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Published in:
Energy

DOI:
10.1016/j.energy.2023.129494

Published: 15/12/2023

Document Version
Publisher's PDF, also known as Version of record

Energy 285 (2023) 129494

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy

Prediction of heavy-duty engine performance for renewable fuels based on fuel property characteristics

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ARTICLE INFO

Keywords:
Renewable fuels
Fuel properties
Heavy-duty vehicles
Fuel economy
GHG emissions
End-use modeling

ABSTRACT

Renewable drop-in fuels can bring timely and efficient defossilization of the current fleet of heavy-duty vehicles. In the present study, different blends of renewable components with standard diesel were analyzed in the context of end-use performance. Based on experimental data from driving cycles, a novel modeling approach was applied to develop a state-of-the-art mathematical model that enables an accurate estimation of fuel consumption and tailpipe CO_2 emissions from heavy-duty vehicles relying solely on fuel properties. The predictions revealed strong agreements with experimental data confirmed by the high coefficient of determination (0.975). The final model represents fuel properties' collective impact on heavy-duty vehicle's fuel economy over the Braunschweig cycle where heating value, density, and cetane number showed the strongest impact (p-values < 0.01). The developed model was applied to simulate the effect of alternative diesel fuels on end-use performance. The increase in mass-based fuel consumption was observed for FAME (14%), oxymethylene ether blends (up to 65%), moderate contents of butanol and pentanol blends (up to 11%), while neat HVO improved fuel economy (6%). The introduced model can be applied to the assessment of renewable liquid fuel blends in heavy-duty transport and serves as a support for industry and decision-makers.

1. Introduction

Global transportation is heavily dependent on fossil resources. As a result, it is responsible for 24% of all anthropogenic CO_2 emissions [1]. At the same time, around 95% of energy carriers used in transport are still of fossil origin mostly supplied by a few countries like the United States, Saudi Arabia or Russia among others [2,3]. In the European Union (EU), thanks to Renewable Energy Directive (RED) implemented in 2009, the renewable energy share in transport met the 10% target by 2020 [4] and more ambitious goals beyond the RED II Directive are suggested [5]. Out of 7.2 Gt of CO_2 emitted by whole transportation in 2020, around 30% originated from the heavy-duty segment including trucks and buses [6]. Looking at the current EU market, there are over 6 million trucks and almost 700 thousand buses on European roads with an average lifetime of 14 and 13 years, respectively. In comparison, the new-built EU sales in 2020 reached 250 thousand trucks and 30 thousand buses [7–9]. Based on the above-mentioned key figures for the heavy-duty vehicle market, the technological transition will be a long-term process that additionally depends on fleet operator [10] and purchasing decision [11]. Therefore, a rather limited pace of fleet renewal is anticipated in the next decade and it is the main motivation behind the use of renewable drop-in fuels of both biogenic and non-biogenic origin.

The clear advantage of drop-in fuels lies in their compatibility with the current infrastructure. Hydroteaetd Vegetable Oil (HVO) and Fatty Acid Methyl esters (FAME) are examples of renewable components that could be directly blended with fossil diesel and used in existing compression ignition (CI) engines of heavy-duty vehicles. Renewable diesel represented by HVO belongs to the group of paraffinic fuels with high cetane number following EN 15940 standard. On the other hand, traditional biodiesel (FAME) from the transesterification process is standardized according to EN 14214. Even though both fuel types can originate from the same feedstock (vegetable oil or animal fat), there are notable differences in fuel properties [12].

Traditional biodiesel is more viscous and has higher density than reference diesel while paraffinic fuels do not meet the density limits from EN 590 standard. Blending FAME with fossil diesel improves the lubricity of the final fuel [13] while there is no such effect for HVO. FAME being an oxygenated compound reduces the toxicity of emissions, especially particulate matter as well as carbon monoxide and unburned hydrocarbon emissions [14,15], however, some unregulated emissions like formaldehyde tend to increase [16]. In heavy-duty CI engines, the emission reductions can be significant already at moderate (20% volumetric) concentrations of biodiesel in blends with fossil

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https://doi.org/10.1016/j.energy.2023.129494
Received 29 June 2023; Received in revised form 1 October 2023; Accepted 27 October 2023
Available online 31 October 2023

Nomenclature

Abbreviations

ADEME	French Environment and Energy Management Agency
BTL	Biomass-to-Liquid
CI	Compression ignition
CO_2	Carbon dioxide
EU	European Union
FAME	Fatty Acid Methyl Esters
GHG	Greenhouse Gases
GREET	Greenhouse gases, Regulated Emissions, and Energy use in Technologies model
GTL	Gas-to-Liquid
HHDDT	Heavy Heavy-Duty Diesel Truck
HVO	Hydrotreated Vegetable Oil
IEA	International Energy Agency
LHV	Lower Heating Value
MOVES	Motor Vehicle Emission Simulator
OMEs	Poly-oxymethylene dimethyl ethers
RED	Renewable Energy Directive
UDDS	Urban Dynamometer Driving Schedule
VECTO	Vehicle Energy Consumption calculation Tool

