Modeling the end-use performance of alternative fuels in light-duty vehicles

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ABSTRACT

Present study investigates the end-use performance of alternative liquid fuels in the current fleet of unmodified light-duty vehicle (LDV) engines. Two mathematical models have been developed that represent the way that various fuel properties affect fuel consumption in spark-ignition (SI) and compression-ignition (CI) engines. Fuel consumption is represented by the results from the New European Driving Cycles (NEDC) in order to reflect the end-use impact. Data-driven black-box modeling and multilinear regression methods were applied to obtain both models. Additionally, quantitative analysis was performed to ensure the statistical significance of inputs (p-value below 5%). Fuel consumption (output) of various alternative fuels can be estimated with high accuracy (coefficient of determination above 0.96), knowing fuel properties (inputs) such as lower heating value, density, cetane/octane number, and oxygen content. The validation procedures confirmed the quality of predictions for both models with the average error being below 2.3%. The model performance for the examined fuels such as hydrotreated vegetable oil (HVO) and ethanol blends showed significant CO_2 reduction with high accuracy. Moreover, both models could be used to estimate CO_2 tailpipe emissions and are applicable to various liquid SI/CI fuels for LDV engines.

1. Introduction

Transportation is considered to be one of the major contributors to global carbon dioxide emissions. Constantly increasing demand of the sector, including all modes: air, water, and land obligates the development of greening solutions. However, an effective and direct way of reducing CO_2 emissions should be highly focused on commercially existing technologies. Current engines, which are powering the present fleet, are expected to be in service for at least next decade. In addition, the recent forecasts predict the predominance of internal combustion engines (ICE) even in the next 30 years [1]. Therefore, immediate action towards fossil-free transport should support drop-in solutions compatible with existing infrastructure. Taking this fact into account, the main attention in the present study is put on fuels produced from sustainable bio-based

feedstock such as various alcohols (i.e. methanol, ethanol, butanol) for spark-ignition (SI) engines and biodiesel (FAME), hydrotreated vegetable oil (HVO) and gas-to-liquid (GTL) fuels for compression-ignition (CI) engines. The aforementioned fuels reveal a decent potential for reducing the carbon footprint of the light-duty vehicle (LDV) sector. Alternative liquid components could be used as a neat fuel (i.e. HVO) but usually are blended with fossil counterparts to comply with blending-wall limitations (FAME or ethanol). Nevertheless, their impact on existing engines has to be carefully investigated, before implementation.

The focus of the present study is on the modeling of the impact of alternative fuel properties on engines' performance in the LDV transport sector. Moreover, this work aims at development of tools, which support the end-use performance assessment. The end-use performance is represented by changes in fuel consumption and CO_2 emissions from the level of regular passenger car users. The motivation behind it is to support the market acceptance and roll-out of Renewable-Energy-Source fuels (RESfuels) [2]. Main considerations are on drop-in fuels whereas technologies looking at future generations of engines are not covered by the scope of this paper. The impact of new fuels on existing engines can be

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investigated through expensive and time-consuming test runs. Multiple studies have analyzed the combustion behavior based on in-cylinder pressure, heat release rate, and local emissions (CO, THC, NO_x, PM). For example, Singh et al. [3] investigated the performance of hydro-processed renewable diesel using direct injection (DI) CI engine. In another study, Rakopoulos et al. [4] examined biofuels including vegetable oil, biodiesel, ethanol, butanol, and diethyl ether. Numerous articles also look at the shift of engine performance when the concentration of alternative fuel changes. Usually measurements are done for few samples with different blending ratios, i.e. Mourad et al. [5] tested propanol blends in passenger vehicle according to a specific driving cycle. The approach in the present study is different and concentrates on alternative fuels and their properties from a global perspective. Instead of looking at one single engine or vehicle and corresponding test results, this work investigates the whole LDV fleet with distinction on CI and SI engines. Alternatively to engine tests, the prediction of end-use performance for renewable fuel is attempted by modeling based on measured fuel properties and experimental data available in the literature. Nevertheless, the development of such a model that links fuel properties with engine performance is a complex task, especially when aiming at versatility. The task demands in-depth analysis of the entire problem, selection of the most suitable approach, proper modeling techniques and validation methods. Hence, the objectives of the present work are as follows:

1. Selection of the approach and choosing the representation of end-use performance.
2. Gathering the data of tested alternative fuel blends together with the associated fuel consumption.
3. Selection of the most important fuel properties in terms of engine performance.
4. Building models for fuel consumption analysis in SI and CI engines for LDV sector.
5. Internal and external validation of both models.

The engine performance can be represented by different parameters, such as brake specific fuel consumption (BSFC), brake power, brake torque, and brake mean effective pressure (BMEP). Many studies have been analyzing the way that fuel consumption of LDV engines is affected by various factors. Zhou et al. [6], performed an extensive review of published models predicting the fuel consumption. Presently, there are models representing the impact of travel ([7–10]), weather([11–13]), vehicle ([14–21]), roadway([9,22–24]), traffic ([25–29]), driver ([18,30–32]), specific location and population ([33]) and fuel additives ([34,35]). Fig. 1 summarizes examined approaches and published models

predicting fuel consumption based on different variables. The pink color indicates the novelty of the present study, in which the focus is paid on the impact of fuel properties on fuel consumption.

When considering drop-in renewable fuels, properties of the fuel blend are of the key importance. Qian et al. [36] tried to bridge the fundamental fuel properties with combustion characteristics for diesel surrogates. However, the prediction of engine performance based on alternative fuel blend is rarely found in the literature. Nevertheless, it is in the interest of fuel producers and engine manufacturers to see how fuel properties are affecting emissions. Tsurutani et al. [37] looked at straightforward correlation between single physiochemical fuel property (i.e. cetane index or aromatics content) and diesel engine performance in terms of NO_x and PM emissions. Tsurutani et al. draw some valuable conclusions, however, they did not develop any models. On the contrary, Najafi et al. [38] used results of experimental analysis and developed an artificial neural network (ANN) with a back-propagation algorithm. In that study, engine power, torque, brake specific fuel consumption (BSFC), brake thermal efficiency (BTE), volumetric efficiency and emission components were determined for different gasoline-ethanol blends and engine speeds. Ghobadian et al. [39] used also the same methodology with ANN in the study focused on biodiesel from waste cooking oil. Instead, Gogoi et al. [40] proposed a cycle simulation model incorporating a thermodynamic based single zone combustion model to predict the performance of diesel engine for biodiesel blends. However, the research was narrowed to the blends of standard diesel and biodiesel from Karanja oil. In another study, effects of density together with ignition timing, air-fuel ratio and compression ratio in ethanol-gasoline blends were investigated by Yucesu [41] and correlated with BSFC and engine torque by means of ANN again with back-propagation algorithm. Despite the aforementioned studies related to alternative fuels application in a specific engine, in this work, the prediction of engine performance for the whole LDV fleet is considered. It is a new approach, which enables global insight on fuel properties and their effect on end-user.

