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# Modelling the end-use performance of alternative fuel properties in flex-fuel vehicles

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A B S T R A C T

Renewable fuels and fuel-optimized engines play a key role in the time- and cost-effective decarbonization of current mobility. The present work introduces a state-of-the-art mathematical model that allows for the first time an accurate estimation of fuel consumption in flex-fuel vehicle engines by considering the impact of the most significant fuel properties exclusively. These engines are optimized to a higher concentration of non-drop-in fuels such as E85. Based on the literature data, a matrix was built with fuel properties as multiple independent variables and fuel consumption as a response variable. A multilinear regression with quantitative analysis was applied to develop a fuel consumption model for FFVs. The most significant fuel properties turned out to be octane sensitivity, vapor pressure, lower heating value, and density. All properties in the final model have a unique and important impact on fuel consumption, secured by extremely low p-values ($P \ll 1$ %). The model reached very high accuracy represented by R-Square of 0.994, which turned into 1.41 % of the average absolute error in internal validation and only 1.9 % in external validation. The present study shows that in all alternative fuel cases, flex-fuel vehicles performed with better fuel economy than standard spark-ignition light-duty vehicles. Moreover, high concentration alcohol blends reduce energy consumption as well as tank-to-wheel $CO_2$ emissions despite their higher fuel consumption. The developed model can be applied to fuel consumption estimations in FFVs from single chemical compounds to commercial fuel products including new fuel blends.

## 1. Introduction

Transport grows dynamically, in 2018, the sector's energy consumption of about 2.8 Gtoe [1] was mainly relying on fossil fuels (over 95 % [2]) which corresponded to emissions of about 8.2 Gt of $CO_2$ accounting for 24.6 % of total world $CO_2$ emissions [1]. The road mode covers 74.5 % of transport emissions which translates to 6.1 Gt of $CO_2$ emissions. This could be further split into road passenger transport (including cars, motorcycles, buses, and taxis) 3.7 Gt and road freight (trucks and lorries) 2.4 Gt of $CO_2$ emissions [3]. Therefore, road passenger transportation accounts for 45.1 % of transport emissions and 11.1 % of world energy sector emissions (33.5 Gt of $CO_2$) [1].

Currently, there are around 1.4 billion vehicles on roads worldwide [4,5], where in Europe there are around 268 million passenger cars

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*Abbreviations:* ABS, Absolute Value; ANN, Artificial Neural Network; BMLR, Best Multiple Linear Regression; BSFC, Brake Specific Fuel Consumption; C, Carbon; C2G, Cradle-to-Grave; CO, Carbon monoxide; $CO_2$, Carbon dioxide; CR, Compression ratio; DC, Driving Cycle; DI, Direct Injection; E, Ethanol; E10, EN228 compliant gasoline with up to 10% ethanol vol. content; E85, Fuel consisted of max. 85% ethanol and 15% gasoline; EC, Energy Consumption; EGR, Exhaust Gas Recirculation; EMS, Engine Management System; EN228, European gasoline standard; EPA, United States Environmental Protection Agency; ETBE, Ethyl *tert*-Butyl Ether; EU, European Union; EV, Electric Vehicle; FC, Fuel Consumption; FFE, Flex-Fuel Engine; FFV, Flex-fuel vehicle; FTP, Federal Test Procedure; G, Gasoline; GHG, Greenhouse Gases; H, Hydrogen; HC, Unburned hydrocarbon emission; HDV, Heavy Duty Vehicle; HHV, Hydraulic Hybrid Vehicles; HP, Horsepower; HVO, Hydrotreated Vegetable Oil; iBu, Isobutanol; ICE, Internal Combustion Engine; ICEV, Internal Combustion Engine Vehicle; IV, Independent Variable; LDV, Light-duty vehicle; LHV, Lower heating value; $LHV_{mass}$, Lower heating value mass-based; $LHV_{vol}$, Lower heating value volume-based; M, Methanol; MLP, Multilayer Perceptron; MLR, Multi-Linear Regression; MON, Motor octane number; nBu, *N*-butanol; NEDC, New European Driving Cycle; $NO_x$, Nitrogen Oxides; O, Oxygen; PDF, Probability Density Function; PFI, Port fuel injection; R, Renewable component; RON, Research octane number; S, Octane Sensitivity; SI, Spark ignition; SS, Steady-State; SSO, Steady-State Operation; THC, Total Hydrocarbon; TRL, Technology Readiness Levels; TTW, Tank-To-Wheel; TWC, Three-way catalyst; UDC, Urban Driving Cycle; VP, Vapor Pressure; VVT, Variable Valve Timing; WLTP, Worldwide Harmonised Light Vehicles Test Procedure; WTW, Well-to-wheel.

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(10.8 years lifetime), 33.2 million vans (10.9 years lifetime), 6.6 million trucks (12.4 years lifetime) and around 770 thousand buses (11.4 years lifetime) [6]. Light-duty vehicles (cars and vans) constitute the vast majority of the market (over 97 %), and when it comes to the share of powertrains in Europe there were around 3.3 million electric vehicles (EV) in use in 2020, which accounts for 1.12 % of European LDV fleet, whereas remaining 98.88 % are internal combustion engine vehicles (ICEVs) [7]. Global light-duty vehicle sales are expected to maintain levels of over 80 million vehicles annually with an increasing tendency toward 90 million in 2025[8]. In 2025 it is predicted that 84 % of global vehicle sales will be ICEVs whereas EVs will account for the remaining 16 % [9]. Taking into the account lifetime of LDVs, and continuous sales of new ICEVs, in 2040 there will be around 1.2 billion ICEVs on the roads worldwide [10]. To meet the global climate targets the production of renewable fuels has to increase dramatically. In 2018, road transportation utilized 2Gtoe of crude oil, which is nearly half of the world's final consumption of crude oil including all sectors [11]. The electricity use in transport was equivalent to 33.5 Mtoe [11], whereas the use of renewable fuels to 88.4 Mtoe [12]. When comparing those figures, it could be noticed that the magnitude of the decarbonization challenge of road transportation is so high that all sustainable solutions are needed in very high quantities to tackle climate change.

Currently, the majority of commercial renewable fuels are produced from biomass, which according to M. F. Demirbas et al. could be considered as the best option in sustainable energy development with the large potential for securing the fuel supply in the future [13]. Recent studies show that renewable fuels have a very low well-to-wheel (WTW) and cradle-to-grave (C2G) environmental impact, which in some cases is significantly lower compared to EVs [14,15]. Another important aspect is that renewable fuels bring very efficient and immediate decarbonization, especially when speaking of drop-in fuels that do not require new powertrains or refueling infrastructure. Good examples are hydrotreated vegetable oil (HVO) known also as renewable diesel or renewable gasoline that could be used respectively in the existing fleet of compression ignition and spark ignition engines. Although renewable fuels are very often more expensive in production compared to their fossil counterparts [16], they have a great potential to reduce not only carbon dioxide emissions, but also regulated and unregulated emissions [17,18,19]. In that respect, renewable fuels can reduce the costs of exhaust after-treatment systems, where an extreme example is modern hydrogen dedicated internal combustion engine, which eliminates the vast majority of exhaust emissions while keeping NOx emissions at very low levels [20].

An alternative to drop-in solutions, Flex-Fuel Vehicles (FFV) allow the use of non- drop-in renewable fuels in high concentrations such as ethanol in 85 % known also as E85. In Brazil, even neat ethanol (E100) is available for FFVs, D. R. Cassiano et al. investigated the end-use performance and emissions of E27 and E100 fuels in FFV during real traffic conditions in Fortaleza city located in Brazil [21]. Such high-concentration ethanol blends could be safely utilized in Flex-Fuel engines thanks to the number of technical advantages over regular SI engines. Ethanol attracts water which might accelerate the corrosion of materials [22], this is why in FFVs ethanol compatible materials are utilized in fuel tanks, fuel pumps, fuel injection systems, and other engine components. Additionally, fuel pumps and injectors of FFVs are designed to operate at higher flows due to the lower calorific content of ethanol. Another aspects of high ethanol blends are related to cold start issues which in modern FFVs are resolved by advanced injection strategies [23]. The technological advancements of FFVs lead to a significant increase in energy conversion efficiency as well as to the reduction of greenhouse gas emissions [24]. In practice, the Engine Management System (EMS) of FFVs receives the signals from the lambda sensor as well as from the sensor of ethanol concentration in the fuel tank. Based on that data, EMS adjusts engine operating parameters including boosting pressure, injection timing and quantity, ignition timing, intake and exhaust flow handling systems, and Exhaust Gas Recirculation (EGR) system [23]. Such optimizations allow FFVs to utilize more efficiently high ethanol content fuels (e.g. better resistance for knocking combustion) compared to regular gasoline-calibrated SI engines. FFVs become an even more attractive option when considering the manufacturing cost of their engines, which is only 180 EUR higher compared to the production cost of 2265 EUR for modern downsized Gasoline Direct Injection (GDI) SI LDV engine [25]. FFVs have been produced since the 1990s and it is estimated that by 2018 around 60 million FFVs were manufactured [26], this accounts for around 4.29 % of the on-road vehicle fleet. Around half of the FFV fleet is concentrated in Brazil (30.5 million LDVs). The second major market is the US with 21 million registered FFVs, subsequently Canada with 1.6 million, and Europe with around 250 thousand vehicles (led by Sweden). In 2022, FFVs are continuously produced by manufacturers, however, their market share and penetration remain low. When looking at the development trends of FFVs, G. Azhaganathan, and A. Bragadeshwaran classified them into six generations (produced from 2003, 2006, 2008, 2009, 2013, and 2019) [23]. In general, progressively with FFV generations, higher ranges of compression ratios were introduced along with improvements in engine power and torque. Cold start issues were resolved by first auxiliary gasoline injection, then electrical heaters, and finally through advanced injection strategies.

The future development trends are oriented toward hybrid solutions combining Flex-Fuel Engine (FFE) with electrical motors and batteries, that will increase further the energy efficiency of the modern hybrid FFVs [27]. Bridging renewable fuels with hybrid powertrains in the FFVs both with batteries but also with hydraulics allows harnessing the kinetic energy of the vehicle while braking, which in consequence improves the fuel economy significantly [28]. When it comes to batteries, Ö. Andersson et al. [29] investigated the Life Cycle Assessment (LCA) of electrified vehicles with renewable fuels, and showed that such powertrain/fuel combinations can provide a substantial reduction of $CO_2$ emissions, reaching levels well below the fully electrified vehicles both in the current scenario (2020) as well as distant future (2050), even despite very high share of sustainable electricity in the grid. The case is similar with hydraulic hybrid vehicles (HHV), T. P. Barbosa et al. proved that HHV has a potential of reducing up to 47.2 % the $CO_2$ emissions, and 20.7 % $NO_x$ emissions levels in the real-world driving cycles [30]. Additional engine optimizations such as operation under lean burn conditions can further reduce $NO_x$ emissions [31]. The reduction of $NO_x$ emissions, as well as lower $CO$ emissions with the growing percentage of ethanol in blends with gasoline, was observed by C. Dardiotis et al. in two FFVs over various driving cycles [32]. Moreover, alcohol fuels such as methanol, ethanol and butanol increase thermal efficiency, reduce total hydrocarbon (THC) and $NO_x$ emissions in the dual-fuel engines as observed by Z. Chen et al. [33].

Fuel-dedicated engines can increase energy conversion efficiency to much higher levels compared with FFVs and regular SI engines. A. Boretti presented an optimized direct injection (DI) turbocharged engine with a compression ratio (CR) of 13:1 powered by pure ethanol (E100) that used 43 % less fuel energy when compared to regular SI engines [34]. Moreover, for low knocking tendency fuels, the CR of dedicated engines could be increased much further, which in turn will lead to additional strong improvements in fuel economy and heavy reduction of $CO_2$ emissions. Such a case was investigated by X. Zhen et al. in a study where knocking of methanol was tested in an SI engine of 17.5 CR [35].

