Poly Aromatics	Total Aromatic	Slope
Density	1.00												
Viscosity	*0.48*	1.00											
Cetane No.	***0.09***	*0.39*	1.00										
Cetan Index	***0.06***	*0.42*	0.68	1.00									
T10	0.82	0.87	*0.37*	*0.37*	1.00								
T50	0.83	0.96	*0.34*	*0.37*	0.96	1.00							
T90	0.91	0.88	***0.22***	***0.21***	0.90	0.94	1.00						
T95	0.86	0.76	***0.21***	***0.16***	0.83	0.84	0.96	1.00					
Energy Density	0.99	0.75	***0.11***	***0.08***	0.85	0.86	0.93	0.87	1.00				
Mono Aromatics	0.50	*0.49*	***0.07***	***0.01***	*0.31*	*0.41*	*0.49*	0.50	*0.43*	1.00			
Poly Aromatics	*0.31*	*0.36*	***0.04***	***0.00***	***0.15***	***0.25***	***0.28***	***0.25***	***0.25***	0.87	1.00		
Total Aromatic	*0.47*	***0.24***	***0.00***	***0.03***	***0.19***	***0.23***	*0.36*	*0.37*	*0.40*	0.78	0.60	1.00	
Slope	0.63	*0.48*	***0.04***	***0.01***	*0.40*	*0.49*	0.67	0.76	0.60	0.70	*0.44*	0.56	1.00

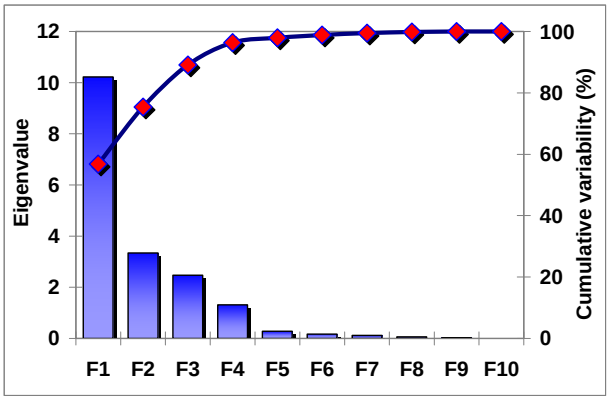
PRINCIPAL COMPONENT ANALYSIS (PCA)

Regression analysis can help in determining the underlying relationships between fuel specifications, chemistry, and engine performance. Principal Component Analysis (PCA) is used as preferable engineering tool to regression analysis in this work, because of its ability to deal with co-linear variables, which have the relationship to each other and potential to uncover “hidden” relationship between the variables. PCA introduced by Pearson (1901) and Hotelling (1933) **[12]** to describe the variation in a set of multivariate data in terms of a set of non-correlating variables. The privilege of PCA is to consider in such a way, that most of the important dimensions will be involved. Especially in diesel-HCCI engines, fuel is ignited kinetically and fuel properties or chemistry play a more effective rule than in conventional engines where ignition is controlled by injection timing. PCA has several advantages as an adjunct to conventional regression analysis for the type of study examined in this investigation. Principal component analysis (PCA) is a mathematical method designed to reveal the relationship between two or more (often many) variables. This analysis determines the significance of the correlations of the variables. By using PCA, useful information from multivariate elemental properties can be extracted as well and it can assist to reduce the dimensionality of a data set while retaining most of original information in the data **[7].** Principal Component Analysis helps to determine these relationships for many elements and properties simultaneously. It offers a technique to reduce the information dimensionality of a dataset consisting of a large number of interrelated variables obtained from a combinatorial experiment. Utilization of this analysis on a well organized database by projection methods can be performed, in a way that minimizes the loss of information, especially for the fuels with certain physical and chemical properties as well as different composition and different fuel molecular structure in the current fuel matrix. A PCA model designed for the current fuel properties including physical and chemical properties. In PCA, new variables known as “Eigenvectors” are constructed as combinations of the original variables in such a way that the new variables are orthogonal and independent of each other. In favorable circumstances, the “Eigenvectors” represent identifiable and distinctive features present in the data that are sufficiently generic as to support the understanding of the physical processes at play.

Table 3 shows the correlation matrix for the selected fuel properties. It is obvious, that the mol mass and ACN (Average Carbon Number) are positively correlating (r=1). Either of the two variables could have been removed without effect on the quality of the results. On the other hand, cetane number and total aromatic in the current fuel matrix have more or less no correlation to each other and they can be considered as independent properties (r = 0.01). The other important table and the corresponding chart are related to a mathematical object, the “Eigenvalue”, which reflect the quality of the projection from the N-dimensional initial table (N=18 in our case) to a lower number of dimensions. It can be seen that the first “Eigenvalue” equals 10.225 and represents 56.8% of the total variability. This means that if the data represent on only one axis, it could still be able to see 56.8% of the total variability of the data. Each “Eigenvalue” corresponds to a factor, and each factor to a one dimension. A factor is a linear combination of the initial variables, and all the factors are non-correlating (r=0). The “Eigenvalue”, and the corresponding factors, figure 17, are sorted by descending order of how much of the initial variability they represent (converted to %). Ideally, the first two or three “Eigenvalue” will correspond to a high percentage of the variance, ensuring that the maps based on the first two or three factors are a good quality projection of the initial multi-dimensional table **[13]**. In the study for all fuels, the first two factors allow us to represent 75.37% of the initial variability of the data. Same analysis can be implemented for aromatic and non aromatic fuels. In this case, fuel matrix divided to two groups and for each group certain PCA analysis performed. Correlation matrices present in appendix and will give a significant comment that with each fuel matrix consideration the results can be a bit varied and need to be taken into account for the further analysis. From this separate investigation, common correlating properties are derived. An example of some non-correlating properties is shown in figure 18. Cetane number shows less inter relation with density and no relation to slope, LHV aromatics and C/H ratio, although these properties can have relation with each other. For further study if cetane selected then these properties can be chosen separately with cetane as non-correlating properties.