2. Methodology

Modeling the impact of fuel properties on LDV engine performance could be achieved in many ways. Therefore, it is important to specify targets regarding the applicability of models at the initial stages. Present study is aiming at development of two models, one for SI and the second for CI LDV engines. The final models should be applicable to the whole fleet of its kind, regardless of the variations in engine size, weight of the vehicle and etc. Additionally, models should represent the real impact from the end-user perspective. In order to satisfy these objectives, the first step is related to an extensive analysis of options and selection of the general approach. In the next step, it is important to decide input and output data representation mode. The core part is focused on modeling and validation techniques. Generally, three possible approaches to this problem can be distinguished: steady state, driving cycles and through combustion characteristics. The following sections will analyze possible approaches and select the most suitable one.

2.1. Steady-state approach

In the steady state approach, engine performance could be represented by the Brake Specific Fuel Consumption (BSFC) or Brake Thermal Efficiency (BTE). The first stage of the analysis is related to the literature review, where 8 sources were selected for further studies. The first 4 sources ([42–45]) are related to spark ignition (SI) engines, and the remaining part ([46–49]) to compression ignition (CI) engines (Table 1).
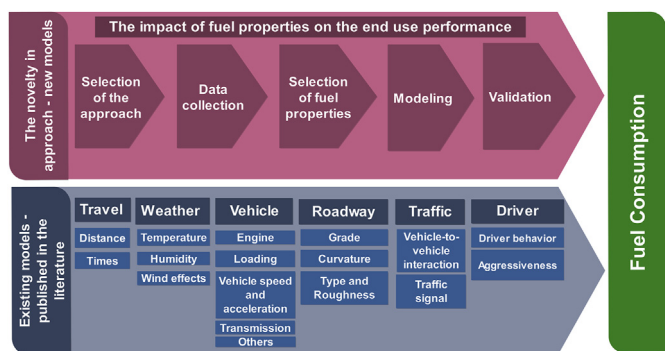

Fig. 1. The novelty of the present study in comparison to already examined approaches in modeling the engine performance of light-duty vehicles.

In the above listed sources, only 4-stroke engines were analyzed. In the case of SI, blends of ethanol with gasoline were tested. In the case of CI blends, blends of Rapeseed Methyl Ester (RME) with standard diesel were investigated. The engine performance results from SI sources are compared based on the Wide Open Throttle (WOT) and 3000 rpm (Fig. 2a). Whereas, the steady-state operational conditions for CI engines were oscillating at 2000 rpm for various load points (Fig. 2b). The vertical axis represents BSFC percentage change relative to the standard gasoline (Fig. 2a) or standard diesel (Fig. 2b) used in the experiments. The horizontal axis represents the increasing concentration of alternative fuel, which in the SI case is ethanol and CI case RME. When analyzing the outputs, a significant incompatibility between the steady state measurement results is observed between different sources, even for the same engines' operating conditions. The reason behind this outcome can be assigned to the impact of the test engine's characteristics on the results. Additionally, there is a strong dependency of BSFC and BTE on engine operation conditions (engine speed and load). This excludes the possibility to create a single uniform model for a given engine type (SI or CI), and hence the steady-state approach is not considered in the rest of the study.

2.2. Driving cycles approach

The second possible approach is through the driving cycles. They include specified velocity profiles designed to represent the real-driving related fuel consumption (FC). Driving cycles are significantly more suitable to represent the end-use impact, because they include a large number of steady-state points together with transient conditions. The result from driving cycles is just one number of fuel consumption for each tested fuel, which is very beneficial from the modeling perspective. In the case of steady-state runs, FC varies depending on the speed and load point of the engine. Moreover, driving cycles are designed to reflect the decent average from the ride in busy cities, roads, and highways. There are different types of cycles such as the New European Driving Cycle (NEDC) or Worldwide Harmonised Light Vehicles Test Procedure (WLTP). However, in this work, the NEDC is selected and the primary reason behind it is the availability of test data. Table 2 includes significant parameters of the cycle.

The NEDC includes 4 Urban Driving Cycles and one Extra Urban Driving Cycle, Fig. 3 represents the velocity profile of NEDC.

The driving cycles approach in comparison to the steady-state approach match significantly better the objectives of the present study. The third possible approach is through the analysis of combustion characteristics and comprehensive engine modeling. However, that option is much more complex due to the impact of an extensive number of parameters. Therefore, driving cycles approach is selected in the present study.

2.3. Modeling procedure

This section analyzes the modeling objectives and introduces selected solutions. Fig. 4 presents the structure of the problem and all involved interrelations. It can be understood in such a way that blending the standard fuel *S* with an alternative fuel *R* results in a new fuel having different properties (A, B, C, D) than *S* and *R* separately. Subsequently, diverse properties affect fuel consumption in their specific way, which furthermore affects CO_2 emissions. Various properties of fuel blends and their end-use performance were reported in scientific publications. However, the target of this work is to discover the mechanisms in the middle of the problem, between the change of fuel properties and the final state of fuel consumption. Hence, the targeted model represents how fuel properties and their change affect the fuel consumption of LDV engines. In order to make the data from various sources comparable, and to achieve a uniform model, both input and output parameters are characterized by percentage changes relative to the standard fuel (gasoline for SI and diesel for CI engines) used at each source.

The problem consists of multiple input parameters and one output parameter, where the majority of relations are assumed to be linear. Therefore, multi-linear regression was chosen as a general modeling method. Multi-linear regression is a more complex form of linear regression, which represents the relationship between one dependent variable and several independent variables (Equation (1)).

$$y(x) = \varphi_1(x) \cdot \beta_1 + \ldots + \varphi_n(x) \cdot \beta_n + \varepsilon(x) \qquad (1)$$

where, *y* - dependent variable, *x* - independent variable, $\varphi_i(x)$ - explanatory variable, β_i parameter of explanatory variable, $\varepsilon(x)$ - error.

Referring to Fig. 4, the Equation (1) could be expressed as follows:

$$\alpha = a \cdot A(X_R) + b \cdot B(X_R) + c \cdot C(X_R) + d \cdot D(X_R) \qquad (2)$$

where, α - relative change of fuel consumption [% change in reference to l/km], X_R - alternative fuel's volumetric concentration in the blend with standard fossil based fuel, $A(X_R) \ldots D(X_R)$ - relative change of fuel properties [% change relative to standard fossil fuel], *a* ... *d* - properties coefficients, *R* - alternative fuel, *S* - standard fossil-based fuel.

Calorific content, density or octane/cetane number are examples of fuel properties (see Section 2.4 for selection of fuel properties). Values of different properties for the given alternative fuel blend are compared to standard fossil fuel and relative changes in properties [$A(X_R)$] are calculated according to Equation (3) (for the property A as an example below).