### 1.1. *Current fuel consumption models for light-duty vehicles*

The vehicle engine performance represented by Fuel Consumption (FC) or GHG emissions, could be influenced by many factors. Generally, the FC influencing parameters could be divided into external factors such as driving route, roadway characteristics, traffic type, and intensity, weather, etc. and internal factors related to the engine of the vehicle (powertrain), fuels [36] and additives [37,38]. In the extensive study of M. Zhou et al. existing vehicle FC predicting models are summarized [39].

When it comes to external factors, K. Ahn et al. modeled the effect of route choice on FC and demonstrated that the choice of a faster highway route is not always the best in terms of FC and GHG emissions [40]. Besides fuel economy, H. C. Frey showed that the choice of route and its duration affects significantly local emissions [41]. The effect of travel route on FC was also investigated and modeled by K. Boriboonsomsin et al. [42], M. Barth et al. [43] and B. Luin et al. [44]. Furthermore, the type of roadway (road gradient such as up-down slopes) has a great impact on fuel economy. M. A. S. Kamal et al. developed a nonlinear model for economical vehicle drive based on road gradient conditions obtained from digital road maps, which led to significant fuel savings [45]. Additionally, the effect of road slope, driving behavior, as well as vehicle load (passengers) on FC and GHG emissions was assessed and quantified by S. Carrese et al. [46]. The next factor affecting the FC of vehicles is the traffic. D. Biggs et al. developed the detailed fuel consumption model called ARFCOM, which can estimate the FC from cars to 40-tonne trucks, dependent on traffic-related variables [47]. Modeling the vehicle fuel consumption based on traffic variables was also performed by J. Kropiwnicki [48] and S. Wörz et al. [49]. Whereas, Y.T. Zhang et al. developed a fuel consumption model for hybrid vehicles based on operation of ICE, electric machine (EM) and battery [50].

The influence of traffic lights on fuel consumption and GHG emissions were modeled and simulated by T. Tielert et al. [51] and B. Asadi et al. [52]. When it comes to the interaction between the driver and traffic lights, M. Sanchez et al. presented that there are possibilities of 25 % savings in fuel consumption within the range of urban areas [53]. Driving pattern factors such as acceleration, deceleration, stops, speed oscillations, gear shifting, etc. clearly influence both FC and GHG emissions of LDVs as examined by E. Ericsson [54]. The impact of driving patterns on vehicle fuel consumption was modeled by X. Zhou et al. [55]. The effects of driving aggressiveness on vehicle performance were studied by I. M. Berry [56], while J. Van Mierlo et al. highlighted that technical solutions and educational programs are possible measures to reduce the influence of driving style on emissions and fuel consumption. Additionally, the importance of effective traffic management in congested areas was highlighted by S. Zhang et al. [57] in the study where fleet-total fuel consumption and $CO_2$ emissions were modeled for Macao registered vehicles.

Proceeding with significant factors, weather conditions influence the FC and GHG emissions of LDVs, M. Rahimi-Gorji et al. applied a multilayer perceptron (MLP) artificial neural network (ANN) and regression technique to develop two mathematical models showing the impact of air pressure, temperature and humidity on brake specific fuel consumption (BSFC) of the LDV engine [58]. It is important to note that climate conditions shift also travel modes in traffic and affect activity levels as presented by S. Saneinejad et al. [59]. One of the most important internal factors affecting the vehicle FC is related to the engine, J. Yanowitz et al. studied the FC and GHG emissions of 6 FFVs of different production years (different millage), displacements, CR, with direct and port injection of the fuel. All vehicles were powered by both E10 and E40, the results show clearly that both engine itself and the type of fuel have a great impact on fuel economy [60].

When the engine and fuel are constant, engine operating conditions influence the FC. LDV engines are not operating at the one steady-state (SS) point of load and speed (as in the case of marine engines), but combine a large number of SS points and transient conditions. Optimization of engine-fuel maps is therefore essential to improve FC and GHG emissions [61,62]. An analytic model for fuel consumption estimations based on powertrain variables over vehicle cruising and accelerating conditions was developed by M. Ben-Chaim [63]. R Joumard et al. developed a model for FC and emissions estimation during urban driving as a function of the vehicle type and its instantaneous speed and acceleration [64]. Similar studies and modeling work was performed by I. El-Shawarby et al. [65], whereas S. Park et al. developed the FC and GHG emission model for not only LDVs, but also HDVs [66].

Besides the powertrain effects, fuel type plays a very important role when thinking of the end-use performance. Standard fossil fuels have their regulated norms such as EN228 for European market gasoline, therefore their FC is very similar. Currently, while the sustainable energy transition gains momentum, the importance and role of alternative fuels are dynamically rising. Such fuels differ in their chemical composition when compared to standard fossil EN-228 gasoline, which in consequence affects also fuel properties [67,68]. Different fuel properties translate into variations in fuel consumption [69], which for the standard fleet of spark-ignition and compression ignition engines was modeled by Y. Kroyan, et al. [70]. A similar methodology was applied by M. Wojcieszyk et al. in the development of the FC model for marine engines [71].

Taking into consideration the lack of a model for end-use analysis of alternative fuel properties in the fleet of SI engines optimized more towards renewable fuels than regular SI-LDVs as well as the high importance of co-optimization of fuels and engines to explore better the potential of alternative fuels in achieving higher performance, reduce the energy consumption and lower the environmental impact [72]. The present work aims to contribute to that niche by developing a state-of-the-art mathematical model that will allow for the first time accurate estimations of fuel consumption in FFV engines based on alternative fuel properties exclusively.

### 1.2. Outline of the novelty

As it was presented in the previous chapter, there is no mathematical model available in the literature that represents the direct impact of fuel properties on fuel consumption in FFV engines. The current work develops and introduces an accurate mathematical model that will allow fast and cost-free estimations of fuel consumption in FFV engines for all kinds of liquid fuels from single chemical compounds to ready fuel products (consisting of thousands of molecules).

The outline of the present work is as follows:

- Section 3.1: Analyzes the collected data from published experimental campaigns of alternative fuels, their properties and performance in FFV engines.
- Section 3.2: Introduces a state-of-the-art mathematical model called FFV- FC that allows for the first time accurate estimations of FC in FFV engines using solely fuel properties. Additionally, based on the developed database, it shows which fuel properties are the most significant for the performance in FFV engines.
- Section 3.3: Explores the performance differences between FFVs and regular SI-LDVs when operating on alternative fuels.
- Section 3.4: Applies the FFV-FC model to simulate the end-use performance metrics for top gasoline blendstocks. This section discovers attractive blending ratios of alternative fuels with regular gasoline, leading to improved energy consumption and reduced $CO_2$ emissions.

## 2. Methodology

The objective of this work is to develop a mathematical model that will accurately link the collective impact of the most significant fuel properties of alternative fuels with their end-use performance in optimized spark-ignition engines of LDVs such as flex-fuel vehicles (FFV). The target model should represent the impacts from the end-user perspective, apply to the entire fleet of SI FFVs and work well for all kinds of fuels, including single chemical compounds, refinery streams, and ready fuel products. The careful selection of a proper methodology is a key part to meet such objectives.

### 2.1. Selection of the approach

Engine performance represented by fuel consumption could be

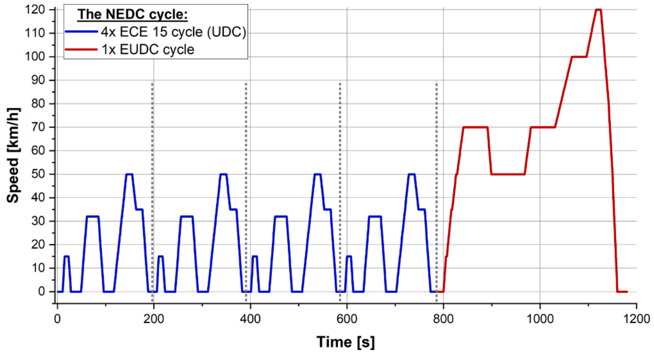

**Fig. 1.** The velocity profile of New European Driving Cycle (NEDC).

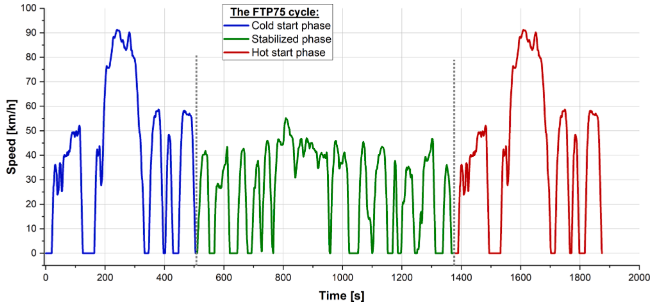

**Fig. 2.** The velocity profile of US Environmental Protection Agency (EPA) Federal Test Procedure (FTP-75).

experimentally measured during the Steady-State Operation (SSO) of the engine or Driving Cycles (DC). The main difference is that during SSO tests the performance is defined for a single point of engine speed and load at a time. In SSO there are no transient engine operation conditions, which are essential when speaking of real-life use of vehicles. On contrary, DC such as Worldwide Harmonised Light Vehicles Test Procedure (WLTP), New European Driving Cycle (NEDC), or the US Environmental Protection Agency (EPA) Federal Test Procedure (FTP) include a significant part of the engine speed and load points together with transient con– ditions. Therefore, when the target is the representation of fuel effects from an end-use perspective, the driving cycles approach is significantly more suitable. Y. Kroyan et al. [70] proved that by comparing the SSO measurement data from various sources, the SSO results were lacking any visible trends. Hence, the driving cycles approach is selected in the present work for further analysis.

Driving cycles are standardized procedures that aim to measure the vehicle engine performance (fuel consumption) and/or tailpipe emissions in an accurate, repetitive, and comparative way. They include a series of data points that represent the speed of a vehicle versus time, which is called a velocity profile, and each driving cycle has its type of velocity profile. As mentioned before, driving cycles include a large number of steady-state points as well as transient conditions. The final result of DC is one average number of for example FC per entire driving cycle expressed in L/100 km that describes well the end-use performance. In that sense, the DC approach is much more attractive when comparing FC of various alternative fuels, as DC produces much clearer trends when comparing the data from different origins. When it comes to FFVs the vast majority of DC data available in the literature are related to the NEDC or FTP-75 driving cycles. Fig. 1 represents the velocity profile of the NEDC driving cycle, whereas Fig. 2 shows the speed/time data for FTP-75.

The NEDC cycle consists of Urban Driving Cycle (UDC) and The Extra-Urban Driving Cycle (EUDC). UDC known also as ECE-15 was introduced in 1970, and is intended to reflect driving in the busy European cities (low engine load, and maximum speed of 50 km/h) [73]. Whereas, EUDC introduced in 1990 represents high-way driving, characterized by high speeds (max. 120 km/h, and for low power vehicles max. speed 90 km/h) [74]. The entire NEDC includes 4 UDC phases (from 0 s to 780 s) and 1 EUDC (from 780 s to 1180 s). The FTP-75 cycle consists of a cold start transient phase with an ambient temperature of 20–30 °C from 0 to 505 s, stabilized phase from 506 s to 1372 s, and a hot start transient phase from 1372 s to 1877 s. However, after the stabilized phase, the engine is turned off for around 10 min (min 540 s, max 660 s). That period is known as a hot soak, and right after it, the hot start transient phase begins. The FTP-75 cycle is presented in the Fig. 2.