Symbols

$\gamma(X_A), \zeta(X_A), \eta(X_A), \mu(X_A)$	relative changes of fuel properties γ, ζ, η, μ for alternative fuel blend compared with reference diesel
α	relative change of fuel consumption - percentage change compared with reference in kg/100 km
α_{abs}	absolute value of fuel consumption in kg/100 km
γ, ζ, η, μ	set of physicochemical properties
ρ	density of the fuel
$a_\gamma, a_\zeta, a_\eta, a_\mu$	regression coefficients corresponding to properties γ, ζ, η, μ, respectively
X_A	volumetric concentration of alternative fuel A in a blend with reference diesel D
z	carbon content of the fuel [wt.%]
A	alternative fuel blending component
B	diesel fuel blend containing FAME
Bu	diesel fuel blend containing butanol
D	fossil diesel - reference fuel
Et	diesel fuel blend containing 2-ethylhexanol
G	diesel fuel blend containing GTL
H	diesel fuel blend containing HVO
Mix	Fuels consisting of four components including HVO, OME, FAME, and 2-ethylhexanol
O	diesel fuel blend containing OME
P	diesel fuel blend containing pentanol

diesel [17,18]. It is also non-toxic and biodegradable but oxidation stability might be an issue when considering fuel storage [19]. Cold flow properties are also worse than in the case of fossil diesel [20]. Additionally, the use of FAME was found to cause the engine oil dilution [21], increase its acidity and worsen oxidation stability [22]. Another challenge relates to deposit formations, which are particularly adverse for direct injection systems in modern engines [23]. As such, neat FAME is not a fully drop-in solution, and therefore, its content in commercial diesel fuel is limited to 7% on a volumetric basis following EN 590 standard used in the EU. Variations in FAME properties result from feedstock used in the transesterification process [19,24] and could be predicted from fatty acid composition by the use of statistical methods [25].

Unlike FAME, the quality of HVO is not very dependent on the raw material used in the hydrotreatment process [26]. The paraffinic diesel is of superior quality that was found to reduce tailpipe CO_2, particulates and nitrogen oxides emissions [27–29]. Therefore, it can be used either as a neat or as a blending component in modern high-speed CI engines for buses or trucks. The same stands for gas-to-liquid (GTL) or biomass-to-liquid (BTL) fuels produced by Fischer–Tropsch synthesis [30,31] that are covered by EN 15940 standard. Both types of fuels including paraffinic diesel (HVO, BTL, GTL) and traditional biodiesel (FAME) were thoroughly investigated in the present study and subject to the modeling work with a focus on the end-use performance. However, this study is not limited to HVO and FAME but focuses also on potential diesel components that could be blended in the future with either fossil or renewable diesel.

1.1. End-use performance prediction for heavy-duty vehicles

Fuel consumption of the vehicle is affected by multiple factors including vehicle type, travel distance, roadway characteristics, traffic conditions, driver behavior and weather as reviewed by Zhou et al. [32]. Those factors were taken into account in previous studies when predicting the end-use performance of the vehicle. Recent modeling efforts focused also on renewable fuels including blends of biodiesel [33], ternary blends of FAME, bioethanol and fossil diesel [34] or animal fat [35] used in CI engines. Among all the investigated factors, however, the effect of fuel properties on end-use performance was not modeled as highlighted in Fig. 1. The current work addresses this niche by investigating and modeling the collective impact of the most significant fuel properties on fuel consumption in a fleet of heavy-duty vehicles.

In the case of heavy-duty vehicles, an extended literature review revealed previous studies aiming at end-use performance prediction. The results are gathered in Table 1. However, the end-use performance model that connects fuel properties with fuel consumption or CO_2 emissions is missing in the available literature. In contrast to all previously discussed modeling efforts, the present study considers blends with variable composition and treats fuel properties as a starting point and input for modeling. The collective effect of fuel properties on heavy-duty engine performance is assessed and modeled using statistical methods. This approach aims to identify the most critical fuel properties with respect to fuel consumption in CI engines of the entire heavy-duty fleet. To the knowledge of the authors, this particular approach enabling accurate analysis of various fuel blends in heavy-duty transport has not been performed so far. Additionally, in the scope of this work are liquid fuels ranging from single components to various blends including commercial diesel. At this point, a unique methodology is suggested to support the deployment of new fuel blends in the existing heavy-duty fleet by predicting fuel consumption and CO_2 emissions based on a known set of fuel properties.

1.2. Outline of the novelty

As discussed above, there is no model that directly bridges fuel properties with fuel consumption of CI engines used in a heavy-duty fleet. The current work presents an accurate tool that will enable instant evaluation of fuel consumption for all types of liquid fuels used as drop-in solutions in heavy-duty vehicles. The outline of the current study encompasses following sections:

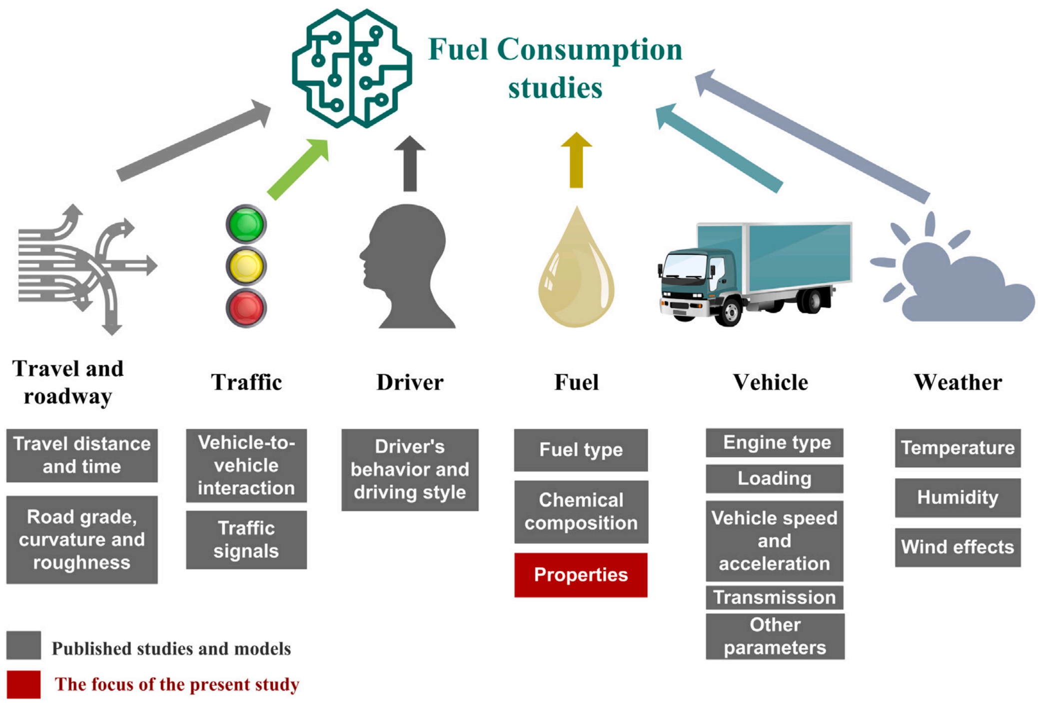

Fig. 1. Set of fuel properties as a new factor affecting fuel consumption of heavy-duty vehicles.

Table 1
Reviewed modeling efforts focusing on the end-use performance of heavy-duty vehicles equipped with compression ignition engines.

Reference	Prediction of engine performance for heavy-duty vehicle
Demir et al. [36]	Review and numerical comparison of six emissions models that reflect driving conditions
Wang et al. [37]	Fuel consumption model dependent on the driving conditions while indicating the optimum speeds and 'eco-freight strategies'
Perugu et al. [38]	Approximation of particulate matter emissions and resulting local air quality using fleet spatial activity data
Ligterink et al. [39]	The estimation method of emissions dependent on velocity and payload with improved predictions for nitrogen oxides
Zamboni et al. [40]	Statistical investigation of the speed patterns to estimate fuel consumption and related emissions
Seo et al. [41]	Estimation of the fleet CO_2 emissions by the bottom-up approach and validation by chassis dynamometer tests
Zacharof et al. [42]	Estimation of fleet representative CO_2 emissions utilizing different sampling methods
Prussi et al. [43]	Comparison of different fuel options in terms of CO_2 emissions and expanded energy over the well-to-wheel perspective
Zhang et al. [44]	Comprehensive statistical analysis while investigating the influence of test cycle and fuel property on HD diesel engine
Tucki [45]	Tool for modeling CO_2 emissions in vehicle's driving tests for neat renewable fuels including FAME, rapeseed oil and butanol
Vijayagopal et al. [46] and Gao et al. [47] (Autonomie)	Autonomie tool - driving cycles' simulations that can be applied to the evaluation of fuel consumption for various engine technologies
Wang et al. [48] (GREET)	Greenhouse gases, Regulated Emissions, and Energy use in Technologies model (GREET) - analytical tool for GHG emission analysis over the lifecycle
Vallamsundar and Lin [49] (MOVES)	Motor Vehicle Emission Simulator (MOVES) model used in the US to estimate emissions at national, regional or project scale
Fontaras et al. [50] (VECTO)	Vehicle Energy Consumption calculation Tool (VECTO) used in the EU for HD vehicle legislation purposes

- Section 2 which in detail describes the applied approach in data analysis;
- Section 3.1 which summarizes collected data from various experimental campaigns and investigates inter-dependencies between fuel properties and fuel consumption for heavy-duty vehicles;
- Section 3.2 which evaluates the effect of driving conditions and test cycle on end-use performance;
- Section 3.3 introduces a state-of-the-art mathematical model that enables the prediction of fuel consumption in the fleet of heavy-duty vehicles based on fuel characteristics;
- Section 3.5 that applies the model in the prediction of fuel consumption for new fuel components including bio- and e-fuels and their blends with fossil or renewable diesel to support decisions of fuel and automotive industries as well as policymakers.

2. Methodology

The main aim of the study was to develop a novel mathematical model that would enable accurate prediction of fuel consumption in heavy-duty compression-ignition engines based on fuel properties exclusively. Additionally, the model was targeted to the entire fleet of heavy-duty vehicles, regardless of their detailed engine characteristics. This work encompassed an extensive literature review and data collection from various sources. Gathered information enabled assessment and comparison of the performance of renewable fuels in the existing heavy-duty powertrains equipped with CI engines. Fuel consumption and CO_2 emissions were under the research scope with an emphasis on the end-user perspective. The liquid drop-in fuels for CI engines were explored including FAME, HVO, GTL, and BTL.

2.1. Driving cycle test procedures

New fuel blends can be evaluated on an engine test bench or chassis dynamometer. The latter one serves legislation purposes but at the same time, the test procedure is more challenging as it requires a bigger test cell to accommodate the truck or bus and could be done only in institutes with relevant infrastructure. Tests on chassis dynamometer take into account the vehicle's properties, selected driving pattern that corresponds to real driving operation as well as give the possibility to test in-use engines instead of new ones. Therefore, heavy-duty vehicle tests on chassis dynamometer reflect the real driving conditions better than those on test benches, while providing results meaningful directly to the end-user (i.e. fuel consumption in g/km instead of g/kWh). Field test with the use of a portable emission measurement system is an alternative to laboratory efforts but the outcomes highly depend on the driving profile, selected route and traffic and it is difficult to make a direct comparison between various fuel blends. Hence, in this work, it was decided to use experimental results from driving cycles as a trade-off between laboratory and field tests.