Table 1
Test engines parameters from the chosen sources.

| Source	Reference	[42]	[43]	[44]	[45]	[46]	[47]	[48]	[49]
	Year	2010	2009	2009	2016	2011	2017	2007	2006
Test	Load	Wide Open Throttle (WOT)				105Nm	medium	20Nm	5 Bar
	Speed [RPM]	3000				1900	2100	1500	2200
Engine characteristics	Type	Spark-ignition 4 stroke				Compression-ignition 4 stroke			
	Injection	MPFI				DI	DI	DI	DI
	Aspiration					turbo	nat.	nat.	nat.
	Cylinders	4	4	1	4	4	2	1	4
	Valves	8	8		16	16			
	Bore [mm]	70	71	80,26	79	103	92	98	110
	Stroke [mm]	64,9	83,6	88,9	81,5	132	75	102	125
	Displacement [cm3]	999	1323	1798	1598	4400	1000	700	4750
	Compression ratio	10:01	9.7:1	10:01	10.5:1	18.3:1	20.5:1	15.5:1	16:01
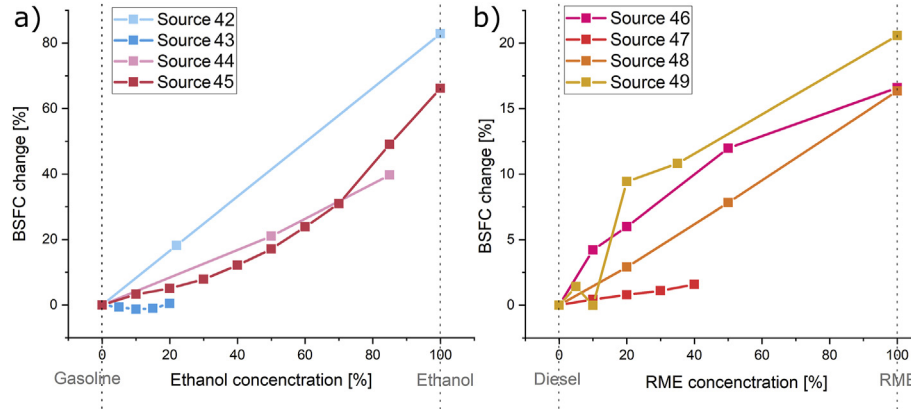
Fig. 2. The impact of alternative fuel concentration on BSFC at steady state conditions. On the left side SI engines powered by ethanol blends with gasoline and on the right side CI engines powered by RME blends with diesel.

Table 2
Parameters of NEDC.

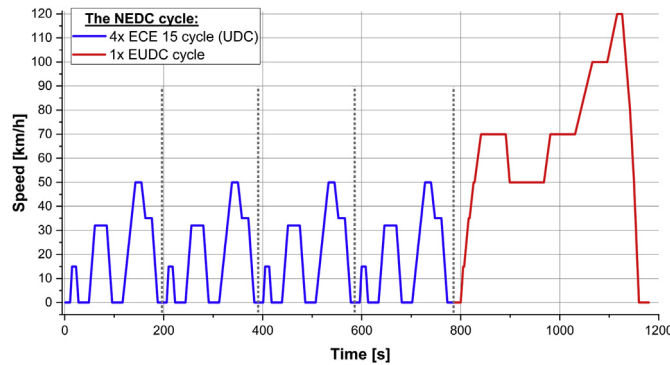|	Units		NEDC
Start condition			cold
Duration	s		1180,00
Distance	km		11,03
Mean velocity	km/h		33,60
Max. velocity	km/h		120,00
Stop phases			14,00
Durations:			Shares:
Stop	s	280,00	23,70%
Constant driving	s	475,00	40,30%
Acceleration	s	247,00	20,90%
Deceleration	s	178,00	15,10%

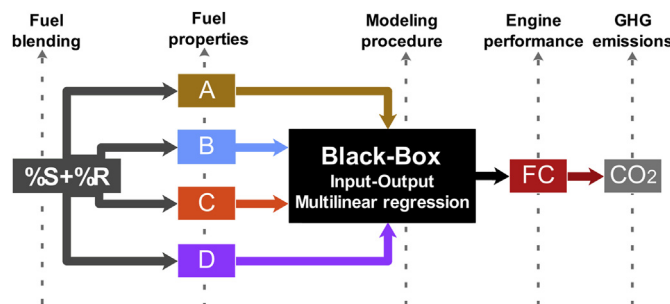**Fig. 3.** Velocity profile of NEDC (based on [50]).

Fig. 4. Structure of the problem, %S - concentration of the standard fuel in the blend with alternative fuel - %R.

$$A(X_R) = (A_R(X_R) - A_S) / A_S \cdot 100\% \qquad (3)$$

where, $A_R(X_R)$ - value of specific fuel property [A] for alternative fuel blend dependent on concentration of alternative fuel X_R, A_S - value of specific fuel property [A] for standard fuel (gasoline or diesel).

The modeling procedure is carried out using the least-squares method [51]:

$$J_\theta = \sum_{x=1}^{N} \varepsilon^2 = \sum_{x=1}^{N} \left(y(x) - \varphi^T(x) \cdot \theta \right) \qquad (4)$$

where, J_θ - least-squares objective function.

As presented in Equation (5), CO_2 emissions are calculated using the outputs of fuel consumption, density and carbon content in the fuel. The coefficient (44.01/12.0107) is a molar mass relation, between carbon dioxide and carbon. The following Equation (5) represents the calculation methodology.

$$\delta = \alpha_{abs} \cdot \rho \cdot z \cdot \frac{44.01}{12.0107} \qquad (5)$$

where, δ - CO_2 emissions [g/km], α_{abs} - absolute value of fuel consumption [l/km], ρ - density of the fuel [g/dm^3], z - mass-based carbon content in the fuel [%], $\frac{44.01}{12.0107}$ - molar mass ratio between carbon dioxide (44.01 g/mol) and carbon (12.0107 g/mol).

The mass-based concentration of carbon in the fuel can be calculated as follows:

$$z = (X \cdot z_R \cdot \rho_R + (1 - X) \cdot z_S \cdot \rho_S) / \rho \qquad (6)$$

where, X - volumetric fraction (concentration) of alternative fuel [%], ρ_R - density of pure alternative fuel [g/dm^3], ρ_S - density of standard diesel or gasoline [g/dm^3], z_R - carbon content in alternative fuel [%], z_S - carbon content in standard gasoline/diesel fuel [%].

The model's accuracy is characterized and controlled by R-square, standard error, t-value and p-value for the *t*-test. The validation procedure is executed against the data used for modeling - internal validation, and the data that were not taken into the modeling process - an external validation.

2.4. Selection of fuel properties in the model

The selection of fuel properties inside the model is performed in

two stages. The first one is taking into account only fuel properties that were measured in each chosen source. Various literature sources used for collection of data for the modeling purpose included only part of these properties, but not all of them. Therefore in order to reduce the error, only fuel properties that were reported commonly at each source were taken for further analysis. Table 3 represents significant fuel properties that affect SI and CI engine performance, operation and emissions.

The second step executed the final selection through the quantitative analysis (the *t*-test). Only fuel properties that proved to be significant together, survived in the final model. The *t*-test is a statistical significance test based on the hypothesis that help to discover whether there are interrelations between applied input properties or not, by checking the difference among used groups of data. The *t*-test includes two hypotheses, the so-called "null hypothesis" and an alternative hypothesis. The "null hypothesis" H_0 states that there is no difference between the groups, whereas the alternative hypothesis H_1 says that there is a difference, and it is examined against the H_0. In other words, when there is strong enough evidence against the null hypothesis, the null hypothesis is rejected, and the groups are considered to be significant. Further details of the methodology is provided in the Appendix A.

Final properties used in the model development and tested by significance analysis are:

- net calorific value mass-based, net calorific value volume-based, density, research octane number, reid vapor pressure, and oxygen content in SI case;
- net calorific value mass-based, net calorific value volume-based, density, viscosity, cetane number, and oxygen content in CI case.