When comparing the NEDC to FTP-75, it could be noticed that NEDC tests are usually performed in cold start conditions, whereas FTP-75 investigates both cold and hot start. The duration of NEDC (the 1180 s) is shorter than FTP-75 (1877 s), also the distance driven in NEDC (11.03 km) is 6.74 km shorter compared to FTP- 75 (17.77 km). Average velocities are similar, for NEDC 33.6 km/h and FTP-75 34.12 km/h, whereas the maximal velocity of NEDC 120 km/h is higher than that of FTP-75 91.25 km/h.

### 2.2. *Data*

The FC driving cycle data for various alternative fuels tested in FFVs are coming from 13 different sources marked in the paper as: A [75], B [60], C [76], D [77], E [78], F [32], G [79], H [80], I [81], J [82], K [83], L [84], M [85]. All sources include empirical data, where measurements were taken while running driving cycles using real vehicles (no simulation data involved). Based on inputs the database of 85 observations of

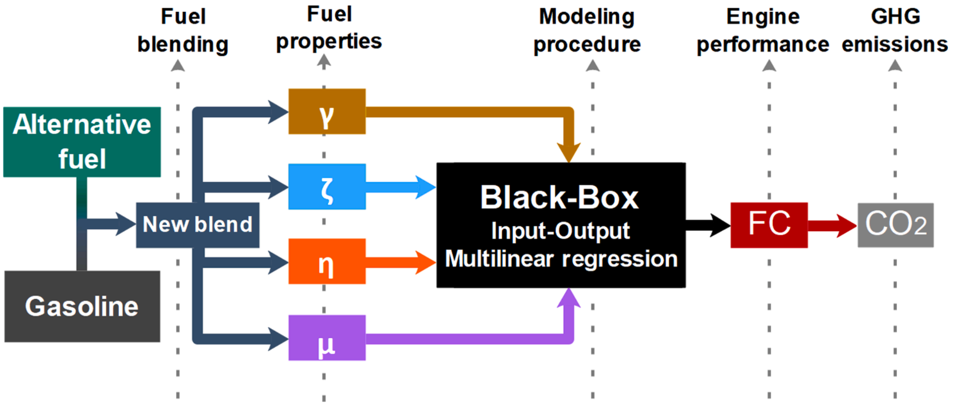

**Fig. 3.** The research problem - letters" $\gamma, \zeta, \eta, \mu$" represent fuel properties such as RON, MON, density, viscosity, calorific content, etc. The fuel consumption (FC) relative to standard gasoline is estimated based on the FFV-FC model that uses fuel properties as inputs. The carbon dioxide emissions are subsequently calculated based on the carbon content of the fuel and results of FC.

FC for various fuels was constructed. The FTP-75 driving cycle was performed in 7 sources (A, B, C, D, I, J, K, and L), whereas the NEDC in 5 sources (E, F, G, H, and M). When it comes to differences in terms of relative changes of fuel consumption when using the same fuels but different driving cycles, A. Olmos et al. [86] showed in the case of E22 and E100 that those relative differences of FC when comparing FTP-75 with NEDC are negligible. Therefore, FTP-75 and NEDC results could be compared to each other. Information about FFVs and their engines used in each source for alternative fuel testing is provided in the Appendix A.

### 2.3. Model development and validation

Alternative fuels such as methanol or ethanol differ in their fuel properties from standard EN228 gasoline. The same applies to blends of renewable fuels with gasoline, the new blend will differ in its fuel properties compared to the base fossil counterpart. The difference in fuel properties is reflected subsequently in the engine performance measures including FC and $CO_2$ emissions. The Fig. 3 visualizes the research problem where fuel properties such as Research Octane Number (RON), Motor Octane Number (MON), density, viscosity, calorific content, etc. are represented by letters" $\gamma,\zeta,\eta,\mu$". The target of this work is to develop a model that will find the direct relationship between fuel properties and fuel consumption in FFVs.

Many individual fuel properties influence the FC to a certain degree. In the modeling procedure, all fuel properties are taken in as Independent Variables (IV). As the modeling problem includes multiple IVs (fuel properties) and a single dependent variable (fuel consumption), multilinear regression (MLR) was selected for the development of the model. As fuel properties are interrelated and affect the performance of engines collectively, the modeling procedure incorporates quantitative analysis, to find the ultimate combination of the most significant fuel properties, where each of them has its unique influence on FC. Additionally, all variables (input and output) are represented as percentage changes relative to standard fossil gasoline. This step allows to better observe trends based on data coming from various sources (different FFVs, fuels, measurement equipment, etc.). Additionally, the relative changes approach makes the final model more universal and applicable, as when such changes are known they could be easily calculated and extrapolated to all kinds of FFV engines. The following equation (1) represents the function of the step-wise Best Multiple Linear Regression (BMLR) that was applied in the modeling part.

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

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

Referring to Fig. 3, the Equation (1) could be expressed as follows:

$$\alpha = a_\gamma\cdot\gamma(X_R) + a_\zeta\cdot\zeta(X_R) + a_\eta\cdot\eta(X_R) + a_\mu\cdot\mu(X_R) \qquad (2)$$

where $\alpha$ - relative change of fuel consumption [% change in reference to l/km], $X_R$ - The volumetric concentration of the alternative fuel in the blend with standard gasoline, $\gamma(X_R),\zeta(X_R),\eta(X_R),\mu(X_R)$- relative change of fuel property $\gamma,\zeta,\eta,\mu$ [% change relative to standard gasoline], $a_{\gamma,\zeta,\eta,\mu}$ - coefficients of property $\gamma,\zeta,\eta,\mu$.

As mentioned before, all variables are represented as changes relative to standard gasoline (expressed in %), and they are calculated in the following way:

$$\gamma(X_R) = (\gamma_R - \gamma_G)/\gamma_G\cdot 100\% \qquad (3)$$

where $\gamma(X_R)$- the value of specific fuel property [$\gamma$] for alternative fuel blend dependent on the concentration of alternative fuel [$X_R$], $\gamma_G$ - value of specific fuel property [$\gamma$] for standard gasoline, $\gamma_R$ - value of specific fuel property [$\gamma$] for neat alternative fuel.

The least-squares method is used to approximate the solution during the regression analysis in the modeling stage [87] - Equation (4).

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

where $J_\theta$ - least-squares objective function.

The modeling which includes quantitative analysis aims to ensure the statistical significance of all independent variables. It means that their p-values have to be lower than the significance level of 5 % (P-value ≤ 0.05) in the final model while achieving the highest possible R-Square. The p-value is a data-based measure that oscillates between 0 and 1 and represents the probability of observing the results outside the range of statistical significance. In practice, the lower p-value the less interrelated is given independent variable from other variables that co-exist in the model. Low p-values ensure that each variable has its unique and particularly important impact, which in consequence leads to more accurate and stronger models. The p-value is calculated based on the *t*-value (result of the Student's *t*-test - statistical hypothesis test) and probability density function (PDF). More details about the p-value calculation are described by Y. Kroyan et al. [70]. The step-wise BMLR method has an iterative approach where IV is added or removed after each iteration. The modeling begins with no variables in the model, then each possible variable is being added to the model, and the respective p-value calculated (statistical significance testing). In case the variable has a p-value greater than 0.05 (5 %) it is rejected from the model, however, when the p-value remains below 0.05 level that variable stays in the model. The process is continued and repeated for each possible IV until all variables are tested and the model is completed. This specific iteration is known as forward stepwise regression, where the final model reaches the highest possible R-square while including the most significant independent variables. The coefficient of determination (R-square) and standard error control the accuracy during the modeling.

There are three options to evaluate carbon dioxide emissions of any fuel-powertrain combination: Tank-To-Wheel (TTW), Well-To-Wheel (WTW), and Cradle-To-Grave (CTG). TTW $CO_2$ emissions take into consideration only tailpipe (exhaust) emissions, without considering the environmental impact related to feedstock production, conversion into fuel, and logistics involved in the process. Meanwhile, the WTW approach counts carbon dioxide emissions from feedstock to tailpipe, by taking into account all the steps mentioned above. However, the most robust approach is known as Cradle-To-Grave (CTG) which besides including all the assessments of the WTW part, it counts also carbon-dioxide emissions involved with the production and recycling of the vehicle and powertrain.

Once the fuel consumption model for FFV is completed, it is used to calculate the TTW carbon dioxide $CO_2$ emission. For that purpose, the outputs of the FC model are utilized together with density, the carbon content in the fuel, and the coefficient (44.01/12.0107) which represents the molar mass relation between carbon dioxide and carbon. Equation (5) represents the calculation methodology:

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

where $\delta$ - $CO_2$ emissions [g/km], $\alpha_{ABS}$ - absolute value of fuel consumption [l/km], $\rho$ - density of the fuel [g/dm$^3$], $z$ - mass-based carbon content in the fuel [%], 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 gasoline can be calculated in the following way:

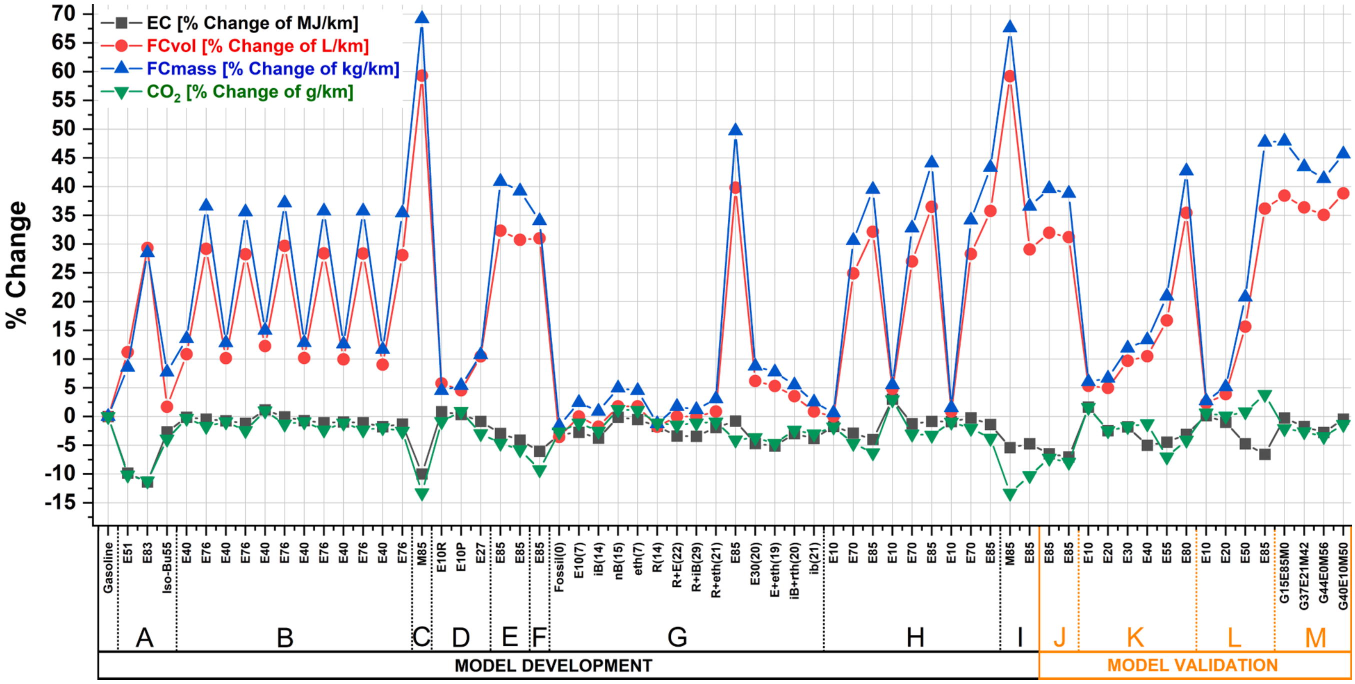

**Fig. 4.** The end-use performance results for alternative fuels relative to standard gasoline. Chart based on the data sources specified in Section 2.2.