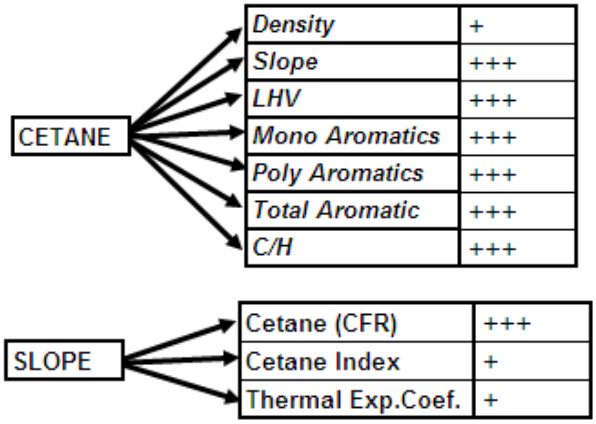
Table 3 Correlation matrix for PCA analysis for all fuels

Fuel properties	Density @ 15 °C	Viscosity @ 40°C	Cetane (CFR)	Cetane Index	T95	Slope	T95-T80	LHV	Energy Density	Mono Aromatics	Poly Aromatics	Total Aromatic	Mol mass	C/H	ACN
Density	**1**														
Viscosity	**0.84**	**1**													
Cetane	0.31	**0.64**	**1**												
Cetane Index	0.24	**0.70**	**0.82**	**1**											
T95	**0.92**	**0.87**	0.46	0.40	**1**										
Slope	**0.76**	0.59	0.19	0.09	**0.89**	**1**									
T95-T80	0.27	0.01	-0.04	-0.26	0.46	**0.71**	**1**								
LHV	**-0.93**	**-0.68**	-0.17	-0.03	**-0.81**	**-0.69**	-0.32	**1**							
Energy Density	**0.99**	**0.86**	0.33	0.29	**0.93**	**0.76**	0.26	**-0.89**	**1**						
Mono Aromatics	**0.69**	**0.62**	0.24	0.13	**0.62**	0.57	0.05	**-0.80**	**0.64**	**1**					
Poly Aromatics	0.51	0.43	0.18	0.02	0.45	0.48	0.03	**-0.64**	0.46	**0.94**	**1**				
Total Aromatic	**0.69**	0.45	0.01	-0.12	0.54	0.54	0.14	**-0.83**	**0.62**	**0.91**	**0.83**	**1**			
Mol mass	**0.86**	**0.96**	0.60	**0.65**	**0.91**	**0.64**	0.14	**-0.66**	**0.90**	0.45	0.26	0.34	**1**		
C/H	**0.96**	**0.73**	0.13	0.09	**0.84**	**0.71**	0.27	**-0.95**	**0.94**	**0.70**	0.48	**0.77**	**0.74**	**1**	
ACN	**0.86**	**0.96**	0.60	**0.65**	**0.91**	**0.64**	0.14	**-0.66**	**0.90**	0.45	0.26	0.34	**1.00**	**0.74**	**1**



	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10
Eigenvalue	10.225	3.342	2.468	1.312	0.280	0.163	0.120	0.061	0.028	0.001
Variability (%)	56.805	18.564	13.709	7.289	1.558	0.904	0.668	0.341	0.154	0.008
Cumulative %	56.805	75.369	89.078	96.367	97.925	98.830	99.497	99.838	99.992	100

Figure 17 Eigenvalue and factors



+++: strongly uncorrelated, | r | <0.3

++: uncorrelated, 0.3 < | r | <0.4

+: weakly uncorrelated, 0.4 < | r | <0.5

Figure 18 Some uncorrelated properties for the current fuel matrix

TEST BENCH CONDITIONS AND TEST PROCEDURE

Figure 19 depicts the layout of the test bench. Engine received an external charge through an external charging system equipped with a 3-stage screw compressor, which is cooled through an intercooler and mixed up with EGR gas before inducting to the engine. Air and fuel mass flow measured directly at the test bench and via a special injection control device, so called IBC, the injection pattern was controlled. During the tests centre of combustion was controlled especially for DoE tests to impose the same centre of combustion for all different fuels. By these adjustments beginning of main injection has been influenced by centre of combustion. EGR rate could be also adjusted by exhaust back pressure valve.

ENGINE SPECIFICATION

The engine assembled with a cylinder displacement volume of 2.136 liters, based on the MAN D28 series of engines. The compression ratio lowered to 15.2 from 17.5 for the purpose of homogenous combustion.