The tool used for data analysis and mathematical modeling is an OriginLAB software, where iteration method used while doing the regression was the Levenberg-Marquardt Algorithm (LMA), based on least-squares method [52].

2.5. Selected sources of the data for modeling

Experimental data for modeling were obtained from publicly available literature sources (journal papers), where different alternative fuels were tested in unmodified LDV engines under the NEDC.

Five sources of data were selected for modeling the end-use

performance in spark-ignition engines, where two of them were used for validation of the model. The first one [53] was testing 5%, 10% and 20% blends of n-butanol with gasoline. The test engine was 4 cylinder/16 valves, Euro 3, multi-port fuel injection (MPFI) passenger car engine having totally 1.2 L displacement. The second source [54] was testing different blends of isobutanol (iBu16, iBu68) and ethanol (E10, E22, and E85) with gasoline. The test engine had 2.0 L of total displacement, 4 cylinders/16 valves, direct injection (DI) and Euro 4. The third source [55] was examining the combustion performance and emissions of ethanol blends with gasoline (E5, E10, E25, E50, E85). The tests were performed in two vehicles, the first one had naturally aspirated, 1.2 L of total displacement SI engine, 4 cylinders/16 valves, port fuel injection (PFI), Euro 5 passenger car. The second vehicle, had 1.4 L engine, turbocharged, DI and also Euro 5. For an external validation purposes data published by Bosmal Automotive Research and Development Institute were selected [56,57]. In both sources blends of ethanol with gasoline from 5% to max. 85% were tested in an unmodified LDV SI engines.

Six data sources were selected for modeling the end-use performance in compression-ignition engines, where two of them were used for validation of the model. The first one [58] was measuring the performance of 30% RME and 30% HVO blends with diesel. The test engine had 1.25 L displacement (4 cylinders), DI and turbocharged. The emission control was Euro 5 and the tests were performed under NEDC. The second source [59] was testing the combustion performance of HVO, GTL and FAME biodiesel in CI engine having 2 L displacement (4 cylinders), DI, turbocharged and Euro 5. In the third source [60], hydrocracked fossil oil blends with HVO were analyzed. Their performances were tested in 2 L, 4 cylinders, DI, turbocharged engine compliant with Euro 5. The last source [61] was analyzing the combustion performance and emissions of biodiesel, enzymatic biodiesel, and HVO. The test engine was 2 L, 4 cylinders, DI, turbocharged compliant with Euro 6. For external validation purposes data from Bosmal Automotive Research and Development Institute were used. In the case of first data source for validation [62], blends of high RME content (30%, 50%, and pure RME - 100%) were tested in LDV CI engine over the NEDC. Whereas, the second one [63] in addition to the high-concentration Fatty Acid Methyl Ester - FAME blends with standard fossil-based diesel, was testing the low concentration RME blends (B7, B15) and higher content HVO blends (30%).

3. Results

The results for both SI and CI case are presented in this chapter. Each subsection represents modeling matrixes, plots of each fuel property impact on engine performance, obtained models, their quantitative analysis results and the two-stage validation (against an internal and external data).

3.1. SI case

In the chosen sources of data, fuel properties such as Research Octane Number (RON), Reid Vapor Pressure (RVP), Net Calorific Value volume-based (NCVvol), Net Calorific Value mass-based (NCVmass), density, oxygen, and carbon contents were measured and reported. Therefore, they are selected further for the modeling part. The following Table 4 combines data from all three sources and represents them as a percentage changes relative to fossil-based gasoline tested at each source together with alternative fuels. In result, gasoline values are zero and represent no change in fuel consumption. Oxygen and carbon contents are represented as percentage mass contents of carbon or oxygen per mass of fuel. The carbon content is not taken into account for fuel consumption modeling. However, it is used for carbon dioxide emissions

Table 3
Fuel properties affecting SI and CI engine performance and emissions.

SI	CI	SI	CI
Duration of injection		**Ignition characteristics and quality**	
Heating value		Octane number	Cetane number
Density		Octane index	Cetane index
		Autoignition temperature	
		Flammability limits	
Combustion characteristics		**Exhaust emissions and fouling**	
Heat of vaporization	Viscosity	Existent gum content	
Vapor pressure		Aromatics content	
Volatility		Sulfur content	
Density		Carbon residue	
Oxygen content		Ash	
		Total contaminants	
Operational aspects		**Safety, storage and refueling**	
Existent gum content	Cloud point	Flash point	
	CFPP	Corrosiveness	
Lubricity		Toxicity	
Density		Oxidation stability	
Viscosity		Compatibility with materials	
Freezing point			

Table 4
Modeling matrix for SI part.

Sources		Fuels	RON	RVP	NCVvol	NCV mass	Density	O2	C	FC
				% change	% change	% change	% change	%m/m	%m/m	% change
[53]		**Gasoline**	0,0	0,0	0,00	0,00	0,0	0,00	84,31	**0,00**
		nBu5	0,2	−4,3	0,16	−0,95	1,1	1,08	83,33	**0,60**
		nBu10	0,5	−25,1	−0,62	−1,89	1,3	2,16	82,36	**2,44**
		nBu20	0,9	−30,3	−1,60	−3,78	2,3	4,33	80,41	**3,12**
[54]		**Gasoline**	0,0	0,0	0,00	0,00	0,0	0,10	86,60	**0,00**
		Gasoline2	7,4	8,3	−3,24	−3,24	0,0	2,50	84,70	**1,64**
		E10	4,2	8,3	−2,87	−4,17	1,4	4,00	82,70	**4,22**
		E22	7,4	10,4	−7,56	−8,80	1,4	8,10	78,50	**7,62**
		E85	11,6	−17,7	−27,78	−31,48	5,4	30,10	56,90	**46,29**
		iBu16	3,2	−10,4	−2,64	−3,94	1,4	5,30	82,90	**1,99**
		iBu68	9,5	−27,1	−9,97	−14,58	5,4	22,50	73,10	**12,19**
[55]	Vehicle 1	**E5**	0,0	0,0	0,00	0,00	0,0	1,74	82,70	**0,00**
		E10	1,7	−1,2	−1,51	−1,79	0,5	3,47	81,09	**3,30**
		E25	5,8	−4,1	−6,02	−2,76	1,3	8,68	76,26	**6,49**
		E50	8,6	−12,1	−13,56	−19,70	2,7	17,35	68,21	**16,61**
		E85	12,4	−44,4	−24,11	−27,65	4,9	29,50	56,93	**35,20**
	Vehicle 2	**E5**	0,0	0,0	0,00	0,00	0,0	1,74	82,70	**0,00**
		E10	1,7	−1,2	−1,51	−1,79	0,5	3,47	81,09	**−0,10**
		E25	5,8	−4,1	−6,02	−2,76	1,3	8,68	76,26	**5,28**
		E50	8,6	−12,1	−13,56	−19,70	2,7	17,35	68,21	**14,86**

calculation (together with density and fuel consumption).

Fig. 5 represents the relation between various fuel properties and FC in SI ICE of LDV.