**Table 1**
Average end-use performance measures (EC, FCvol, FCmass, tailpipe or TTW $CO_2$ emissions) of alternative fuel blends tested in data sources (A [75], B [60], C [76], D [77], E [78], F [32], G [79], H [80], I [81], J [82], K [83], L [84], M [85]).

| Alternative fuels | Symbol | Nr of observations | EC | Average values of FCvol | FCmass | CO2 | Data from sources |
|---|---|---|---|---|---|---|---|
| Ethanol | E10 | 8 | 0.1 | 3.0 | 3.6 | 0.2 | D, G, H, K, L, G |
| | E20 | 2 | −1.7 | 4.4 | 5.9 | −1.2 | K, L |
| | E30 | 3 | −2.4 | 8.8 | 10.5 | −2.8 | D, G, K |
| | E40 | 7 | −1.2 | 10.4 | 13.1 | −0.8 | B, K |
| | E50 | 3 | −6.3 | 14.5 | 16.8 | −5.5 | A, K, L |
| | E70 | 9 | −1.0 | 28.0 | 34.9 | −2.5 | B, H |
| | E85 | 14 | −4.3 | 33.6 | 40.9 | −5.4 | A, E, F, G, H, I, J, K, L, M |
| Methanol | M85 | 2 | −7.7 | 59.3 | 68.4 | −13.3 | C, I |
| | M56 | 1 | −2.7 | 35.1 | 41.4 | −3.5 | M |
| Isobutanol | iBu55 | 1 | −2.7 | 1.7 | 7.7 | −3.9 | A |
| | iBu14 | 1 | −3.7 | −1.8 | 0.9 | −2.5 | G |
| | iBu21 | 1 | −3.8 | 0.9 | 2.5 | −3.0 | G |
| Nbutanol | nBu15 | 1 | −0.1 | 1.8 | 5.0 | 1.2 | G |
| Ethyl *tert*-butyl ether | ETBE7 | 1 | −0.5 | 1.8 | 4.5 | 1.1 | G |
| Renewable component | R14 | 1 | −1.7 | −1.8 | −1.2 | −1.1 | G |
| Binary blends | iBu + ETBE20 | 1 | −3.0 | 3.5 | 5.5 | −2.4 | G |
| | R + E22 | 1 | −3.4 | 0.0 | 1.8 | −1.5 | G |
| | R + iBu29 | 1 | −3.4 | 0.0 | 1.2 | −1.1 | G |
| | R + ETBE21 | 1 | −1.9 | 0.9 | 3.1 | −0.9 | G |
| | E + ETBE19 | 1 | −5.1 | 5.3 | 7.7 | −4.7 | G |
| Tertiary blends | G37 + E21 + M42 | 1 | −1.7 | 36.4 | 43.5 | −2.6 | M |
| | G40 + E10 + M50 | 1 | −0.5 | 38.8 | 45.7 | −1.4 | M |

$$z = (X \cdot z_R \cdot \rho_R + (1 - X) \cdot z_G \cdot \rho_G)/\rho \tag{6}$$

where $X$ - volumetric fraction (concentration) of alternative fuel [%], $\rho_R$ - density of neat alternative fuel [g/dm$^3$], $\rho_G$ - density of neat gasoline [g/dm$^3$], $z_R$ - carbon content in alternative fuel [%], $z_G$ - carbon content in gasoline [%].

The energy consumption (EC) is calculated on a basis of FC and calorific content:

$$\varepsilon = \alpha_{ABS} \cdot LHV_{ABS} \tag{7}$$

where $\varepsilon$ represents the energy consumption in [MJ/km] and $LHV_{ABS}$ is a lower heating value of a given fuel expressed in [MJ/L].

The final model is validated against the internal data (used for modeling) as well as external data coming from multiple sources that were not taken into the modeling process.

## 3. Results and discussion

This section focuses on the results of the current work, with special attention to:

1. Analysis of the FFV performance data represented by volumetric and mass- based fuel consumption, energy consumption, and $CO_2$ emissions.

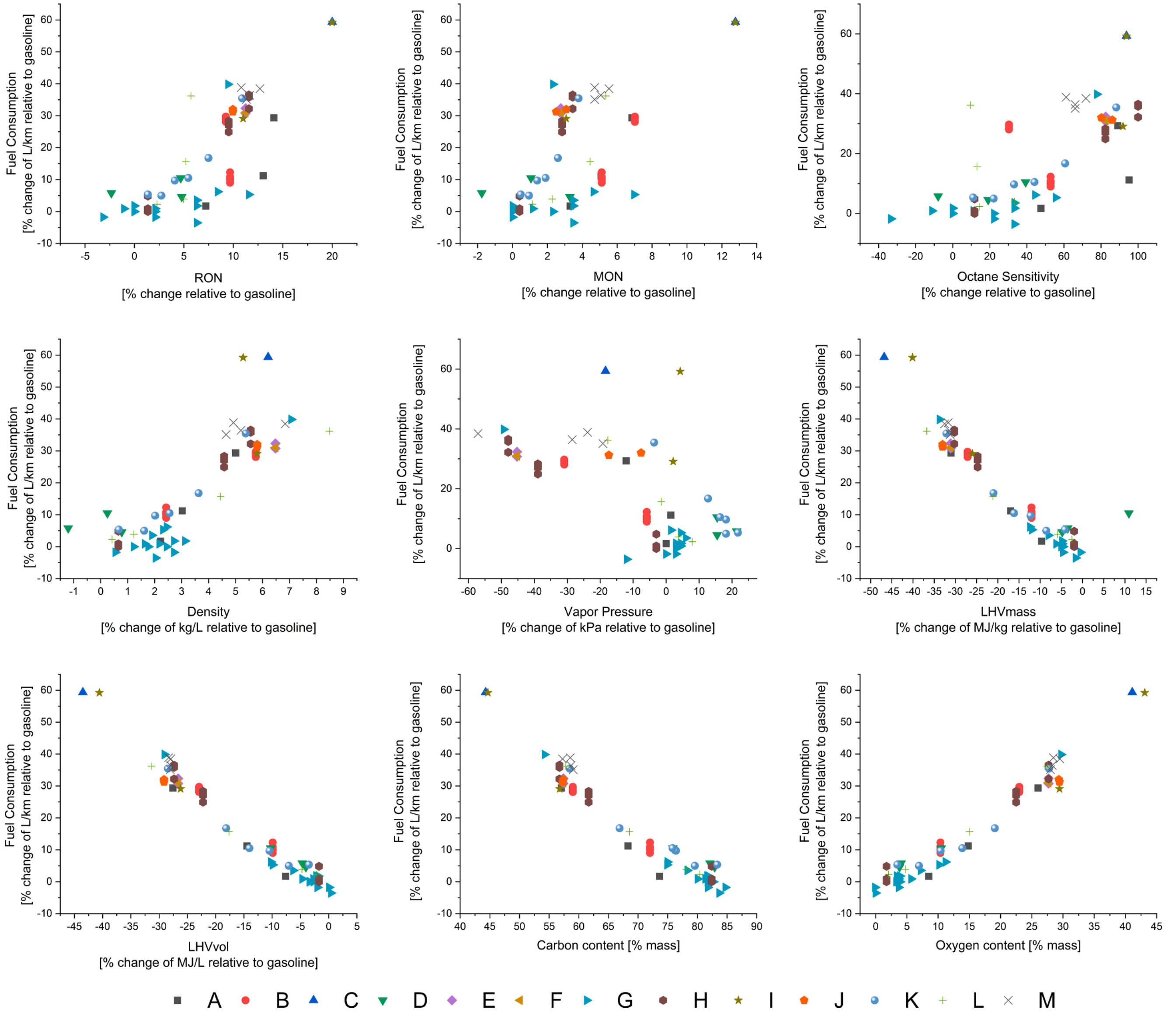

**Fig. 5.** The change of fuel properties against the change of fuel consumption in FFVs.

**Table 2**
Modeling results, the most important fuel properties for FCvol in FFV engines are LHVvol, S, Density and VP (P-values much bellow 1% in all cases). The FFV-FC model has very high accuracy represented by the R-Square of 0.994.

| Variable | Coefficient | Std. Error | *T*-value | P-value |
|---|---|---|---|---|
| LHVvol | −1.653 | 0.064 | −25.842 | 0.000 |
| S | −0.061 | 0.014 | −4.470 | 0.000 |
| Density | −1.575 | 0.285 | −5.528 | 0.000 |
| VP | −0.079 | 0.023 | −3.467 | 0.001 |
| R-Square | 0.994 | | | |

2. Presentation of the developed model for fuel end-use analysis in FFVs as well as its internal and external validation.
3. Simulation of the fuel consumption in FFvs vs regular spark-ignition engine vehicles for various renewable fuels. The analysis and discussion about the performance benefits in fuel-optimized engines in comparison to regular SI engines designed for standard fossil gasoline.

### *3.1. The FFV performance data*

Based on 13 independent sources 85 rows of data were collected, 65 rows of data (about 76 %) coming from 9 sources were used for model development, whereas 20 rows (about 24 %) of data from 4 sources for external validation of the model. Different alcohol-based alternative fuels were tested, such as ethanol, methanol, isobutanol, *n*-butanol, and ethyl *tert*-butyl ether (ETBE) in various concentrations with standard gasoline as well as combinations of their binary and tertiary blends. All fuels were tested in FFVs produced from the year 1993 up to 2017, in engines with displacements ranging from 1.6 to 5.7l (4–8 cylinders), power oscillating between 92-381HP (148-544Nm torque), compression ratios from 9.0:1 to 11.7:1, both with port- and direct- injection of the fuel, as well as naturally aspired and turbocharged. Therefore, the data that were collected represent a wide range of FFV engine types, more details can be found in the Appendix A.

The end-use performance data of tested alternative fuels are plotted as volumetric and mass-based fuel consumption (FCvol and FCmass), energy consumption (EC), and $CO_2$ emissions in the Fig. 4. The dataset contains 62 tests of alternative fuels and 23 runs with standard gasoline. The most commonly tested fuel in the dataset was ethanol in

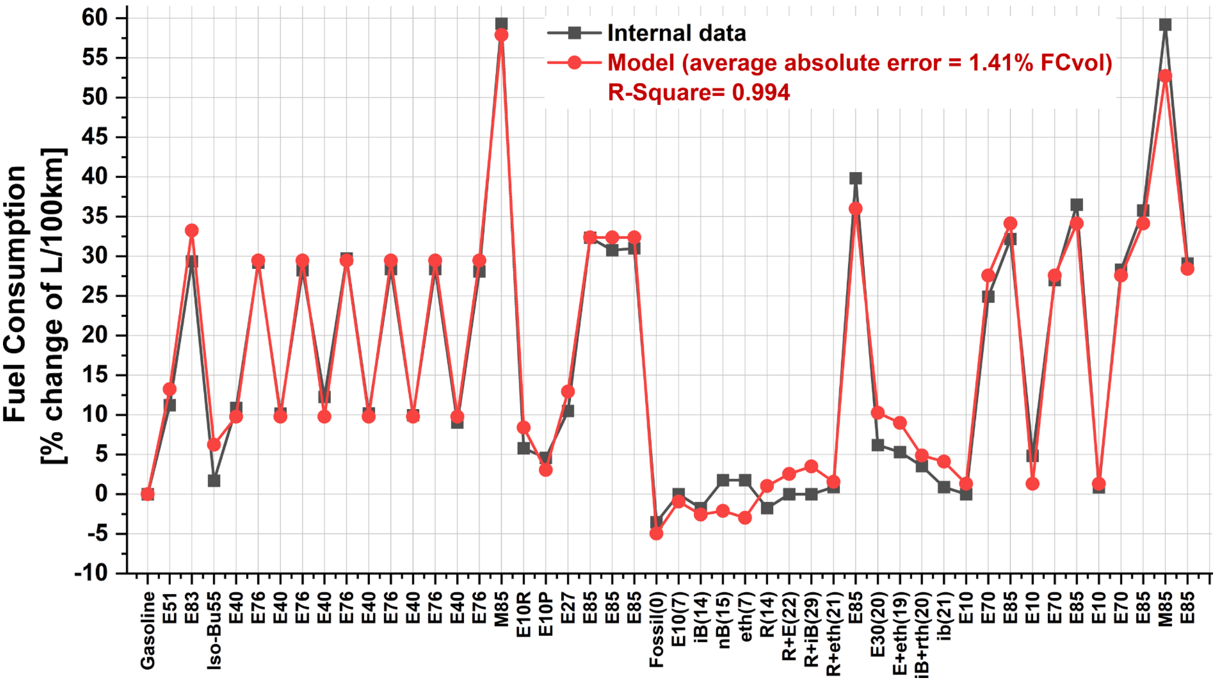

**Fig. 6.** Internal validation of the FFV-FC model against the data used for model development from the following sources: A [75], B [60], C [76], D [77], E [78], F [32], G [79], H [80], I [81].