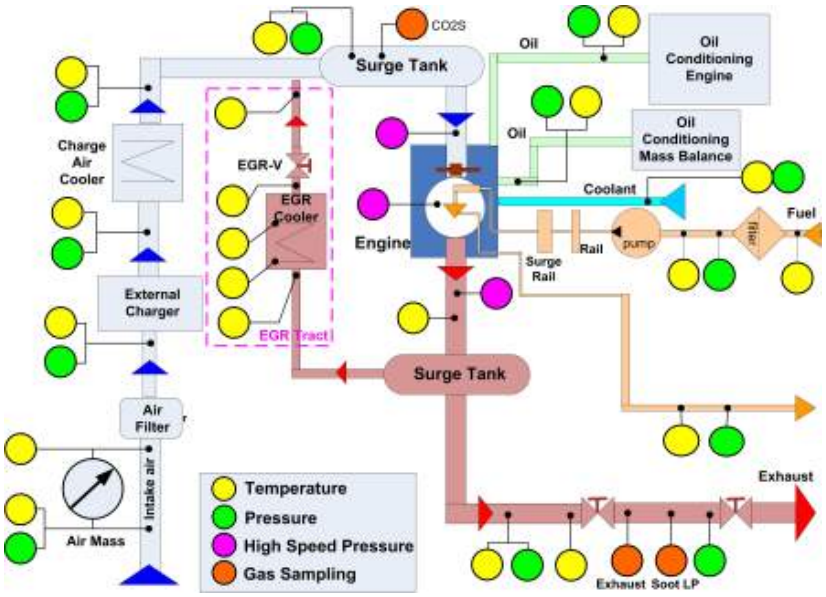


Figure 19 Test bench set up

Table 4 Specification for the Single Cylinder Engine

TECHNICAL SPECIFICATION	*Value*	*Unit*
Engine displacement	2.1361	L
Piston stroke	128	mm
Bore diameter	166	mm
Compression ratio	15.17:1	-
Valves per cylinder	4	-
Max cylinder peak pressure	200	bar
Fuel injection system	Common Rail System	
Maximum injection pressure	2000	bar
Hydraulic flow rate (HD)	1400	cc/min
Number of spray holes	6	-
Hole diameter	0.207	mm
Spray cone angle	80	deg
Charging method	External , compressor	
EGR system	External EGR+ Cooler	

The measurement systems include cylinder pressure, inlet and exhaust manifold pressure indication. The injection parameters rail pressure and injector current signal are also recorded using high-speed data acquisition. Further, a variety of pressures and temperatures for monitoring and control are displayed and recorded at 5 Hz. Hydrocarbon emissions are measured using an FID (Flame Ionization Detector), while a CLD (Chemiluminescence Detector) is employed to measure NOx emissions. Particulate emissions are only indirectly measured, in that the Smoke Number using an AVL Smoke meter (heated) is used to correlate the particulate mass.

HOMOGENIZATION

The A and C (1220 and 1780 1/min) speeds were chosen from the European Stationary Cycle (ESC) for detailed analysis. The homogeneous operating region was estimated to lie between the 25% and 70% load range corresponding to each speed. DoE tests have been performed by variation of EGR rate, boost pressure, rail pressure and start of injection for pilot injection as DoE parameters. At the full load points, only heterogeneous tests were executed. First, main injection optimization was conducted first. At part load points no

limitation of peak firing pressure was expected, resulting in an early main injection around 30 ° CA before TDC. During course of investigation more advanced injections were also investigated. At full load, injections happened at maximum 10 °CA before TDC, due to peak pressure limitation. The desired load was set with the main injection. Then the first pilot was introduced from 95° CA as earlier than this would result in fuel liner contact. The quantity of pilot injection was varied making sure that the load remains constant. This was done to avoid considerable engine load of the pilot quantity. Ideal was to inject as much fuel as possible in the pilot injections to increase homogenization.
A second pilot was established, keeping an average 10° CA distance between two injections. This distance was calculated based on time for full needle opening and closure.
With a very early pilot, a high CO and HC were produced which gave an idea of wall contact, so pilots were shifted towards late. A low NOx was a direct result of early pilot as it helped reduce the peak temperatures. To produce low smoke values, rail pressure variations were investigated and the beneficial pressure was adjusted as optimum. Post injection helps to reduce high smokes. At A25 and C25 points, post injections were not engaged, as the smoke values were already very low and a post injection would have caused a higher NOx generation. The main injection was already very early giving sufficient time for oxidation of particles. High EGR rates were considered to reduce the NOx and at the same time the boost pressure was increased to offset high values of smoke. Optimization was tried between the two parameters as well as timing to get best setting. Various injection strategies with respect to injection timing was tested and evaluated based on NOx, smoke, fuel consumption, CO, HC and combustion stability. Noise was also taken as additional criteria for the entire investigation. Figure 20 shows the full load curve of the engine together with the selected points for investigation. For each operation point, the utilized injection pattern is also mentioned. At A100 and C100 operating points , heterogeneous combustion were implemented and for A25, C25, A70, C60 points partly homogeneous combustion were introduced. The dominating criterion for the injection strategy is described in figure 20. For each selected operating point, most of fuel matrixes have been tested , DoE test implemented and the proper model have been analyzed. Highlighted points are the selected DoE points. The main injection was varied to the point where the heat released has reached 50%, i.e. CA50. Because of limitation in some fuels all DoE tests have not been completely done at C60 point. As an example, a conventional heterogeneous combustion DoE model for C100 point is shown in figure 21. Model points are created virtually which are around 5000 points that surrounding the measured points, base point and validation points were measured at the test bench. Validation points were used for determining the accuracy of the model or the equipment respectively. Base point is also a start point or the available calibration status to begin the DoE Test. Optimization in this case performed for NOx at EU V level, i.e. lower than 3.5 g/kWh. It has to be also mentioned that for all fuels at defined operating points, the same DoE plan was applied to have the same influence of engine parameters for all fuels.

TEST RESULTS AND ANALYSIS

For each DoE test, 53 operating points with different combination of DoE parameters were tested and it was repeated with the same condition for the next fuel. PCA analysis determined the most uncorrelated fuel properties. Now the test results can be analyzed for engine outputs and engine outputs together with most independent properties which will be described in this session.
The main results are presented in figures 22 to 25 for both A25 and C25 points, as well as in figures 26 to 29 for C60 points respectively.