In general, higher RON values allow earlier spark timing, which in consequence leads to lower FC. This effect could be particularly observed in engines that are able to utilize this performance benefit - higher compression ratios (CR). However, in Fig. 5, the growth of RON represents higher values of fuel consumption. The reason for this observation is the influence of other fuel properties such as lower NCV of those high RON blends. In the case of density, larger values are associated with higher fuel consumption. This effect is also influenced by other fuel properties similar to the case of RON, alcohols have higher density but lower NCV and higher oxygen content. The impact of NCVmass and NCVvol on FC is very intuitive and such strong impacts may dominate over other properties such

as RON and Density. Oxygen content affects directly NCV decreasing it respectively to the percentage concentration in the fuel, which in turn increases fuel consumption almost linearly. When it comes to the Reid Vapor Pressure, despite the fact that there are no clear visible trends, fuels with higher RVP oscillate in the regions of lower FC. The conclusion that could be withdrawn at this stage is that it is difficult to observe the influence of each single fuel property separately on engine performance. Fuel properties are interrelated and they affect engine performance collectively. Therefore, the present study investigates the joint impact of fuel properties in the next steps, during the modeling procedure.

Modeling results are summarized in Table 5. In the final model, oxygen content, density, NCVvol, and RON represent fuel consumption with high accuracy (R-Square 0.989). The p-value for each fuel property is bellow 5%, which means that all of them are
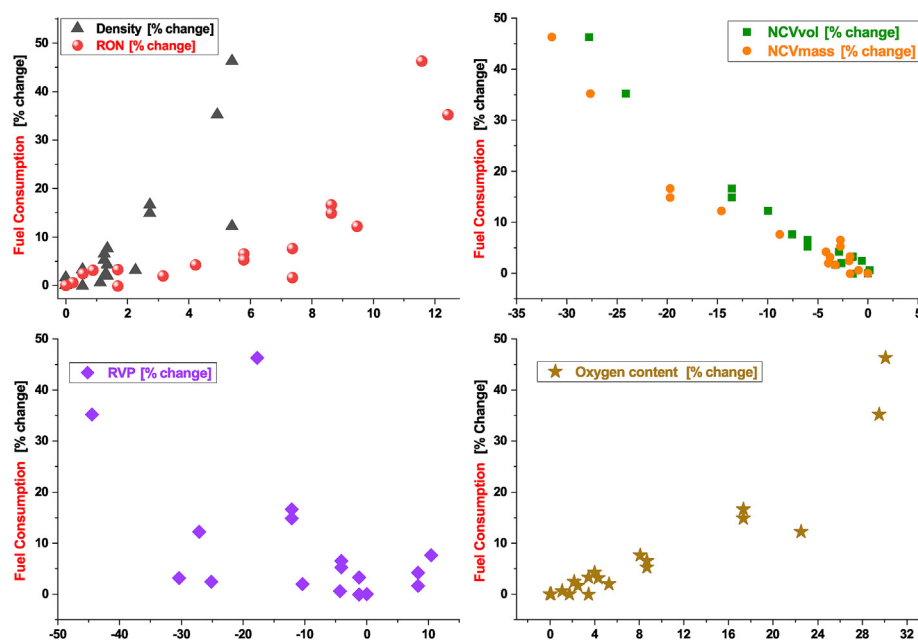

Fig. 5. The dependency of fuel consumption on SI fuel properties.

Table 5
SI part's modeling results.

Fuel property	Coefficient's value	Standard Error	T-value	P-value
O2	**−0,613**	0,253	−2,419	0,028
Density	**1,883**	0,661	2,847	0,012
NCVvol	**−2,220**	0,179	−12,382	1,31E-09
RON	**−0,771**	0,170	−4,538	3,36E-04
R-Square (COD)	0,989		Adj. R-Square	0,987

Bold values of coefficients are the most significant.

significant.

The following Equation represents the final model for fuel consumption of SI part:

$$\alpha_{SI} = -0.771 \cdot A - 2.220 \cdot B + 1.883 \cdot C - 0.613 \cdot D \qquad (7)$$

where, α_{SI} - fuel consumption [relative change], A - RON [relative change], B - NCVvol [relative change], C - Density [relative change], D - Oxygen content [relative change].

Fig. 6 shows the compatibility of model predictions with data used for modeling and carbon dioxide emissions. The model performs very well against the internal data, especially when considering that they originate from various parts of the world (India, Poland, and England), and tests were carried out in four different vehicles powered by fuels coming from local markets.

The second part of the validation is testing the model against the data that were not taken into the modeling procedure - Fig. 7. Two sources of data were taken into the validation. The results show that the model has a very good prediction of fuel consumption. The average absolute error of the model versus source [56] is just 1.1%, whereas in the case of source [57] 2.28%.

3.2. CI case

In the case of CI, fuel properties such as cetane number (CN), viscosity, NCVvol, NCVmass, density, oxygen, and carbon contents were measured and reported in literature sources used for modeling. The following Table 6 combines data from all four
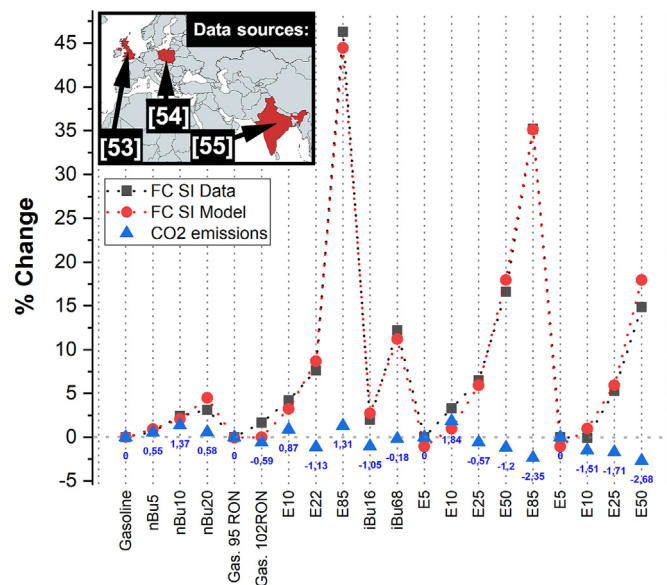
Fig. 6. Internal validation of the SI model against the fuel consumption values from data ([53–55]), with additional change in carbon dioxide emissions.
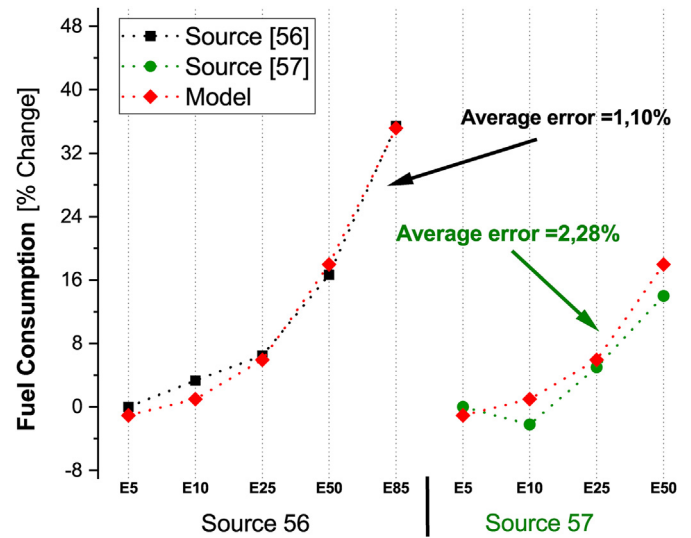
Fig. 7. External validation of the SI model against the data from sources [56,57].

sources and represents them as a percentage change relative to fossil-based diesel tested at each source together with alternative fuels.