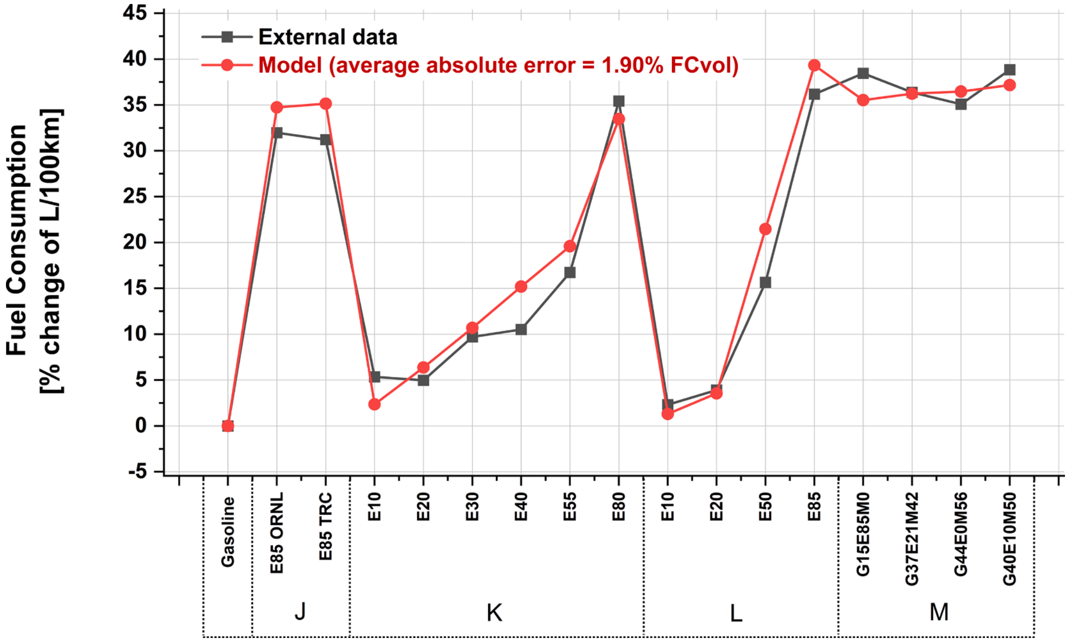

**Fig. 7.** External validation of the FFV-FC model against four independent sources of data: J [82], K [83], L [84], M [85].

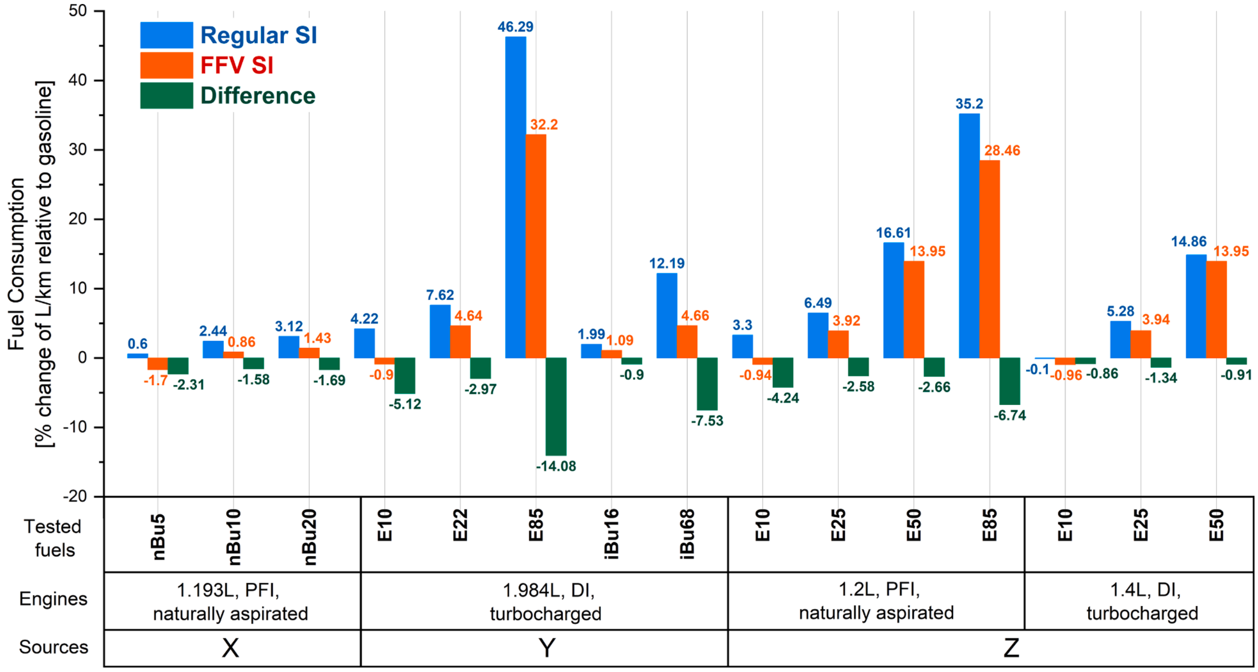

**Fig. 8.** The performance of alternative fuels in FFvs vs regular SI-LDVs. The data of FC for regular SI-LDvs comes from experimental campaigns published in sources X [89], Y [90], and Z [91]. Whereas the FC for FFvs was simulated by applying the developed in this study FFV-FC model.

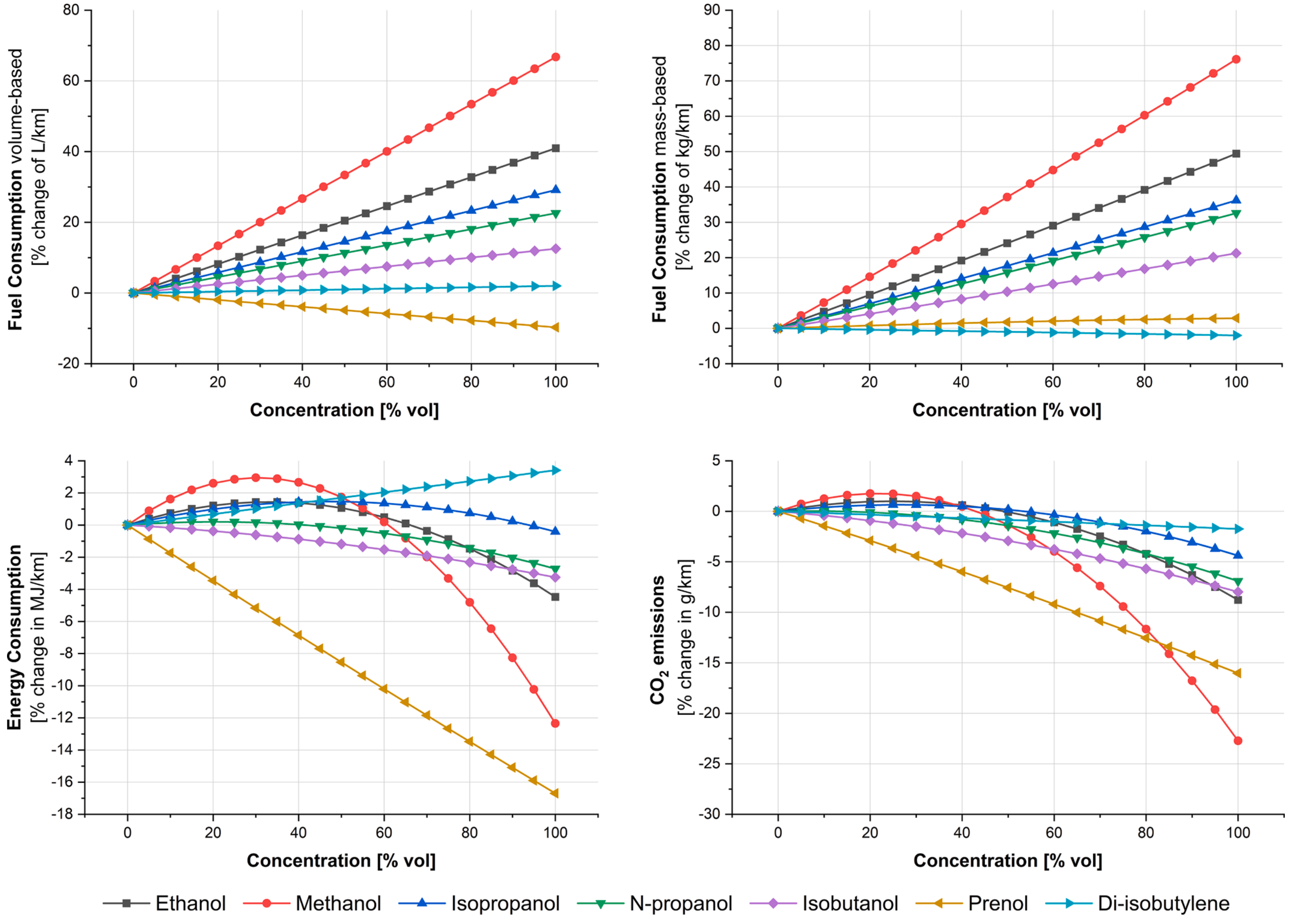

**Fig. 9.** The end-use performance of renewable gasoline blendstocks.

concentrations ranging from 10 % (E10) to 85 % (E85) with gasoline. It could be noticed that with the growing concentration of ethanol the fuel consumption notably increases compared to gasoline, reaching on average 33.6 % higher FCvol and 40.9 % higher FCmass for E85. The reason for such difference in FC is the calorific content LHV of ethanol (21.1 MJ/L or 26.7 MJ/kg) which is significantly lower compared to gasoline (about 32 MJ/L or 43 MJ/kg). However, despite the higher FC, ethanol blends provide better energy conversion efficiency (partially because of the higher RON), which is reflected in the 4,3% lower EC of the E85 blend. All other ethanol blends have lower EC compared to their fossil counterpart as well. Because of ethanol's significantly lower carbon content compared to gasoline, tank-to-wheel (TTW) $CO_2$ emissions of ethanol blends are also lower, even despite their much higher fuel consumption. In the case of E85 $CO_2$ emissions are 5.4 % lower.