There are multiple driving cycle test procedures to examine heavy-duty vehicle performance. Each driving cycle is characterized by its own driving profile that is expressed by the velocity in a specified time. While testing, the heavy-duty vehicle needs to follow a velocity profile over the specified time. Braunschweig, ADEME, Urban Dynamometer Driving Schedule (UDDS), or Heavy Heavy-Duty Diesel Truck (HHDDT) are examples of driving cycles considered in this study. The differences are based on velocity levels, acceleration/deceleration rates, time of engine operation in transient conditions or duration of the test. For instance, Braunschweig or ADEME cycles represent the operation of the bus in urban conditions while UDDS or HHDDT are tests designed for heavy-duty trucks. As illustrated in Fig. 2 the velocity profile of the Braunschweig cycle is heavily varying over time while for the UDDS cycle the engine operation is much less transient. Even though both tests are meant for heavy-duty vehicle operation in urban areas, the differences are significant.

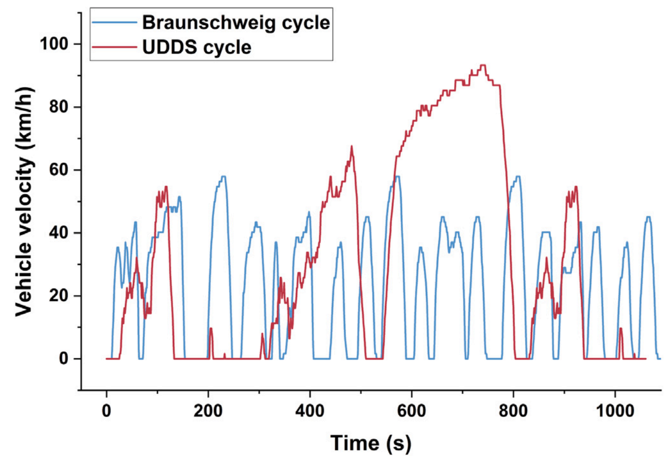

Fig. 2. Differences between driving profiles of test cycles (Braunschweig and UDDS) for a heavy-duty vehicle. Plot based on data retrieved from DriveCAT tool [51].

2.2. Experimental tests of alternative fuels - input data

This section presents data collected from the literature whereas results from experimental tests on heavy-duty vehicles are considered as input for the modeling work. After an extensive review, eight literature sources were selected and experimental data retrieved. Karavalakis et al. [52] tested two trucks on a chassis dynamometer according to UDDS and HHDDT Transient driving cycles while blends of ultra-low sulfur diesel, HVO and FAME were assessed. In another study, Murtonen et al. [53] used a chassis dynamometer and a separate engine test bench to assess the performance of neat alternative drop-in fuels including GTL, HVO and FAME under the Braunschweig driving cycle among other conditions. In the work by Na et al. [54], FAME and HVO blends with fossil diesel were tested in a heavy-duty truck on a chassis dynamometer under UDDS and HHDDT cycles. Fuels like HVO, GTL and FAME from various feedstock were blended with fossil diesel and tested in heavy-duty trucks on the chassis dynamometer by Hajbabaei et al. [55]. Erkkila et al. [56] investigated HVO behavior in several city buses on a chassis dynamometer according to the Braunschweig cycle. Also, the International Energy Agency (IEA) has been focusing on alternative fuels within the Advanced Motor Fuels framework. In Annex 37, Nylund et al. [57] investigated several fuel blends over multiple driving cycles on a chassis dynamometer in the case of city buses. Tested fuels included binary or ternary blends of HVO, GTL and FAME from different types of feedstock with EN 590 diesel. The end-use performance tests were accomplished in two independent laboratories, which resulted in 180 cases with various combinations of vehicle, fuel and driving cycle type. In another IEA study reported in Annex 38, Mizushima [58] and Sato [59] used a commercial vehicle equipped with a CI engine while test results encompassed fuels like FAME, HVO and BTL and their blends with fossil diesel.

2.3. Model development

In the present study, the fuel-centric approach was selected, meaning that alternative fuels and their blends with reference diesel were of the highest interest, in particular drop-in solutions. Fuel's physicochemical properties were expected to have a detrimental effect on the heavy-duty vehicle. In previous experimental studies on renewable fuels in compression ignition engines [60,61], it was clearly shown that the changes in properties like cetane number, oxygen content or composition significantly affect the engine performance. In connection to this study, the collective impact of different fuel properties on engine performance was already demonstrated for passenger cars [62], flex-fuel light-duty vehicles [63], marine medium-speed engines [64], and aircrafts [65]. In passenger cars equipped with modern compression ignition engines, the most significant properties affecting fuel consumption turned out to be the lower heating value (LHV), density and cetane number [62], while in the marine engine case, the CO_2 emissions were predicted by density, heating value and viscosity [64]. The results from the aforementioned studies represented the behavior of renewable fuels and their blends in the existing fleet from the end-user perspective. It was a necessary part of the input for the holistic assessment of selected advanced biofuel options, especially important for decision-makers in the scope of the AdvanceFuel Horizon2020 project [66]. Whilst heavy-duty fleet is responsible for a significant part of anthropogenic CO_2 emissions as presented in Section 1, predictions for new fuel blends compatible with existing infrastructure are important indicators. Therefore, the model that reveals the effect of fuel properties on fuel consumption was targeted in the present study.