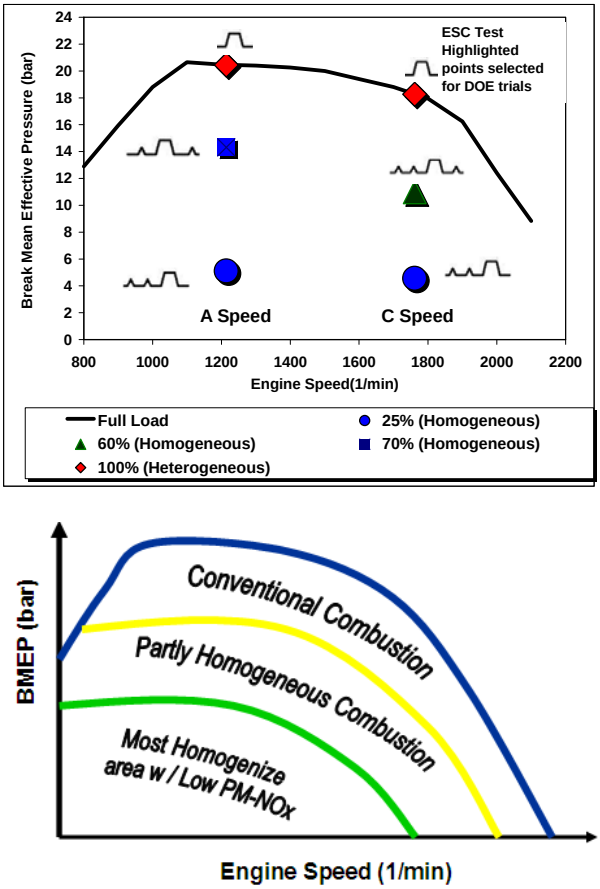


Figure 20 Selected operating point and the relevant injection strategy for DOE trials.

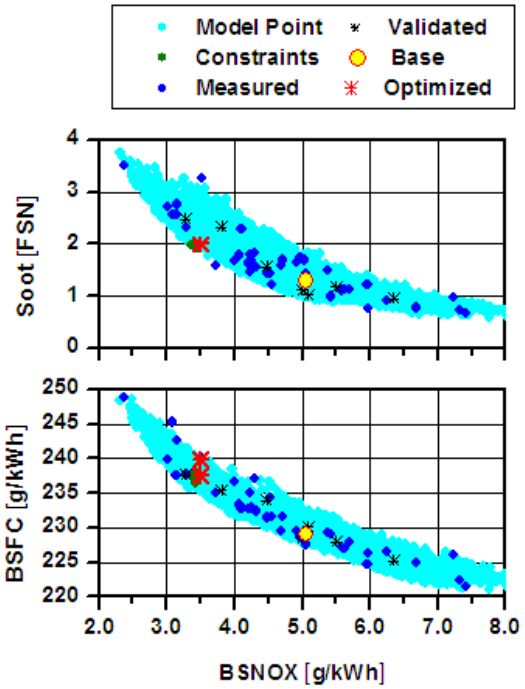


Figure 21 Example of DOE model optimization

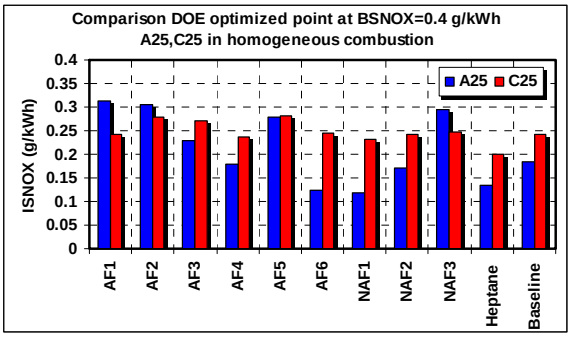


Figure 22 A25, C25, ISNOx optimization at BSNOx < EUVI

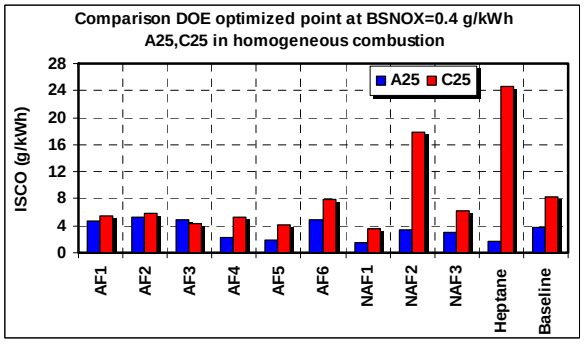


Figure 23 A25, C25, ISCO optimization at BSNOx < EUVI

Optimization at A25 presents a very promising homogenization achieved with a very low NOx and PM values, in case that a good premixed mixture and beginning of ignition was defined. All fuels show good potential to reduce NOx up to the EU VI level without any problem for particulates, whereas in figure 23 an acceptable carbon monoxide is also achievable. As soon as engine speed increased to C25, the particulates are increasing as the time for premixed mixture and premixed combustion is reduced. At C25, ISCO is increased dramatically for Heptane and NAF2 fuels. On the other hand PM value was highly increased for AF4, AF6, NAF2 and Heptane compared to the other fuels.