Methanol blends reach even further with the reductions of EC and $CO_2$, showing values respectively 7.7 % and 13.3 % lower for M85 compared to gasoline. On the other hand, methanol has even lower LHV (15.8 MJ/L or 19.9 MJ/kg) than ethanol, which translates into an average of 59,3% higher FCvol and 68.4 % higher FC- mass. Among tested alcohols, butanol has the highest calorific content LHV (27.9 MJ/L or 34.4 MJ/kg) which yielded lower differences in FC compared to lighter alcohols, while decreasing both EC and TTW $CO_2$ emissions. Ether ETBE in a concentration of 7 % with Gasoline performs similar to neat gasoline, just with negligibly higher FCvol and $CO_2$ emissions, in both cases, the changes are bellow 2 %.

In source G [79] unknown renewable component (R) was tested in 14 % blend with gasoline and binary blends (no gasoline involved) with 22 % ethanol, 21 % ETBE, and 29 % isobutanol. Based on results, it could be noticed that blending of 14 % R improved negligibly end-use performance measures, and in binary blends with isobutanol and ETBE, values are close to gasoline. An only binary blend of R with 29 % iBu achieves 3.4 % better EC. In other binary blends (iBu + ETBE20 and E + ETBE19) as well as tertiary blends (G37 + E21 + M42 and G40 + E10 + M50) the end-use relations are similar to classical alcohol blends, meaning higher FC measures while lower EC and TTW $CO_2$. Average values of the end-use performance measures are summarized in the Table 1.

The Fig. 5 represents the change of single fuel properties against the change of FCvol. The figure was built based on fuel properties and FCvol reported in data sources. When thinking of the energy content of the fuel, which is essential in energy conversion processes, the higher the energy content (both LHVvol and LHVmass), the lower fuel consumption should be. That relation could be easily observed in the Fig. 5. It could be also noticed that the lower the carbon content and the higher the oxygen content the higher the fuel consumption. However, low reactivity (high RON, and MON) and high-density fuels that were tested are in the vast majority alcohols that also have lower calorific content compared to gasoline. That affects and makes it difficult to observe the specific impact of RON, MON, S, and density separately. As fuel properties are interrelated, it is extremely difficult to draw conclusions when looking at each fuel property individually. This is why the next section focuses on the collective impact of fuel properties, aiming to address the question of which fuel properties together matter the most for fuel consumption in FFVs.

### 3.2. Modeling results

In this section, the modeling results related to the collective impact of the most significant fuel properties on FCvol in FFV engines are presented and discussed. Based on the gathered data that were earlier specified in sections 2.2 and 3.1 a modeling matrix was built that included: RON, MON, Sensitivity (S), Density, Vapor Pressure (VP), LHVmass, LHVvol, carbon content (C), oxygen content (O), and hydrogen content (H) as multiple independent variables (fuel properties), whereas volumetric fuel consumption was selected as a single response variable. The modeling matrix is included in the Appendix B. The results of performed modeling are presented in the Table 2.

Based on the data and modeling the most significant fuel properties for FCvol in FFV engines turned out to be S, LHVvol, Density, and VP. It is worth noticing significantly lower than 1 % P-values of each fuel property which, confirms the unique and important impact of every individual fuel property as well as good strength of the final model. Additionally, R-Square of 0.994, reflects the high accuracy of the developed FFV-FC model. The final form of the FFV-FC model is represented in the following equation:

$$\alpha_{FFV-FC} = -0.061\cdot\gamma - 1.653\cdot\eta - 1.575\cdot\zeta - 0.079\cdot\mu \quad (8)$$

where $\gamma$ stands for sensitivity, $\eta$ for lower heating value volume-based, $\zeta$ for density, and $\mu$ for vapor pressure.

In the internal validation the high R-Square (0.994) of the FFV-FC model translated into the average absolute error of 1.41 % of FCvol. The visual comparison of the model outcomes to the data used for modeling is presented in the Fig. 6.

The FFV-FC model is validated also against the external data that the model has never seen in the training procedure. Four independent sources of data (J [82], K [83], L [84], M [85]) were used, where both ethanol and methanol as well as their tertiary blends with gasoline were tested in FFVs. It could be noticed that the FFV-FC model performed very well in the external validation, by predicting the changes of FCvol very accurately and close to the measured values. That good accuracy is also reflected in a very low average absolute error of 1.90 % FCvol in the external validation (see Fig. 7).

The present analysis is based on limited number of observations related to solely liquid renewable fuels. In that respect the model was not tested against unconventional fuels in a gaseous phase such as hydrogen or ammonia. Nevertheless, the current analysis is valid and applicable to liquid alternative fuels including different alcohols, ethers and their blends with paraffins, isoparaffins, cyclic hydrocarbons and aromatic compounds.

The developed FFV-FC model allows instant, cost-free, and accurate analysis of fuel consumption in FFVs for alternative liquid fuels. Moreover, as the explanatory variables of the model are fuel properties, the FFV-FC model could be applied to end-use performance assessments from single chemical compounds, groups of molecules, refinery streams, to ready fuel products consisted of large number of chemical molecules. Therefore, the FFV-FC model could be applied for analysis from laboratory scale to industrial across the whole spectrum of Technology Readiness Levels (TRL).

### 3.3. Performance differences between FFVs and regular SI-LDVs

This section is focused on the comparison of the fuel consumption between regular SI-LDvs vs FFvs for various alternative fuels. The aim is to investigate whether FFvs are operating more efficiently with alternative fuels than regular SI-LDVs. FFV powered by high RON fuels can achieve higher effective CR through advanced ignition timing, Variable Valve Timing (VVT), and boosting the intake pressure (feedback control of FFV engines adjusts fuel delivery and ignition timing to achieve higher CR) [88]. To make that comparison, the fuel consumption for alternative fuel blends with gasoline at various concentrations was taken into analysis. The FC data for regular SI LDvs were taken from the following three sources; X [89] (blends of *n*-butanol with gasoline), Y [90] (blends of ethanol and isobutanol with gasoline), Z [91] (blends of ethanol with gasoline), where in all cases end-use performance was tested over the NEDC. The fuel properties (S, LHVvol, Density, and VP) of tested blends were taken as inputs to the FFV-FC model to simulate their performance in flex-fuel vehicles. The comparison is presented in the Fig. 8, where the difference in FC for alternative fuels in regular SI-LDvs vs FFvs is revealed.

It could be noticed that in all cases renewable fuels perform with better fuel economy in FFVs. When it comes to ethanol blends with gasoline, high ethanol concentration blends (E85) show the biggest difference in FC while comparing regular SI vehicles with FFVs. FFVs powered by up to 20 % blends of *n*-butanol or isobutanol with gasoline show rather small changes in FC, nevertheless still they perform slightly better in FFVs than regular SI-LDVs. Despite 10 % lower LHVvol of fuel blend containing 68 % isobutanol with 32 % gasoline (iBu68), the fuel consumption in FFVs is only 4.66 % higher compared to neat gasoline. At the same time, iBu68 performs with 7.53 % better fuel economy in FFVs compared to regular SI-LDVs. In European Union, the EN228 standard sets the blending wall of max 10 % ethanol with gasoline for regular SI-LDVs [92]. Based on the data from sources Y and Z, it could be noticed that E10 blends perform on average with 2.47 % higher FC in regular SI LDVs, whereas in FFVs with almost 1 % lower. On the other hand, ethanol blends between E22-E25, perform with higher FC both in regular SI vehicles and FFVs compared to neat gasoline, nevertheless still on average 2.29 % of FC could be saved when using such blends in FFVs.

The 50 % ethanol blend with gasoline was tested in source Z using two vehicles, one naturally aspirated with port fuel injection (PFI), while the second vehicle was equipped with a turbocharged direct-injection (DI) engine. In FFVs, the E50 fuel performs with 2.66 % and 0.91 % lower FC compared to respectively vehicle 1 and vehicle 2. This result is indicating that modern regular SI-LDVs (DI and turbocharged) are utilizing more efficiently ethanol blend fuels compared to their older generations (PFI and naturally aspirated).

### *3.4. Simulation of the end-use performance for renewable gasoline blendstocks*

The FFV-FC model was applied to simulate the end-use performance (FCvol, FC- mass, EC, and $CO_2$ emissions) of renewable gasoline blendstocks in their entire blending spectrum with standard fossil gasoline. The following fuels were chosen for analysis: methanol, ethanol, isopropanol, *n*-propanol, isobutanol, prenol, and di-isobutylene. The selection of components was motivated by the Co-Optima project which highlighted them as the best blendstocks for turbocharged spark- ignition engines [72]. For the simulation purpose, fuel properties of selected gasoline blendstocks were obtained from the Co-Optima project including the fuel properties database from the National Renewable Energy Laboratory (NREL) [93].

Ethanol is the most widely used gasoline blendstock worldwide, it has almost 14.7 % higher RON than gasoline, and around 6 % higher density. However, ethanol is 32 % less calorific (on a volume basis) than gasoline, which results in about 41 % higher FCvol for E100. Nevertheless, E100 has about 39 % less carbon than fossil gasoline, which leads to noticeable reductions in TTW $CO_2$ emissions (-8.7 % for E100 compared to gasoline). Additionally, improved EC could be observed when operating FFV engines with high ethanol concentration blends, reaching a maximum of 4.47 % energy savings for E100. Among analyzed blendstocks, the highest resistance for knocking combustion has isopropanol with the RON rating of 113 and MON 97. Both isopropanol and *n*-propanol have higher FC than gasoline, yet lower when compared to lighter alcohols such as methanol or ethanol. Fuel blends with propanol isomers have similar EC to standard gasoline, with a slight reduction for very high concentration blends (-2.7 % EC for neat isopropanol). Isobutanol is more calorific than propanol, it has 14 % lower LHVvol than gasoline, which yields 12.53 % higher FCvol for iBu100. However, energy conversion for isobutanol is more efficient when compared to gasoline, which could be noticed on the plot of EC.

The most reactive fuel among tested blendstocks is prenol (RON = 93 and MON = 74). Prenol has also the highest density (848 g/L), which combined with very high LHV translated into the lowest values of FCvol and EC for blends with gasoline as well as for neat component. On the other hand, prenol has the lowest vapor pressure of 0.19 kPa at 37.8 °C which from the practical perspective might cause cold-start problems in SI engines. The highest fuel consumption is observed for methanol and its blends with gasoline, because of the low values of their calorific content. Despite that methanol leads to the greatest reductions in TTW $CO_2$ emissions driven by the lowest carbon content (37.48 % mass-based for neat $CH_3OH$) when compared to other blendstocks. Moreover, a great reduction in energy consumption could be observed for blends containing more than 60 % of methanol, reaching a maximum of over 12 % energy savings while running the engine with M100 compared to fossil gasoline. The curve of EC for methanol blends has a strongly nonlinear character, which is caused mainly by the fact that FCvol grows steadily while calorific content decreases fast with increasing concentration of methanol in the blends with gasoline. The same character of the plot could be observed for methanol's $CO_2$ emissions, where similarly FC increases while carbon content drastically decreases for blends containing gradually higher methanol content.

The most similar to gasoline in terms of calorific content is di-isobutylene with LHVvol of 31.675 MJ/L, no oxygen content, and very comparable MON of 87. However, di-isobutylene has a much higher RON value of 106 for the neat component, which lifts octane sensitivity to the value similar to ethanol. The density of di-isobutylene is about 4 % lower compared to gasoline, while vapor pressure for the neat component shows 11.02 kPa at 37.8 °C. When looking into the end-use performance of di-isobutylene, it is almost identical to gasoline fuel consumption both in volume and mass-based comparison. Moreover, the FC similarity is kept across the full concentration spectrum. However, slightly higher energy consumption could be observed that reaches a maximum of + 3.4 % EC for neat di-isobutylene, while TTW $CO_2$ emissions are slightly lower (−1.74 % for the neat component). Fuel properties taken for the simulation of the end-use performance of renewable gasoline blendstocks are in Appendix D, while the Fig. 9 represents the FCvol, FCmass, EC, and $CO_2$ emissions for all blendstocks across the entire concentration range with standard gasoline.