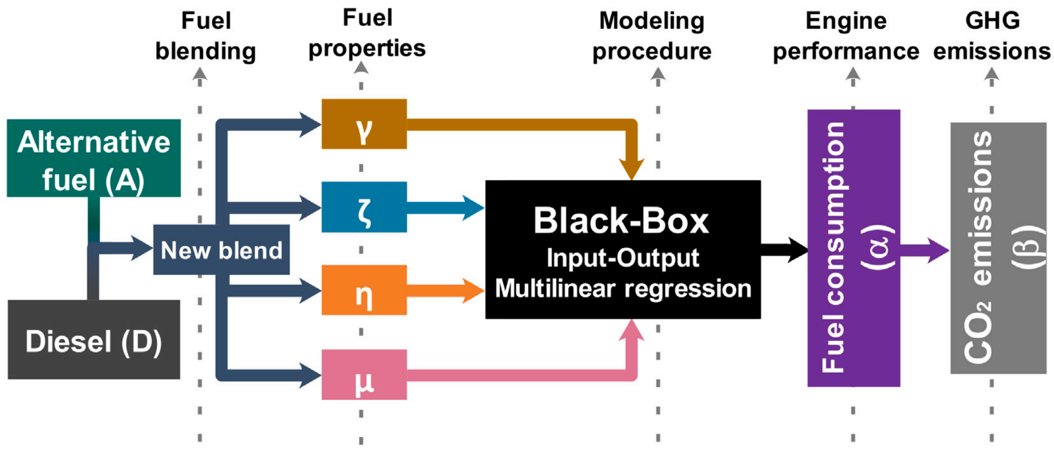

Fig. 3. The novel approach in the analysis of alternative fuels and their impact on heavy-duty vehicle performance. Fuel properties are at the core of the modeling procedure.

The black-box modeling approach (Fig. 3) was explored to predict the end-use performance of the heavy-duty vehicle. In general, the black-box approach is a suitable method for data-driven modeling which enables prediction of the dependent variable treated as an output based solely on independent variables considered as inputs. It results in a functional relationship between input and output while exploring statistical methods. The analysis of input–output dependency is of high importance that allows to find a correlation between the predicted variable and inputs. Instead of applying demanding computational simulations that involve detailed reaction chemistry and combustion models, black-box modeling with statistical methods enables robust analysis of complex mixtures of hydrocarbons represented by their physical and chemical properties in the context of end-use performance. In this study, the aim of the black-box approach is to understand on a general level which properties of renewable fuel blend have critical impact on fuel consumption of heavy-duty vehicles. Therefore, fuel properties of various blends were treated as input parameters. Lower heating value on volume and mass basis, density, viscosity, cetane number, carbon, oxygen and hydrogen contents as well as carbon-to-hydrogen ratio were among the investigated properties of the fuel. The blending procedure of alternative fuel (A) with fossil diesel (D) entails unique characteristics of the fuel product defined by a set of physicochemical properties (γ, ζ, η, μ) as presented in Fig. 3. The role of black-box modeling is firstly to indicate significant properties in the estimation of end-use performance for heavy-duty vehicles and secondly to provide a tool for accurate prediction. Different performance indicators were analyzed and assessed including fuel consumption, tailpipe CO_2 emissions and energy efficiency. Fuel consumption, an output of the model, is the essential factor for the fleet operator or vehicle owner due to cost calculations based on consumed fuels and additional payload related to the mass of the fuel.

In the model development, the selection of consistent data was essential. In principle, the modeling results are no better than available information and outcomes depend on the consistency of data. Therefore, the input collected from the literature was carefully analyzed in terms of investigated fuels and their properties, vehicle or engine characteristics and driving cycle profiles. The created database (Supplementary material) was a starting point for further analysis. The characteristics of the collected database are as follows:

- over 70 fuel blends with drop-in or almost drop-in characteristics;
- matrix of 190 rows from 8 different test campaigns;
- engine displacements in the range of 3–15 L;
- variety of driving cycles (Braunschweig, ADEME, UDDS, HHDDT) with substantial differences, i.e. average speed in the range of 11–60 km/h.

To enable a comparison of experimental results from various laboratories, the relative changes approach was applied to the collected numerical data. The reference fuel was always fossil diesel while all changes in properties for alternative fuels and their blends were referred to the reference fuel used in the same study. It is important to note that fossil diesel could have different specifications depending on geographical location, time of the year or producer but it still should be within allowable limits specified by standards, for instance, EN 590 in the EU. For that reason, the properties of reference diesel are not fixed but vary depending on the experimental campaign. The same convention was valid for end-use performance indicators while test runs with reference diesel were treated as a baseline scenario. All test results for alternative fuel blends were compared to this baseline and expressed in relative changes, too. The collected numerical data were converted to relative change values using Eq. (1). For the final model development, data only from the Braunschweig cycle were used for the model training.

$$\gamma(X_A) = (\gamma_A - \gamma_D)/\gamma_D \cdot 100\% \quad (1)$$

where, $\gamma(X_A)$ - the relative change (compared to reference diesel) of specific fuel property/performance indicator (denoted as γ) for fuel blend with X_A volumetric concentration of alternative fuel A; γ_D - absolute value of specific fuel property/performance indicator for reference diesel; γ_A - absolute value of specific fuel property/performance indicator for alternative fuel blend.

Different modeling approaches were considered including statistical methods and machine learning. Machine learning models are attractive options provided that the database is big enough. With more limited and static data availability, statistical methods are very good options that allow an understanding of the input parameters. Therefore, the final black-box model was built by using the multilinear regression method expressed by Eq. (2).

$$y(x) = \phi_1(x) \cdot \xi_1 + \cdots + \phi_n(x) \cdot \xi_n + \epsilon(x) \quad (2)$$

where, y - dependent variable; x - independent variable; $\phi_i(x)$ - explanatory variable; ξ_i parameter of explanatory variable; $\epsilon(x)$ - error.