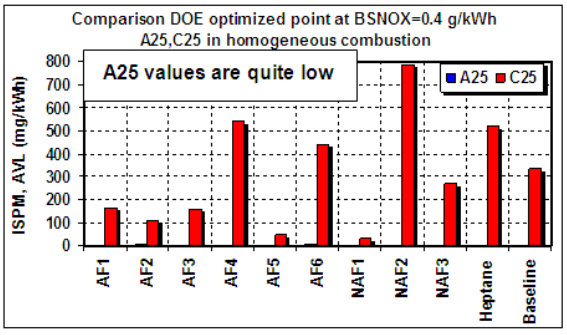


Figure 24 A25, C25, ISPM optimization at BSNOx < EUVI

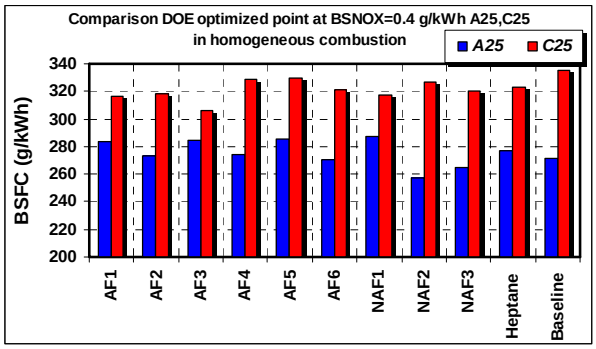


Figure 25 A25, C25, BSFC optimization at BSNOx<EUVI

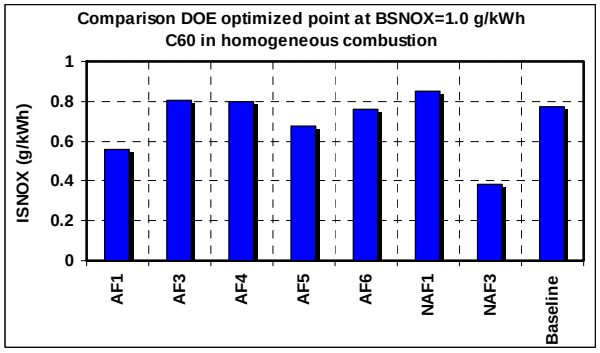


Figure 26 C60, ISNOx optimization at BSNOx = 1 g/kWh

At C60, one of the main important behaviors of all fuels is given by the reduction of particulate matter for all fuels compared to baseline fuel, which signals the potential of these selected specifications. Besides non-aromatic fuels show lower values for particulate than the others, however CO concentrations at these fuel types are higher. The main important idea to reduce the emission in this study focused on the NOx value. Reduction of engine-out NOx to EU VI level leads to reduce a huge investment in exhaust aftertreatment system. That is why within this study minimized concentration of NOx has been considered more than the other issues. Figure 30 shows the changes of the NOx at the same optimization to the baseline diesel fuel application.