## 4. Conclusions

Based on the literature data the present study investigated the end-use performance of alternative fuels in a wide range of FFV engines. The present work developed a state-of-the-art mathematical model (FFV-FC) that accurately predicts the FC in FFV engines based on a known set of fuel properties. The results show that:

The most significant fuel properties for FCvol in FFV engines are octane sensitivity($\gamma$), LHVvol ($\eta$), density ($\zeta$), and vapor pressure($\mu$):

$$\alpha_{FFV-FC} = -0.061\cdot\gamma - 1.653\cdot\eta - 1.575\cdot\zeta - 0.079\cdot\mu$$

All independent variables in the model have p-values significantly lower than 1 % which confirms their unique and important impact on FCvol. The high accuracy of the model represented by an R-Square of 0.994, translated into an average absolute error of 1.41 %FCvol during internal validation and 1.90 % FCvol against the data that the model has never seen (external validation).

- The FFV-FC model applies to end-use performance analysis of alternative fuels from single chemical compounds, groups of molecules, and refinery streams, to ready fuel products in FFV engines.
- Growing ethanol concentration in blends with gasoline leads to an increase of FCvol that in the case of E85 reaches on average 33.6 % higher values compared to neat gasoline. However, despite higher

fuel consumption, E85 operates more efficiently than gasoline in FFV engines, which could be concluded based on 4.3 % lower energy consumption. As the carbon content of ethanol is lower compared to standard gasoline, TTW $CO_2$ emissions of E85 are 5.4 % lower as well. The same relation is observed for methanol, isobutanol blends, as well as binary (iBu + ETBE20, E + ETBE19) and tertiary blends (G37 + E21 + M42, and G40 + E10 + M50).

- The FFV engines perform noticeably better with low reactivity alternative fuels of high knocking resistance when compared to regular SI-LDV engines. The largest fuel savings (FFV vs regular SI-LDV) are observed for high concentration ethanol and isobutanol blends (E85 and iBu68).
- The end-use performance simulations for renewable gasoline blendstocks show that methanol markedly increases FC while drastically reducing the TTW $CO_2$ emissions for high concentration blends with gasoline. The most efficient energy conversion could be observed for prenol with 16.7 % savings in EC, and the second-best reduction (after methanol) in TTW $CO_2$ emissions. On the other side, di-isobutylene blends with gasoline show slightly higher EC, while their FC vol and mass are almost identical compared to standard gasoline. Ethanol, propanol isomers, and isobutanol blends increase FC such that the lighter alcohol the higher FC (strongly influenced by their calorific content). High concentration alcohol blends reduce $CO_2$ emissions, as well as EC.

FFV technology is mature, economically feasible, and relatively easy to increase its market penetration. As it was presented in the current work FFVs utilize more efficiently alternative fuels then regular SI-LDVs. Fuels like ethanol are also relatively easy in production which is an important factor when thinking of the scalability aspects and in turn enhancements of energy security. Moreover, hybridization of the FFVs powered by renewable fuels, as well as advancements in fuel dedicated technologies, can strongly contribute to time and cost-effective decarbonization.

## CRediT authorship contribution statement

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

## 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.

## Data availability

All the research data is directly available on the paper

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## Appendix A. FFV information

Refer Table 3.

**Table 3**
Specification of flex-fuel vehicles used for fuel testing in each source.

| Source | Make | Model | Year | Displ. [L] | Config. | Injection | Power [HP] | Torque [NM] | CR | VVT | Aspiration | Milage [km] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| A [75] | Ford | F-150 | 2013 | 3,7 | V-6 | Port | 302 | 377 | 10.5:1 | Yes | Natural | 22,027 |
| | Chevrolet | Silverado | 2014 | 5,3 | V-8 | Direct | 380 | 416 | 11:1 | Yes | Natural | 1646 |
| | Nissan | Titan | 2009 | 5,6 | V-8 | Port | 320 | 533 | 9.8:1 | Yes | Natural | 33,796 |
| | Toyota | Tundra | 2010 | 5,7 | V-8 | Direct | 381 | 544 | 10.2:1 | Yes | Natural | 27,359 |
| | Dodge | Caravan | 2002 | 3,3 | V-6 | Port | 180 | 285 | 9.3:1 | – | Natural | 177,027 |
| B [60] | GMC | Terrain | 2011 | 3,0 | V-6 | Direct | 264 | 222 | 11.7:1 | Yes | Natural | 16,093 |
| | Ford | Taurus | 2002 | 3,0 | V-6 | Port | 155 | 251 | 9.3:1 | – | Natural | 185,074 |
| | Ford | Fusion | 2011 | 3,0 | V-6 | Port | 250 | 309 | 11.0:1 | Yes | Natural | 17,703 |
| C [76] | Ford | Taurus | 1993 | 3,0 | V-6 | Port | 223 | 271 | 9.8:1 | – | Natural | – |
| D [77] | Chevrolet | Equinox | 2017 | 2,4 | l-4 | Direct | 182 | 233 | 11.2:1 | Yes | Natural | – |
| E [78] | – | – | 2009 | 1,8 | – | Port | 92 | – | – | – | – | – |
| | – | – | 2010 | 2,0 | – | Direct | 132 | – | – | – | – | – |
| F [32] | – | – | 2009 | 1,8 | – | Port | 92 | – | – | – | – | – |
| G [79] | – | – | 2006 | 2,0 | l-4 | Port | 132 | 280 | – | – | – | 62,000 |
| | Ford | Focus | 2003 | 1,6 | l-4 | Port | 103 | 148 | 11.0:1 | Yes | Natural | 38,200 |
| H [80] | Ford | Focus | 2003 | 1,6 | l-4 | Port | 103 | 148 | 11.0:1 | Yes | Natural | 48,700 |
| | Ford | Focus | 2002 | 1,6 | l-4 | Port | 103 | 148 | 11.0:1 | Yes | Natural | 29,800 |
| I [81] | Ford | Taurus | 1993 | 3,0 | V-6 | Port | 223 | 271 | 9.8:1 | – | Natural | 27,352 |
| | Chevrolet | Lumina | 1993 | 3,1 | V-6 | Port | – | – | – | – | – | 28,485 |
| J [82] | Saab | 9–5 BioPower | 2007 | 2,0 | l-4 | Port | 180 | 280 | 9.0:1 | – | Turbo | – |
| K [83] | Mercury | Grand Marquis | 2006 | 4,6 | V-8 | Port | 224 | 369 | 9.38:1 | – | Natural | – |
| L [84] | Chevrolet | Silverado | 2007 | 5,3 | V-8 | Direct | 380 | 416 | 11:1 | Yes | Natural | – |

## Appendix B. Modeling matrix

Refer Table 4.

**Table 4**
The matrix containing the data used for FFV-FC model development.

| Source | Driving cycle | **Fuel blend** | RON | MON | S | Density | VP | LHVmass | LHVvol | C | O | H | **FCvol** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | % change | | | | | %mass | | **% change** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,54 | 0,00 | 17,46 | **0,00** |
| A [75] | FTP-75 | **E51** | 13,02 | 5,08 | 95,12 | 3,02 | 1,43 | −16,97 | −14,46 | 68,28 | 14,83 | 16,89 | **11,21** |
| | | **E83** | 14,10 | 6,85 | 89,02 | 5,00 | −12,14 | −31,03 | −27,58 | 57,05 | 26,01 | 16,94 | **29,35** |
| | | **Iso-Bu55** | 7,21 | 3,31 | 47,56 | 2,22 | 0,00 | −9,65 | −7,65 | 73,61 | 8,49 | 17,90 | **1,71** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **10,86** |
| | | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **29,18** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **10,17** |
| | | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **28,23** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **12,27** |
| B [60] | FTP-75 | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **29,71** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **10,19** |
| | | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **28,38** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **9,96** |
| | | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **28,37** |
| | | **E10** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,00 | 0,00 | 18,00 | **0,00** |
| | | **E40** | 9,68 | 5,11 | 52,81 | 2,43 | −5,87 | −12,03 | −9,90 | 72,00 | 10,38 | 17,62 | **9,03** |
| | | **E76** | 9,25 | 7,02 | 30,34 | 5,75 | −30,92 | −27,11 | −22,93 | 59,00 | 23,00 | 18,00 | **28,08** |
| C [76] | FTP-75 | **M0** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,40 | 0,00 | 13,60 | **0,00** |
| | | **M85** | 20,00 | 12,78 | 93,72 | 6,21 | −18,39 | −46,81 | −43,51 | 44,29 | 41,10 | 14,61 | **59,32** |
| | | **E0** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,58 | 0,00 | 13,42 | **0,00** |
| D [77] | FTP-75 | **E10R** | −2,34 | −1,76 | −7,87 | −1,21 | 21,43 | −3,50 | −4,66 | 82,13 | 4,07 | 13,80 | **5,79** |
| | | **E10P** | 4,78 | 3,29 | 19,10 | 0,78 | 15,48 | −4,78 | −4,04 | 82,90 | 3,82 | 13,28 | **4,58** |
| | | **E27** | 4,68 | 1,06 | 39,33 | 0,25 | 15,48 | 10,95 | −10,25 | 75,86 | 10,48 | 13,66 | **10,48** |
| | | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,80 | 0,00 | 15,20 | **0,00** |
| E [78] | NEDC | **E85** | 11,25 | 2,77 | 82,52 | 6,48 | −45,26 | −31,11 | −26,65 | 57,40 | 27,70 | 14,90 | **32,33** |
| | | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,80 | 0,00 | 15,20 | **0,00** |
| | | **E85** | 11,25 | 2,77 | 82,52 | 6,48 | −45,26 | −31,11 | −26,65 | 57,40 | 27,70 | 14,90 | **30,76** |
| F [32] | NEDC | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,80 | 0,00 | 15,20 | **0,00** |
| | | **E85** | 11,25 | 2,77 | 82,52 | 6,48 | −45,26 | −31,11 | −26,65 | 57,40 | 27,70 | 14,90 | **31,00** |
| | | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,63 | 0,00 | 15,37 | **0,00** |
| | | **Fossil hc** | 6,32 | 3,49 | 33,33 | 2,04 | −11,94 | −1,61 | 0,40 | 83,68 | 0,00 | 16,32 | **−3,54** |
| | | **E10** | 2,11 | 0,00 | 22,22 | 2,45 | 2,99 | −5,05 | −2,72 | 81,68 | 3,60 | 14,72 | **0,00** |
| | | **Ibu14** | 2,11 | 0,00 | 22,22 | 2,72 | 2,99 | −4,59 | −1,99 | 81,76 | 3,70 | 14,54 | **−1,77** |
| | | **nBu15** | 0,00 | 0,00 | 0,00 | 3,13 | 2,99 | −4,82 | −1,84 | 81,64 | 3,90 | 14,46 | **1,77** |
| | | **ETBE7** | 6,32 | 3,49 | 33,33 | 2,72 | 4,48 | −4,82 | −2,23 | 81,83 | 3,40 | 14,77 | **1,77** |
| | | **R14** | −3,16 | 0,00 | −33,33 | 0,54 | 0,00 | −0,46 | 0,08 | 84,72 | −0,10 | 15,38 | **−1,77** |
| G [79] | NEDC | **R + E22** | 0,00 | 0,00 | 0,00 | 1,77 | 2,99 | −5,05 | −3,37 | 81,93 | 3,90 | 14,17 | **0,00** |
| | | **R + iBu29** | 2,11 | 2,33 | 0,00 | 1,22 | 2,99 | −4,59 | −3,42 | 82,67 | 3,30 | 14,03 | **0,00** |
| | | **R + ETBE21** | −1,05 | 0,00 | −11,11 | 2,17 | 2,99 | −4,82 | −2,75 | 81,34 | 3,70 | 14,96 | **0,88** |
| | | **E85** | 9,47 | 2,33 | 77,78 | 7,07 | −49,25 | −33,72 | −29,03 | 54,23 | 29,70 | 16,07 | **39,82** |
| | | **E30** | 8,42 | 4,65 | 44,44 | 2,45 | 1,49 | −12,39 | −10,24 | 74,95 | 11,20 | 13,85 | **6,19** |
| | | **E + ETBE19** | 11,58 | 6,98 | 55,56 | 2,31 | 4,48 | −11,93 | −9,89 | 74,89 | 10,20 | 14,91 | **5,31** |
| | | **iBu + ETBE20** | 6,32 | 3,49 | 33,33 | 1,90 | 5,97 | −8,03 | −6,28 | 78,31 | 7,20 | 14,49 | **3,54** |
| | | **iBu21** | 2,11 | 1,16 | 11,11 | 1,63 | 4,48 | −6,19 | −4,66 | 80,04 | 5,70 | 14,26 | **0,88** |
| | | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,48 | 0,00 | 15,52 | **0,00** |
| | | **E10** | 1,36 | 0,41 | 11,76 | 0,65 | −2,99 | −1,95 | −1,71 | 82,40 | 1,73 | 15,86 | **0,00** |
| | | **E70** | 9,54 | 2,84 | 82,36 | 4,58 | −38,93 | −24,74 | −22,23 | 61,67 | 22,50 | 15,82 | **24,90** |
| | | **E85** | 11,58 | 3,45 | 100,00 | 5,56 | −47,92 | −30,23 | −27,36 | 56,73 | 27,69 | 15,57 | **32,17** |
| | | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,48 | 0,00 | 15,52 | **0,00** |
| H [80] | NEDC | **E10** | 1,36 | 0,41 | 11,76 | 0,65 | −2,99 | −1,95 | −1,71 | 82,40 | 1,73 | 15,86 | **4,83** |
| | | **E70** | 9,54 | 2,84 | 82,36 | 4,58 | −38,93 | −24,74 | −22,23 | 61,67 | 22,50 | 15,82 | **26,99** |
| | | **E85** | 11,58 | 3,45 | 100,00 | 5,56 | −47,92 | −30,23 | −27,36 | 56,73 | 27,69 | 15,57 | **36,51** |
| | | **E5** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 84,48 | 0,00 | 15,52 | **0,00** |
| | | **E10** | 1,36 | 0,41 | 11,76 | 0,65 | −2,99 | −1,95 | −1,71 | 82,40 | 1,73 | 15,86 | **0,88** |
| | | **E70** | 9,54 | 2,84 | 82,36 | 4,58 | −38,93 | −24,74 | −22,23 | 61,67 | 22,50 | 15,82 | **28,30** |
| | | **E85** | 11,58 | 3,45 | 100,00 | 5,56 | −47,92 | −30,23 | −27,36 | 56,73 | 27,69 | 15,57 | **35,78** |
| | | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,40 | 0,00 | 13,60 | **0,00** |
| I [81] | FTP-75 | **M85** | 20,00 | 12,78 | 93,72 | 5,28 | 4,29 | −40,11 | −40,58 | 44,68 | 43,10 | 12,22 | **59,20** |
| | | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,40 | 0,00 | 13,60 | **0,00** |
| | | **E85** | 11,00 | 3,08 | 91,86 | 5,80 | 2,15 | −25,99 | −26,20 | 56,77 | 29,44 | 13,79 | **29,08** |