Applying this mathematical method to the problem presented in Fig. 3, Eq. (2) could be rewritten in the form of Eq. (3):

$$\alpha = a_\gamma \cdot \gamma(X_A) + a_\zeta \cdot \zeta(X_A) + a_\eta \cdot \eta(X_A) + a_\mu \cdot \mu(X_A) \quad (3)$$

where, α - relative change of fuel consumption [percentage change compared with reference in kg/100 km]; X_A - volumetric concentration of alternative fuel A in a blend with reference diesel D; $\gamma(X_A), \zeta(X_A), \eta(X_A), \mu(X_A)$ - relative changes of fuel properties γ, ζ, η, μ for alternative fuel blend compared with reference diesel; $a_\gamma, a_\zeta, a_\eta, a_\mu$ - regression coefficients corresponding to properties γ, ζ, η, μ, respectively.

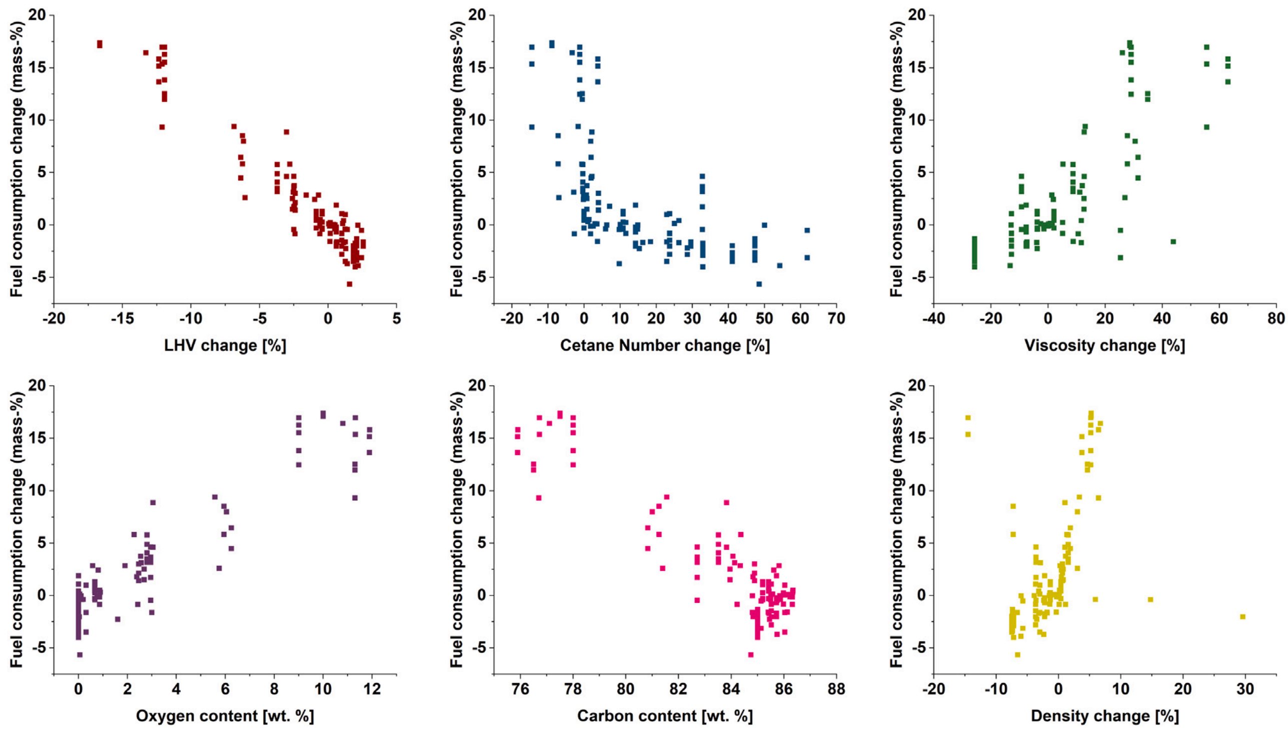

Fig. 4. The dependency between fuel consumption change and fuel property change in case of alternative fuel blends. The relative changes approach is used with fossil diesel as a reference while fuel consumption change refers to the unit of mass per driven distance (kg/100 km).

In the applied stepwise multilinear regression method, the quantitative analysis was executed by monitoring the significance of independent variables and the accuracy of the prediction. The *p*-value, calculated based on the probability density function and Student's t-test, was a data-based significance measure. In the particular case of this study expressed by Eq. (3), the p-values were checked for coefficients corresponding to selected independent variables (fuel properties). In the iterative process of the stepwise multilinear regression method, the properties with p-values above the 5% threshold were removed from the model. Additionally, the coefficient of determination (R-square) of the model was used as the accuracy metric representing the extent to which independent variables explain the dependent variable (fuel consumption) in the regression method. In the approximation of the solution in regression analysis, the least-squares method was used - Eq. (4).

$$J_\xi = \sum_{x=1}^{N} \epsilon^2 = \sum_{x=1}^{N} (y(x) - \phi^T(x) \cdot \xi)^2 \tag{4}$$

where, J_ξ - least squares objective function.

The model with the highest accuracy and all p-values below the threshold was validated both internally using training data, and externally by data never seen in the model development stage. After obtaining the final model for the fuel consumption prediction, CO_2 emissions can be directly derived from the absolute value of fuel consumption using the carbon balance method - Eq. (5).

$$\beta = 10 \cdot \alpha_{abs} \cdot z \cdot 44.01/12.01 \tag{5}$$

where, β - CO_2 emissions [g/km]; α_{abs} - absolute value of fuel consumption [kg/100 km]; z - carbon content of the fuel [wt.%].