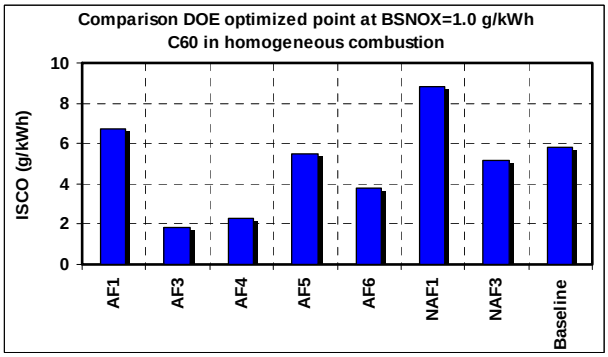


Figure 27 C60, ISCO optimization at BSNOx = 1 g/kWh

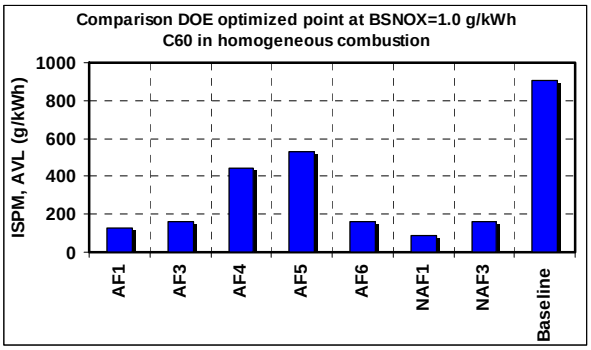


Figure 28 C60, ISPM optimization at BSNOx = 1 g/kWh

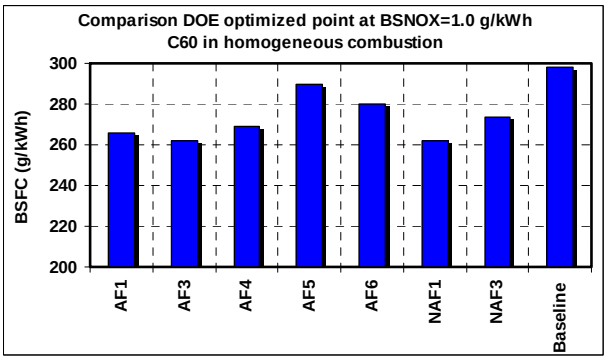


Figure 29 C60, BSFC optimization at BSNOx = 1 g/kWh

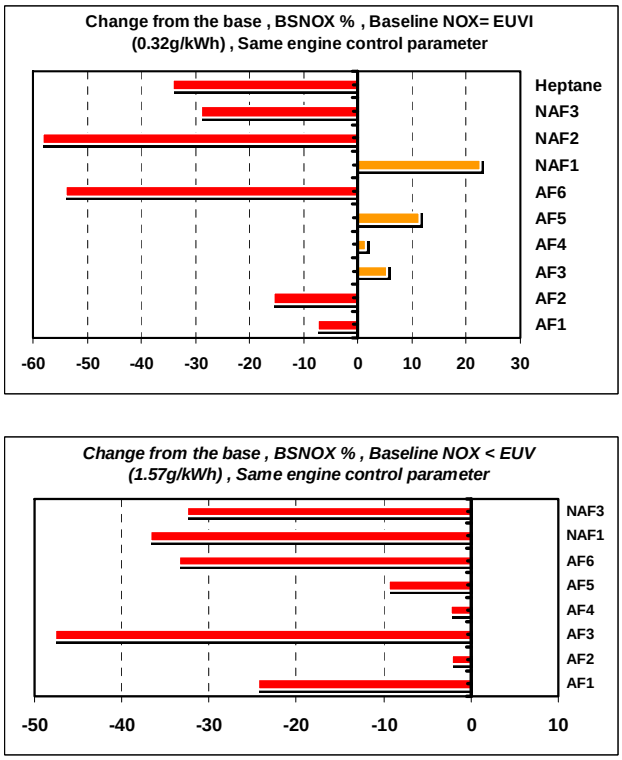


Figure 30 Changes of NOx compare to Baseline

In this analysis, the positive values are relevant to increment of the ISNOx to the baseline and the negative values shows the potential of the proper fuel to reduce the NOx with the same engine parameter setup and boundary conditions as for baseline diesel.

In figures 31-32 NOx and CO emissions versus cetane number are presented whereas it is also important to know the behavior of CO at low NOx conditions. It is clear, that by increasing cetane number at both operating points NOx will be increased, but the deltas of increment are not the same with increasing or decreasing the cetane number, it must be influenced by other facts, properties, which will be discussed by sensitivity analysis.

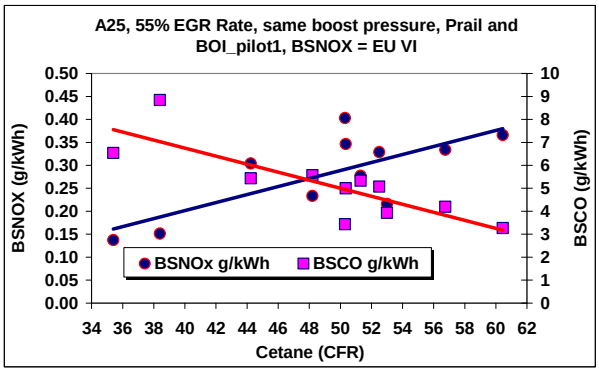


Figure 31 BSNOx, BSCO Vs Cetane at A25

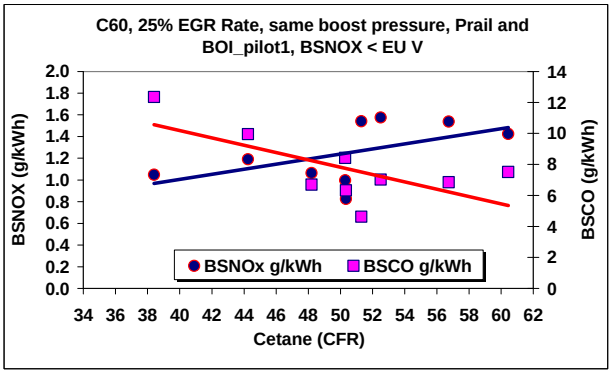


Figure 32 BSNOx, BSCO Vs Cetane at C60

The high cetane number fuels at 25% to 60% load in homogeneous combustion show an increment of NOx as the ignition delay decreased and the beginning of combustion advanced. Carbon monoxide decreased via early ignition and sufficient time for combustion in high cetane number fuels.

Results of the study indicate that the engine is capable to reduce the emissions, especially NOx to EU VI level at 25% load in a wide range of A to C speeds. At A speed and low load points a most homogeneous combustion could be established in order to define very early pilot injection and considering a well-prepared mixture. Increasing speed and load to C speed and load more than 50% causes a part homogeneous combustion up to 60% load in case of adjusting the NOx level between EU V and EU VI level. At A speed point partly homogeneous combustion achieved up to 70% load. More than 70% and 60% load at A and C speed respectively, conventional combustion applied and it was tried to keep the engine at safe and stable combustion.

Sensitivity indices are shown in figure 33-34 for both main operating points. A high value of sensitivity index signals the importance of the variables, in the given case, fuel properties in homogeneous combustion at these operating points and vice versa. It is obvious, that the BSFC has less sensitivity at both operating points to the fuel properties. For the emissions, especially BSNOx, A25 which has the highest homogeneity, is more sensitive to the fuel properties than at C60.