Fig. 8 illustrates the relations between various fuel properties and FC in CI passenger car engines. Fuels having higher cetane number are usually associated with lower fuel consumption. The cetane number is an indicator of ignition quality, which affects engine performance. Higher cetane number fuels are more reactive with shorter ignition delay and it can be reflected in better thermal efficiency. Density as a physical property, which determines mass of fuel per given volume, affects injection in CI engines. Looking closely at Fig. 8, its growth is usually followed by fuel consumption's increase. Whereas, in both cases of volume- and mass-based NCV, lower fuel consumption is usually associated with higher calorific content. However, there is no straightforward relation between NCVvol and FC. It means that not only calorific content affects engine performance but also other properties such as density or cetane number play significant role. It is evident that FAME type of fuels have lower calorific content than fossil diesel or HVO/GTL. This fact is related to the composition of those fuels - the higher the oxygen content, the lower the NCV. The highest oxygen content is actually observed in FAME type of fuels, whereas there is no oxygen in the chemical composition of HVO. In addition, fuels with high viscosity such as biodiesel represent higher fuel consumption than less viscous alternatives such as GTL.

Modeling results correlating FC with CI fuel properties are summarized in Table 7. In the final model, cetane number, density, and NCVmass represent fuel consumption with high accuracy (R-Square 0.966). The p-value for each fuel property is bellow 5%, which means that all of them are significant.

The following Equation represents the final model for fuel consumption of the CI part:

$$\alpha_{CI} = -1.113 \cdot E - 0.076 \cdot F - 1.075 \cdot C \qquad (8)$$

where, α_{CI} - fuel consumption [relative change], E - NCVmass [relative change], F - CN [relative change], C - Density [relative change].

Fig. 9 reveals the compatibility of model outcomes with data used for modeling and carbon dioxide emissions for CI case. Similarly to the SI case, data for modeling were collected from different countries (Poland, Italy, and Spain). The predictions generated by

Table 6
Modeling matrix for CI part.

Source	Fuels	CN	Density	Viscosity	NCVvol	NCVmass	O2	C	FC
		% change	% change	% change	% change	% change	%m/m	%m/m	% change
[58]	**Diesel**	0,00	0,00	0,00	0,00	0,00	0,00	86,20	**0,00**
	B30	3,12	1,85	18,72	−1,95	−3,73	3,40	83,40	**2,07**
	H30	18,55	−3,02	−5,07	−2,00	1,05	0,00	85,40	**2,19**
[59]	**Diesel**	0,00	0,00	0,00	0,00	0,00	0,00	86,20	**0,00**
	B100	21,03	3,79	60,56	−9,93	−13,20	10,37	76,14	**9,92**
	GTL100	64,58	−8,40	−6,77	−4,94	3,77	−0,66	84,82	**−0,88**
	H100	74,91	−7,69	19,12	−4,38	3,58	−0,66	84,68	**−1,33**
[60]	**Diesel**	0,00	0,00	0,00	0,00	0,00	0,00	86,20	**0,00**
	HCK100	0,76	−0,06	11,79	0,71	0,77	0,00	86,20	**−1,54**
	HCK85H15	15,21	−0,40	33,06	0,51	0,91	0,00	86,20	**−1,47**
	HCK70H30	30,04	−1,07	49,57	0,13	1,21	0,00	86,00	**−3,25**
	HCKcni100	22,62	−0,06	11,79	0,71	0,77	0,00	86,20	**−1,85**
[61]	**Diesel**	0,00	0,00	0,00	0,00	0,00	0,00	86,00	**0,00**
	BE100	−2,26	5,19	56,41	−7,70	−12,25	10,93	77,07	**6,94**
	B100	20,53	4,43	67,28	−8,11	−12,01	10,93	77,07	**7,18**
	H100	40,68	−7,15	5,67	−4,25	3,13	0,00	84,61	**1,14**
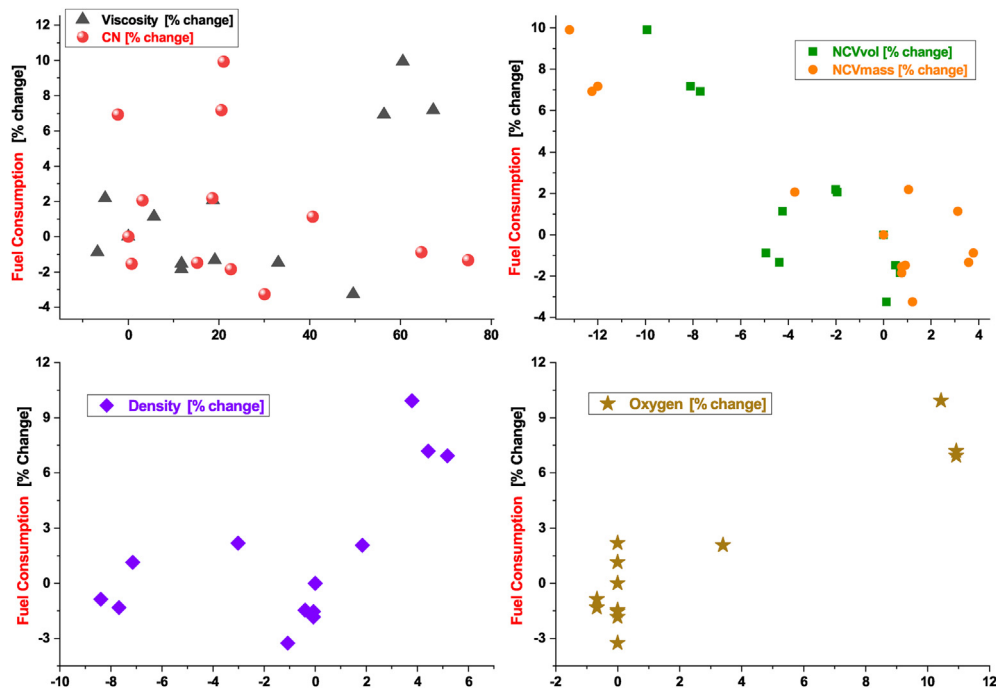
Fig. 8. The dependency of fuel consumption on CI fuel properties.

Table 7
CI part's modeling results.

Fuel property	Coefficient's value	Standard Error	T-value	P-value
NCVmass	**−1,113**	0,083	−13,385	0,000
CN	**−0,076**	0,016	−4,828	0,000
Density	**−1,075**	0,166	−6,460	2,13E-05
R-Square (COD)	0,966		Adj. R-Square	0,961

Bold values of coefficients are the most significant.

the model follow very closely the internal data.

When analyzing carbon dioxide emissions, in the case of bio-diesel (FAME), there is no significant change, even in the region of high concentrations. It means that higher FC and density for bio-diesel is compensated by lower carbon content of FAME fuel.

Whereas HVO and GTL blends represent lower CO_2 emissions in all cases, especially for neat fuels over 10% decrease can be observed. It is a direct consequence of lower density and carbon-hydrogen ration. The reason of lower FC could also be related to the higher CN of those fuels which leads towards the shorter ignition delays, earlier heat release and higher pressures of expanding gases. This chain results in higher thermal efficiency.