The carbon content in the fuel blend can be determined using densities and carbon contents of neat alternative fuel and reference diesel - Eq. (6).

$$z = (X_A \cdot z_A \cdot \rho_A + (1 - X_A) \cdot z_D \cdot \rho_D)/\rho \tag{6}$$

where, X_A - volumetric concentration of alternative fuel [vol.%]; ρ_A - density of neat alternative fuel [kg/m^3]; ρ_D - density of reference diesel [kg/m^3]; ρ - density of final fuel blend [kg/m^3]; z_A - carbon content of neat alternative fuel [wt.%]; z_D - carbon content of reference diesel [wt.%].

3. Results and discussion

3.1. Fuel properties effect on end-use performance

When investigating engine performance for renewable fuels and their blends, the relative changes of gravimetric fuel consumption were plotted versus relative changes of fuel properties as depicted in Fig. 4. The analysis was conducted based on over 120 experimental results (Supplementary material). The fuel consumption change is directly proportional to the oxygen content of the fuel. In general, oxygen atoms in the molecular structure of FAME-type fuels lower the calorific content and more fuel is needed to provide the same power output for the engine. Also, high-viscosity fuels tend to negatively affect fuel consumption, however, the trend is not as evident as in the case of oxygen content. In principle, lower viscosity enables smaller droplet formation, faster evaporation and better mixing inside the combustion chamber. However, too low viscosity may lead to lubrication problems in compression ignition engines. In the case of lower heating value, its change is inversely proportional to fuel consumption meaning the higher the LHV, the lower fuel consumption for the given fuel blend. A similar strong pattern of correlation is observed for carbon and hydrogen contents. For density, no clear trends could be concluded. Despite this observation, density is an important property that affects significantly injection and mixture formation in compression ignition engines while the impact on fuel economy might not be explicitly visible. Cetane number, a measure of fuel reactivity, is another important property of compression ignition engines. High cetane number fuels are characterized by slightly lower gravimetric fuel consumption compared to reference diesel. Even higher potential benefits could be expected in optimized engines which could explore shorter ignition delay times resulting in higher thermal efficiency.

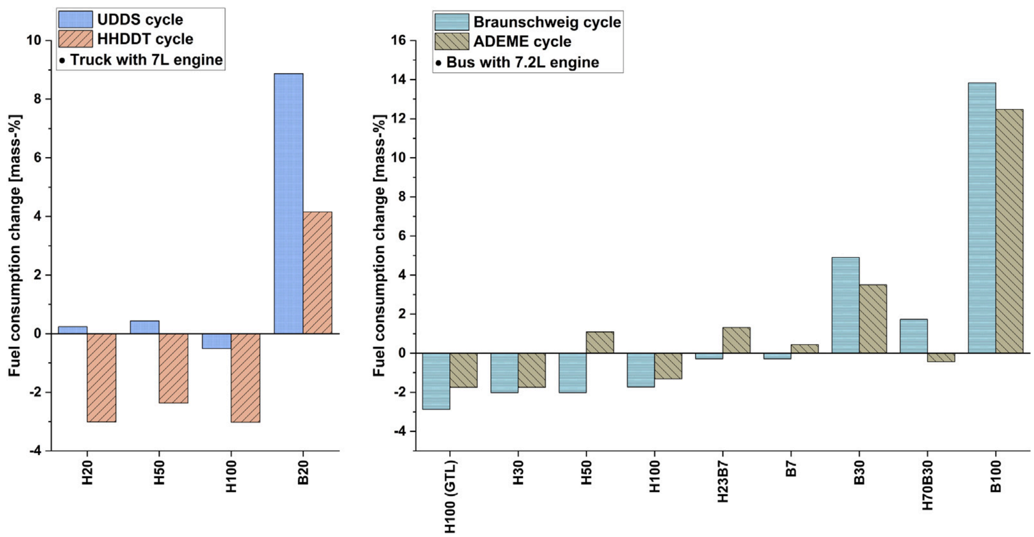

Fig. 5. Comparison of results from different driving cycles for the same fuel blends. Left: UDDS versus HHDDT cycle in case of the heavy-duty truck engine based on [52]. Right: Braunschweig versus ADEME cycle in case of heavy-duty bus engine based on [57]. 'B' denotes FAME-type of fuel blend, 'H' paraffinic fuel blend, while the adjacent number stands for the volumetric concentration of that alternative fuel component in the final blend.

3.2. Effect of the driving cycle on end-use performance

Fuel consumption of heavy-duty vehicles depends on engine operating conditions required by the specific driving cycle [67]. Therefore, in this work, the experimental data for alternative fuels are presented as relative changes compared to the reference scenario with fossil diesel. Even in this approach, there are some differences between results for the same vehicle and fuel but under different operating conditions. As presented in Fig. 5, the same fuel blend can perform better in one cycle than in another one when compared to fossil diesel. Based on data from [52], it is evident that three tested alternative fuel blends of HVO outperformed diesel under the HHDDT driving cycle while no improvement was observed for the UDDS cycle. Also, the biodiesel blend had worse performance under the UDDS cycle. As illustrated in Fig. 5, the 3%–5% differences in gravimetric fuel consumption change are observed between those two cycles for the same truck equipped with a 7.0 L engine and the same test fuel. The reason behind such a discrepancy is a variation in the velocity profile. The HHDDT cycle is much more transient than UDDS and in that case, the engine could benefit from the favorable properties of hydrogenated and oxygenated fuel blends. In another study by [57], the same bus was tested under Braunschweig and ADEME cycles. Both cycles are driving test procedures representing urban driving. In this case, the differences between relative changes in fuel consumption for the same fuel blends are less significant, on average 1.5% difference in relative change of gravimetric fuel consumption (Fig. 5).