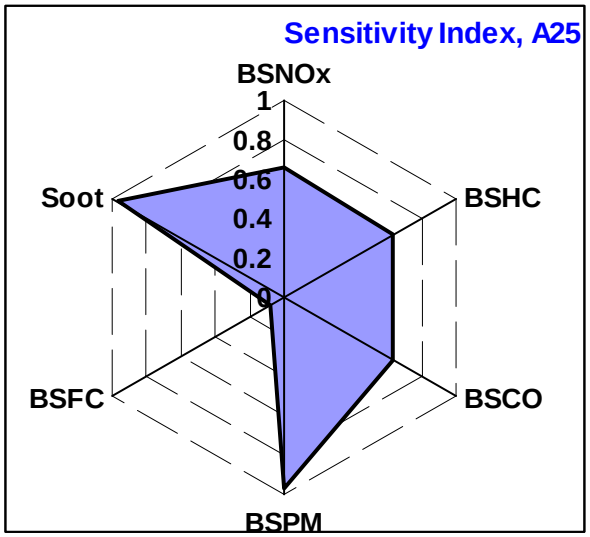


Figure 33 Sensitivity index at A25

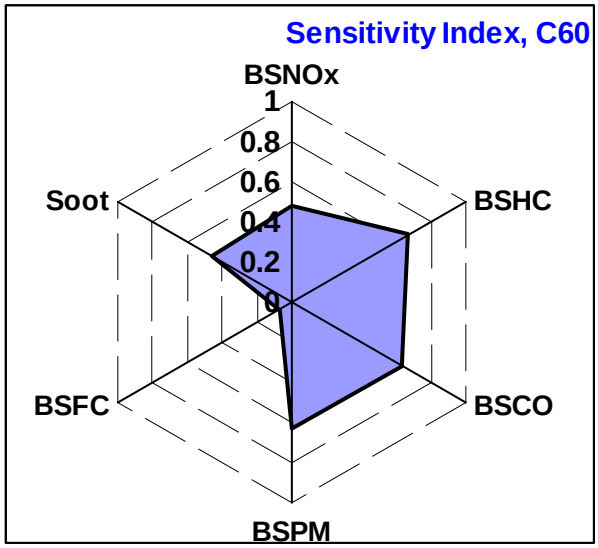


Figure 34 Sensitivity index at C60

To separate the impact of each property to the engine emission, the independent properties have been chosen for further analysis. As part of the analysis, the properties, which have the lowest inter-correlation to cetane number, picked up, which are presented in figure 35. The absolute sensitivity considered to avoid of any confusion and false interpretation.

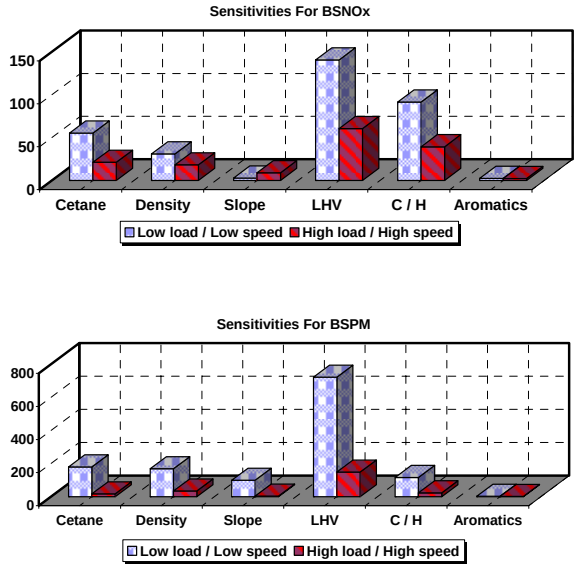


Figure 35 Absolute Sensitivity for NOx and PM

The higher sensitivity shows that even with small changes in this property a certain impact to the engine out emission would appear. For low heating value (LHV), fuels are not scattered in a wide ranges of values, however it influences the fuel energy and causes more effect especially at part homogeneous operation.
The magnitude of the numbers will give an idea of the peaks or the influences.

CONCLUSION

Heavy-duty diesel engines are using EGR in entire engine map and NOx reduction in new emission legislation is one of the big challenges, although there are benefits in using SCR systems, which have been so far developed and applied to these kinds of vehicles, but the cost issue is not negligible. This is why any alternative combustion strategy to reduce the engine-out emission with eliminating some of these aftertreatment systems is noticeable. This paper illustrated potential of some fuels for heavy-duty diesel engines. It was tried to configure the PCA method to derive the most non-correlating fuel properties, which are important later on for new fuel number study. It can be concluded that:

- Non-correlating properties can be derived from each fuel matrix if the analysis and interpretation run in a right way with correct analysis. If high numbers of fuels are available, then the analysis should be done for fuel matrix in several groups to get the best compromise for each fuel properties.

- Correlation between fuel properties can be first investigated by study of the refinery processes which have been implemented for significant matrix. However, some exceptions in case of special refine process as well as the feed stock properties are considerable.

- If any additive used to improve the cetane number or improve any other fuel property, the amount of additive has to be considered in fuel matrix for statistical analysis.

- Sensitivity analysis showed a good criterion to find out the impact of each fuel and properties at certain operating point and to verify the relationship between properties and engine outputs.

Sensitivity analysis for the current fuels considering the most independent properties results the following statements:

- ***Cetane*** number has a significant influence of NOx and PM values in homogeneous operation at low load / low speed area, however in high speed / high load area the influence is a lower.

- ***Density*** has also more impact at low load / low speed than at high load and speed operation point; especially the influence on PM is much higher.

- ***Slope (Boiling characteristics)*** has less influence of NOx but it features a substantial impact on PM at low speed and low load point. At high speed and load area no big influences were observed.

- ***Heating value*** impacts in both area but the influences on PM at low speed / load area is higher.

- ***Carbon to Hydrogen ratio*** has more impacts on NOx and PM at low load / speed area but the impact on high load / speed area is also considerable.

- ***Aromatics*** have no big influence in both areas at more homogeneous combustion. But it has to be highlighted, that the aromatic content of the investigated fuel matrix was not varied too much and the contents were significantly lower as for the baseline fuel.

It has been presented that up to 60-70% load , can be covered by part homogeneous combustion mode, which despite a very good NOx and PM advantages, can potentially offer an economically viable solution by eliminating the need for a complex after-treatment system i.e. SCR systems for NOx and diesel particulate filters (DPF's). For some fuels still there are problems for the high amount of carbon monoxide at part load points which can be covered by further calibration to find out the best compromise between NOx and CO. Further potential for improved emissions behavior can be tapped with the optimization of the engine hardware, combined with the use of higher EGR rates and boost pressure.

All fuels have lower aromatic content than baseline diesel. It has been confirmed that aromatic content in fuels is detrimental for PM emissions, even under part homogeneous conditions. The distillation curve, density and viscosity, which influence the mixture formation, also appear to play an important role in the result. It has been shown in these experiments that a low distillation curve, accompanied by low fuel viscosity delivers good performance. Besides low cetane number of NAF2 fuel causes higher particulate because of the longer ignition delay but the NOx values are always promising for such fuel.