## Appendix C. Validation matrix

Refer Table 5.

**Table 5**
The matrix containing the data used for FFV-FC model validation.

| Source | Driving cycle | **Fuel blend** | RON | MON | S | DensityVP % change | | LHVmass | LHVvol | C | O %mass | H | **FCvol % change** |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| J [82] | FTP-75 | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,40 | 0,00 | 13,60 | **0,00** |
| | | **E85 ORNL** | 9,96 | 3,08 | 80,23 | 5,80 | −7,61 | −33,02 | −29,14 | 57,40 | 29,33 | 13,27 | **31,98** |
| | | **E85 TRC** | 9,96 | 2,51 | 86,05 | 5,80 | −17,39 | −33,02 | −29,14 | 57,30 | 29,44 | 13,26 | **31,21** |
| K [83] | FTP-75 | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 87,00 | 0,00 | 13,00 | **0,00** |
| | | **E10** | 1,36 | 0,47 | 11,03 | 0,67 | 21,82 | −4,16 | −3,51 | 83,33 | 3,47 | 13,20 | **5,35** |
| | | **E20** | 2,72 | 0,95 | 22,06 | 1,61 | 18,18 | −8,55 | −7,07 | 79,57 | 6,94 | 13,49 | **4,98** |
| | | **E30** | 4,09 | 1,42 | 33,09 | 2,02 | 18,18 | −12,24 | −10,47 | 76,39 | 10,41 | 13,20 | **9,70** |
| | | **E40** | 5,45 | 1,89 | 44,12 | 2,55 | 16,36 | −16,17 | −14,03 | 75,81 | 13,88 | 10,31 | **10,51** |
| | | **E55** | 7,49 | 2,60 | 60,66 | 3,63 | 12,73 | −21,02 | −18,15 | 66,88 | 19,09 | 14,03 | **16,73** |
| | | **E80** | 10,90 | 3,79 | 88,23 | 5,38 | −3,64 | −32,10 | −28,45 | 58,46 | 27,76 | 13,78 | **35,43** |
| L [84] | FTP-75 | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 82,09 | 0,21 | 17,70 | **0,00** |
| | | **E10** | 2,29 | 1,14 | 14,29 | 0,42 | 7,95 | −2,51 | −2,10 | 80,41 | 2,07 | 17,52 | **2,31** |
| | | **E20** | 4,99 | 2,28 | 33,33 | 1,22 | 3,75 | −5,87 | −4,72 | 78,12 | 4,77 | 17,11 | **3,91** |
| | | **E50** | 5,20 | 4,44 | 13,10 | 4,44 | −1,50 | −21,13 | −17,63 | 68,53 | 15,03 | 16,44 | **15,65** |
| | | **E85** | 5,72 | 5,35 | 9,52 | 8,48 | −17,69 | −36,74 | −31,38 | 57,72 | 27,47 | 14,81 | **36,18** |
| M [85] | NEDC | **Gasoline** | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 0,00 | 86,50 | 0,00 | 13,50 | **0,00** |
| | | **E85** | 12,70 | 5,53 | 71,84 | 6,84 | −57,07 | −32,54 | −27,95 | 57,26 | 29,50 | 13,25 | **38,45** |
| | | **G37 + E21 + M42** | 11,65 | 5,06 | 66,02 | 5,20 | −28,50 | −31,45 | −27,95 | 58,70 | 28,29 | 13,02 | **36,39** |
| | | **M56** | 11,33 | 4,71 | 66,02 | 4,65 | −19,20 | −31,22 | −28,01 | 59,06 | 28,00 | 12,94 | **35,10** |
| | | **G40 + E10 + M50** | 10,81 | 4,71 | 61,17 | 4,92 | −23,86 | −31,68 | −28,30 | 58,56 | 28,47 | 12,97 | **38,84** |

## Appendix D. Fuel properties of renewable gasoline blendstocks

Refer Fig. 10.

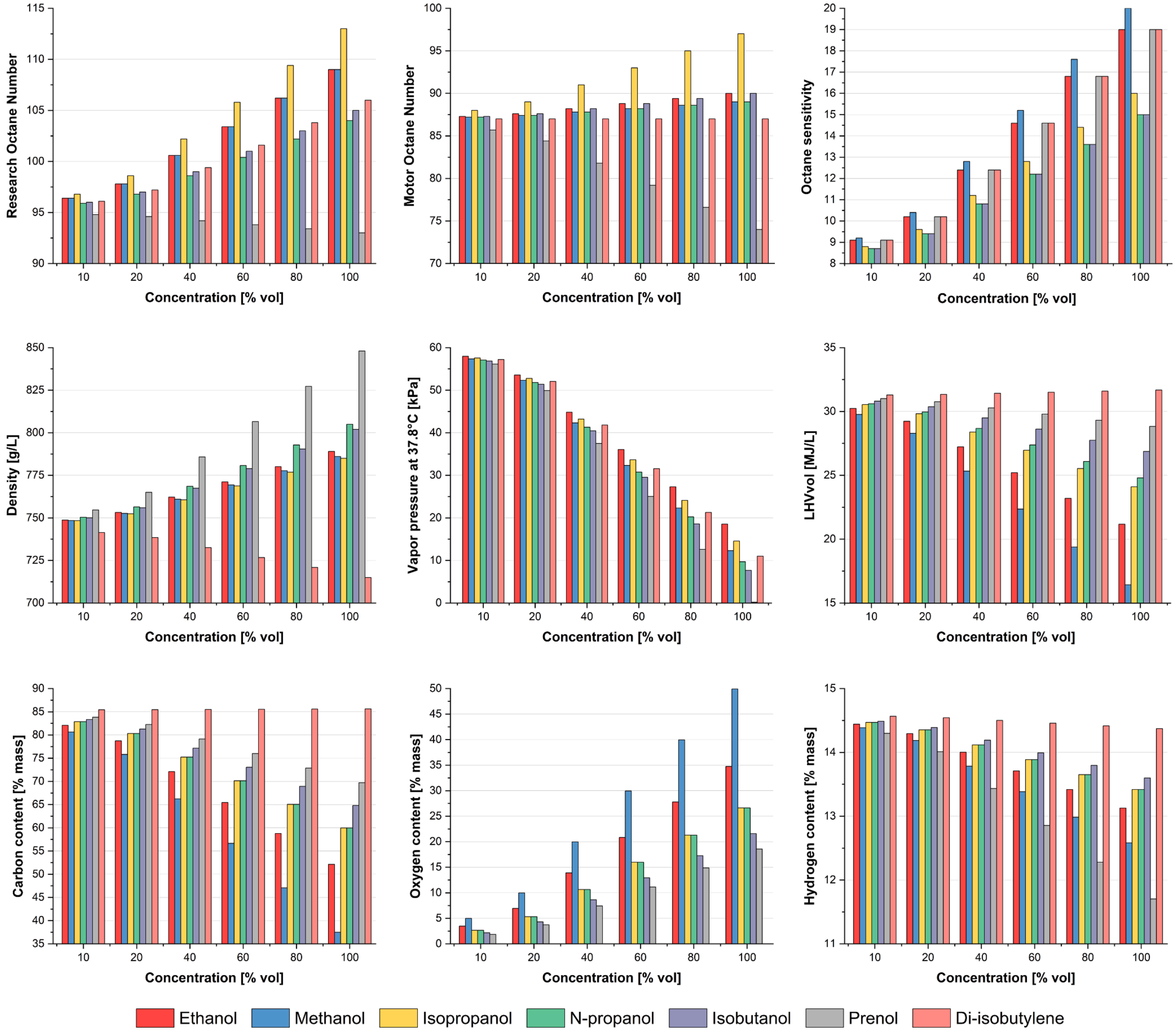

**Fig. 10.** Fuel properties of renewable gasoline blendstocks in the entire concentration spectrum with standards fossil gasoline.

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