The second part of validation is an external one, which is focused on testing the model against data, which were not taken into the modeling procedure - Fig. 10. Two sources of data were used in validation. The results show that the model has a very good prediction of fuel consumption. The average absolute error of model predictions versus experimental data reported in the source [62] is only 0.51%. Whereas, comparing to the source [63], model predictions have around 1.74% of average absolute error
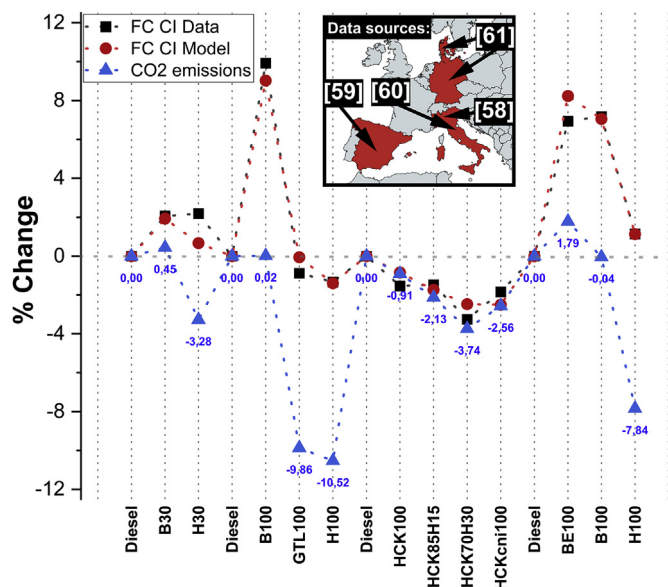
Fig. 9. Internal validation of the CI model against the fuel consumption values from data ([58–61]), with additional change in carbon dioxide emissions.
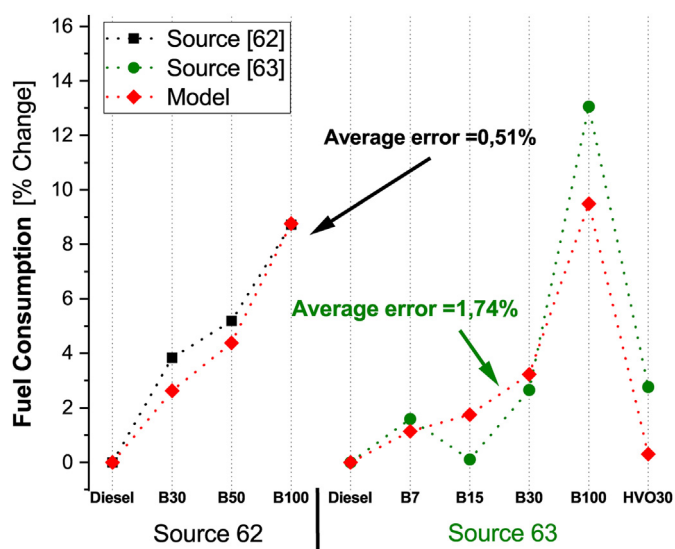

Fig. 10. External validation of the CI model against the data from sources [62,63].

4. Discussion

Current study presented new models for the prediction of fuel consumption in on-road vehicles. The research revealed the collective effect of fuel properties on engine performance in unmodified LDV fleet. Fuels tested in the literature were mainly alcohol-gasoline blends in SI engines and biodiesel (FAME), renewable diesel (HVO) and GTL blends with fossil diesel in CI engines. Three possible approaches were indicated for the modeling purposes, steady-state, driving cycles and combustion characteristics. In the steady-state approach, various limitations were found. The most important was related to the high sensitivity of fuel consumption

on engine operational conditions, the inconsistency of data from different sources, and the strong impact of engine characteristics. Modeling the end-use performance through the combustion characteristics, turned out to be highly complex and associated with a large number of non-fuel related parameters. The driving cycles approach was selected as the most suitable to represent the impact of fuel properties on engine performance from an end-user perspective (not dependent on engine characteristics or operational conditions). By turning the raw values of fuel properties and FC into the relative changes normalized to standard fossil fuel (gasoline for SI, and diesel for CI case), the influence of engine size and configurations were strongly minimized. Additionally, the relative changes allowed to create a consistent database and enabled the possibility for modeling and validation. The stepwise multiple regression, connected with quantitative analysis and internal-external validation, were selected to develop models. Selected fuel properties in the bodies of both SI and CI models satisfy the significance level of 5% (the highest value for p-test was 3%).

4.1. Overall observations

Relative changes of FC over the NEDC and fuel properties in case of unmodified LDV engines turned out to be decently preserved, regardless of the engine size, production year, manufacturer, vehicle, emission control standard, fuel producer, blends that were tested as drop-in fuels, their quality or country where tests were performed.

4.2. Applicability

Developed models are applicable to the whole fleet of unmodified SI and CI LDV engines. They predict the end-use performance of alternative fuels in engines optimized for standard fuel. Additionally, both models can be used to simulate the results of NEDC runs for various fuels. Particularly beneficial is the prediction of fuel consumption based on the few measured properties of the new fuel blend. When utilizing the potential of the linear models, it is possible to estimate the change in FC and CO_2 emissions when NCV, RON/CN, density, oxygen and carbon content are known for considered blend and compared with reference diesel or gasoline. The main scope of this work is related to the final utilization of fuels in LDV engines and related tailpipe emissions, whereas the part concerning the production of fuels by refineries is not included in the analysis. In practice, presented in this paper models can help decision-makers to accelerate development and commercialization of future sustainable fuels by:

- giving a quick, cost-free and user friendly way of performance assessment for new fuels and blends in the current fleet of unmodified engines with a decent prediction quality. Presently, measurements of fuel consumption and emissions are involved with chassis dyno runs of driving cycles (NEDC or WLTP), that are both expensive and time consuming.
- allowing fleet operators to estimate what would be the effect of new fuels in their engines. Especially, when taking into account blends that represent lower CO_2 emissions despite slightly higher fuel consumption.
- supporting policy makers in development of new regulations related to sustainable liquid fuels.

5. Conclusions

In this study, two models were developed for prediction of end-use performance in the current fleet of unmodified ICE of LDVs, one for SI and one for CI engines. Both models represent how relative changes in fuel properties affect collectively the fuel consumption expressed also in the percentage change. The relative changes are referring to the standard gasoline in SI case and diesel in CI case. Based on the results the following conclusions could be withdrawn:

- The most significant properties from the fuel economy perspective in SI LDV are RON (coefficient −0.771), NCVvol (coefficient −2.220), density (coefficient −1.883), and oxygen content (coefficient −0.613). The final model's accuracy is very high, R-square equals 0.989. Additionally, an external validation, when comparing model predictions versus chassis dyno runs proved very good consistency. In the case of two external sources, the average errors were 1.1% and 2.28%.
- The use of alcohol-gasoline blends yielded higher fuel consumption. Nevertheless, in many cases despite the higher fuel consumption, CO_2 emissions are lower (examples of E10, E22, E25, E50, E85 iBu16, iBu68). The reason behind this outcome is associated with the higher engine thermal efficiency of fuels representing high RON. Although thermal efficiency is an engine-related property, it could be affected (within certain limits) by different fuels.
- In the case of CI LDV model, the most significant fuel properties turned out to be NCVmass (coefficient −1.113), CN (coefficient −0.076) and density (coefficient −1.075). The coefficient of determination (COD) is slightly lower for CI case than SI, nevertheless still very high, equals 0.966 (R-square). However, external validation of the model was better for CI case than SI, average errors 0.51% and 1.74% respectively. The reason is mostly related to the maximal changes of FC, which are roughly 4.7 times higher in the SI case when comparing to the CI case.
- The carbon dioxide emissions for biodiesel (FAME), are similar to fossil diesel. However, HVO and GTL blends represent up to 10% lower CO_2 emissions. These trends were also accurately predicted by the developed models.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRediT authorship contribution statement