It can be concluded, that the highest impact of fuel properties exist in the part load and low speed area of the engine map at more homogeneous combustion area. As soon as load is increased, the influence gets minor and at full load area, conventional combustion is dominant.

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DEFINITIONS, ACRONYMS, ABBREVIATIONS

ACN: Average Carbon Number

AFRst : Stoichiometric Air Fuel Ratio

BOI: Beginning of (Fuel) Injection

BSCO: Brake specific CO

BSFC: Break Specific Fuel Consumption

BSNOx: Break Specific NOx Emissions

BSPM: Break Specific Particulate Matter

C/H: Carbon to Hydrogen Ratio

DPF: Diesel particulate filter

DOE: Design of Experiments

EGR: Exhaust gas recirculation

FBP: Final Boiling Point

FSN: Filter Smoke Number

HCCI: Homogeneous Charge Compression Ignition

HFR: Hydraulic Flow Rate

IBP: Initial Boiling Point

ICE: Internal Combustion Engine

ISCO: Indicated Specific Carbon Monoxide Emissions

ISNOx: Indicated Specific NOx Emissions

ISPM: Indicated Specific Particulate Matter Emissions

LHV: Lower Heating Value

PCA: Principal Component Analysis

SA: Sensitivity Analysis

SCR: Selective catalytic reduction

Slope: T95 – T10, in °C

T10: 10% evaporation

T50: 50% evaporation

T95: 95% evaporation

APPENDIX:

Correlation matrix for Aromatic fuels:

Variables	Density @ 15 °C	Viscosity @ 40°C	Cetane (CFR)	Cetane Index	Thermal Exp. Coef.	T95	Slope	T95/T90	T95-T80	LHV	Energy Density	Mono Aromatics	Poly Aromatics	Total Aromatic	Diesel Index	Mol mass	C/H	ACN
Density @ 15 °C	1																	
Viscosity @ 40°C	0.661	1																
Cetane (CFR)	0.419	0.898	1															
Cetane Index	0.188	0.854	0.917	1														
Thermal Exp.Coef.	-0.384	-0.062	0.063	0.125	1													
T95	0.848	0.913	0.684	0.620	-0.254	1												
Slope	0.798	0.523	0.170	0.143	-0.331	0.816	1											
T95/T90	-0.158	-0.443	-0.619	-0.589	0.301	-0.399	-0.177	1										
T95-T80	0.372	-0.278	-0.593	-0.644	-0.652	0.045	0.417	0.440	1									
LHV	-0.772	-0.144	0.076	0.371	0.189	-0.354	-0.478	-0.392	-0.589	1								
Energy Density	0.949	0.808	0.595	0.434	-0.423	0.952	0.823	-0.406	0.206	-0.532	1							
Mono Aromatics	0.877	0.408	0.160	-0.077	-0.039	0.645	0.764	0.088	0.345	-0.857	0.740	1						
Poly Aromatics	0.750	0.294	0.129	-0.119	0.113	0.520	0.672	0.005	0.181	-0.758	0.619	0.958	1					
Total Aromatic	0.775	0.055	-0.213	-0.453	-0.360	0.397	0.695	0.185	0.700	-0.893	0.588	0.878	0.818	1				
Diesel Index	-0.236	0.563	0.749	0.893	0.397	0.218	-0.273	-0.419	-0.839	0.620	-0.007	-0.411	-0.395	-0.774	1			
Mol mass	0.437	0.925	0.921	0.940	-0.184	0.784	0.345	-0.668	-0.396	0.174	0.669	0.088	-0.003	-0.206	0.703	1		
C/H	0.756	0.170	-0.194	-0.331	-0.556	0.463	0.681	0.341	0.867	-0.825	0.600	0.693	0.499	0.850	-0.661	-0.060	1	
ACN	0.437	0.925	0.921	0.940	-0.184	0.784	0.345	-0.668	-0.396	0.174	0.669	0.088	-0.003	-0.206	0.703	1.000	-0.060	1

Correlation matrix for Non-Aromatic fuels:

Variables	Density @ 15 °C	Viscosity @ 40°C	Cetane (CFR)	Cetane Index	Thermal Exp.Coef.	T95	Slope	T95/T90	T95-T80	LHV	Energy Density	Diesel Index	Mol mass	C/H	ACN
Density @ 15 °C	1														
Viscosity @ 40°C	0.978	1													
Cetane (CFR)	-0.105	-0.039	1												
Cetane Index	-0.711	-0.564	0.573	1											
Thermal Exp. Coef.	-0.516	-0.347	0.676	0.969	1										
T95	0.908	0.974	0.114	-0.362	-0.125	1									
Slope	0.913	0.979	0.039	-0.392	-0.162	0.997	1								
T95/T90	0.809	0.910	0.232	-0.172	0.071	0.981	0.972	1							
T95-T80	0.800	0.904	0.231	-0.158	0.084	0.977	0.969	1.000	1						
LHV	-0.991	-0.995	0.017	0.611	0.397	-0.955	-0.956	-0.880	-0.872	1					
Energy Density	0.999	0.970	-0.128	-0.735	-0.545	0.894	0.900	0.789	0.779	-0.986	1				
Diesel Index	0.191	0.329	0.858	0.519	0.705	0.514	0.458	0.647	0.651	-0.310	0.159	1			
Mol mass	0.964	0.997	0.022	-0.506	-0.281	0.987	0.988	0.936	0.931	-0.990	0.954	0.395	1		
C/H	0.998	0.969	-0.164	-0.747	-0.561	0.888	0.898	0.781	0.771	-0.982	0.999	0.131	0.951	1	
ACN	0.964	0.997	0.022	-0.506	-0.281	0.987	0.988	0.936	0.931	-0.990	0.954	0.395	1.000	0.951	1