Yuri Kroyan: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - original draft, Writing - review & editing, Visualization. **Michal Wojcieszyk:** Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing - original draft, Writing - review & editing. **Ossi Kaario:** Conceptualization, Validation, Writing - original draft, Writing - review & editing, Supervision. **Martti Larmi:** Conceptualization, Resources, Writing - original draft, Supervision, Project administration, Funding acquisition. **Kai Zenger:** Validation, Formal analysis.

Acknowledgments

Appendix A

The result of a *t*-test is so called t-value, which is expressed as follows:

$$t = \frac{\overline{x} - \mu}{\frac{\sigma}{\sqrt{n}}} \tag{9}$$

where, $\overline{x}$ - mean of the sample, μ - population mean, σ - standard deviation of the population, n - sample size.

A big number of t-value indicates that the groups are different, while the small one that groups are similar. More likely observations are located by the t = 0.
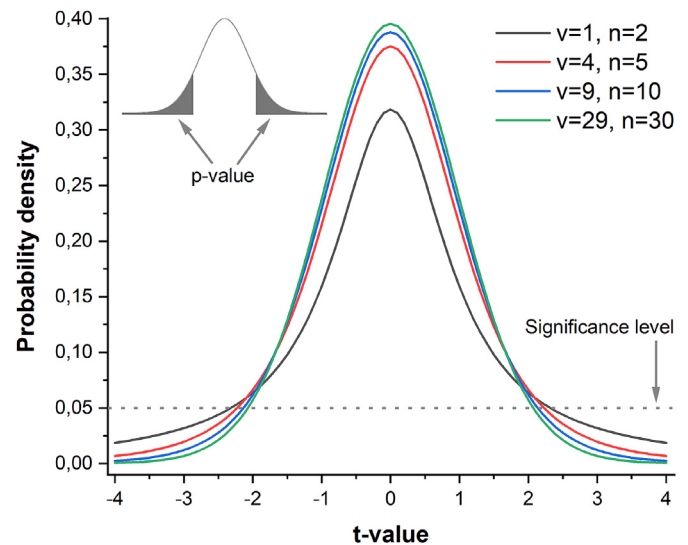

Fig. 11. Probability density on the t-distribution for different sample sizes (n).

The probability of observing the results outside the statistically significant compartments is the so-called p-value. The p-value is a data-based measure and oscillates between 0 and 1, the higher the number the higher the probability of observing the results outside the range of significance. In practice, the p-value is calculated based on the Probability Density Function (PDF) for the t-distribution [64]:

$$f(t) = \frac{\Gamma\left(\frac{v+1}{2}\right)}{\sqrt{v\pi}\,\Gamma\left(\frac{v}{2}\right)} \left(1 + \frac{t^2}{v}\right)^{-\frac{v+1}{2}} \tag{10}$$

where, $v = n - 1$ - degrees of freedom, t - t-test value, Γ - gamma function

$$\Gamma\left(\frac{v}{2}\right) = \int_0^\infty x^{\frac{v}{2}-1} e^{-x} dx \tag{11}$$

$$\Gamma\left(\frac{v+1}{2}\right) = \int_0^\infty x^{\frac{v+1}{2}-1} e^{-x} dx \tag{12}$$

Two areas under the PDF function (on the left and right side from the t-value equal 0) limited on the vertical sides by the observed t-values constitute a p-value (in the double tail event

case). There is a point called significance level, that has to be specified before doing the statistical significance testing. In the present studies the selected significance level is 0.05, which means that there is a 5% risk of obtaining no difference between the groups. The results of p-value are compared to the significance level. When they are smaller than 5% than the null hypothesis is rejected and groups are significant. In the reverse situation, when the p-value is bigger than the significance level, the null hypothesis is accepted and there is no difference between the groups, which in consequence indicates that the parameter is not significant. P-value could be calculated by computer using the data analysis software or estimated based on the p-value tables [65].

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Abbreviations

ANN: Artificial Neural Network
B100: 100% FAME (biodiesel) fuel
B30: 30% blend of FAME (biodiesel) with 70% of fossil diesel
BE100: 100% FAME (biodiesel) fuel produced with the use of enzymes
BMEP: Brake Mean Effective Pressure
BSFC: Brake Specific Fuel Consumption
BTE: Brake Thermal Efficiency
C: Carbon content
CFPP: Cold Filter Plugging Point
CI: Compression Ignition
CN: Cetane number
CO: Carbon monoxide
CO2: Carbon dioxide emissions
COD: Coefficient of determination
CR: Compression Ratio
DI: Direct Injection
E10: 10% blend of ethanol with 90% of gasoline
E22: 22% blend of ethanol with 78% of gasoline
E85: 85% blend of ethanol with 15% of gasoline
FC: Fuel Consumption
GTL: Gas To Liquid
GTL100: 100% Gas To Liquid fuel
H100: 100% HVO fuel
H30: 30% blend of HVO with 70% of fossil diesel
HCK: Diesel fuel produced from the hydrocracking process
HCK100: 100% of diesel fuel produced from hydrocracking process
HCK70H30: 70% blend of diesel fuel produced from hydrocracking process with 30% of HVO
HCK85H15: 85% blend of diesel fuel produced from hydrocracking process with 15% of HVO
HCKcni100: 100% of diesel fuel produced from hydrocracking process enriched with cetane improver
HVO: Hydrotreated Vegetable Oil
iBu16: 16% blend of isobutanol with 84% of gasoline
iBu68: 68% blend of isobutanol with 32% of gasoline
ICE: Internal Combustion Engine
LDV: Light-Duty Vehicle
LMA: Levenberg-Marquardt Algorithm
MPFI: Multi Port Fuel Injection
nBu10: 10% blend of n-butanol with 90% of gasoline
nBu20: 20% blend of n-butanol with 80% of gasoline
nBu5: 5% blend of n-butanol with 95% of gasoline
NCVmass: Net Calorific Value mass-based
NCVvol: Net Calorific Value volume-based
NEDC: New European Driving Cycle
Nm: Newton meter
NOx: Nitrogen oxides
O2: Oxygen content
PDF: Probability Density Function
PFI: Port Fuel Injection
PM: Particulate Matter
RESfuel: Renewable Energy Source fuel
RME: Rapeseed Methyl Ester
RON: Research Octane Number
RPM: Revolutions Per Minute
RVP: Reid Vapor Pressure
SI: Spark Ignition
THC: Total Hydrocarbon Content
WLTP: Worldwide Harmonised Light Vehicles Test Procedure
WOT: Wide Open Throttle