As an important conclusion for modeling purposes, only one driving cycle or at least similar ones should be used in the model development procedure. Due to data availability limitations, similar driving cycles could be used for validation purposes. Braunschweig and ADEME are urban cycles with very transient conditions, applicable to bus driving in the city center. On the other hand, less transient cycles are considered for heavy-duty trucks including UDDS and HHDDT cycles. However, HHDDT and UDDS should not be used simultaneously due to significant variations in velocity profiles. Finally, engines with similar displacements and comparable technologies are preferred in the preparation of a database for modeling purposes.

3.3. End-use performance model

Based on data availability and comparison of various driving cycles (Section 3.2), the final model for the prediction of fuel consumption was built on experimental results from heavy-duty vehicles operated under the Braunschweig cycle. This test procedure on the chassis dynamometer reflects the city driving of the heavy-duty vehicle and is characterized by a transient velocity profile, in which the effect of the alternative fuel is clearly visible. The investigated vehicles were equipped with engines mostly in the range of 7-9L displacement volume. For the model development in total 66 experimental results were used from four independent sources. The experimental outcomes for the Braunschweig test runs are presented in Fig. 6.

It should be noted that paraffinic- and methyl esters-based fuels and their blends with fossil diesel were investigated. The engine performance is presented in terms of relative changes compared to reference tests with standard diesel fuel. Paraffinic fuels (HVO, GTL, BTL) tend to lower the gravimetric fuel consumption, depending on the composition even up to 5% for neat HVO. Characterized by lower density and viscosity paraffinic fuels have also slightly higher gravimetric heating value and significantly higher cetane number. The combination of those properties contributes to better performance in CI engines in terms of fuel consumption on a mass basis. In contrast, FAME-type fuels increase fuel consumption, even by 15% in the case of neat biodiesel. It is mainly caused by lower calorific value originating from higher oxygen content in the fuel. When blending HVO with FAME in a volumetric ratio of 70:30 (Fig. 6), the positive effect of HVO is completely eliminated by FAME and fuel consumption increases by about 2%–5%. The same is observed for lower concentration ternary blends (volumetric concentration ratio of 23:7:70 for HVO, FAME and fossil diesel, respectively), for which the performance is similar to the reference diesel.

In terms of volumetric fuel economy, in the vast majority of cases, the performance of alternative fuels is worse compared to reference diesel. The explanation for this phenomenon can be found in density differences. For paraffinic fuels, lower density contributes to around 5% decrease in fuel economy. In contrast, FAME with a higher density than EN 590 fuel has improved volumetric fuel consumption compared to the gravimetric one. However, for neat biodiesel, volumetric fuel consumption can still be over 10% higher than in the case of reference diesel. In terms of tailpipe CO_2 emissions, the alternative fuel blends tend to have positive effects. The highest reductions are observed for paraffinic fuels, up to 5%. Neat biodiesel could increase tailpipe CO_2 emissions by 5% but only in some cases. Nevertheless, CO_2 measurements provide only part of the complete GHG emission analysis. In the final assessment, also production-related emissions should be considered to properly estimate the environmental footprint of alternative fuel blends.

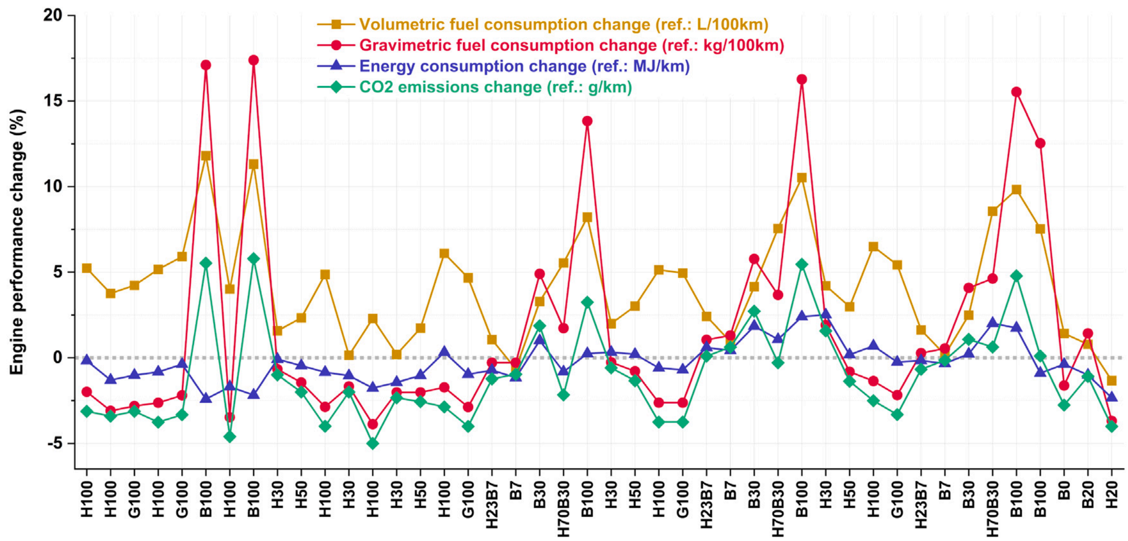

Fig. 6. Engine performance of heavy-duty engines under Braunschweig driving cycle. 'B' denotes the FAME-type of fuel blend, 'H'- renewable diesel (HVO) blend, 'G' - GTL fuel blend, while the adjacent number stands for the volumetric concentration of that alternative fuel component in the final blend.

Table 2
Modeling results from stepwise multilinear regression.

Variable	Coefficient	Std. Error	T-value	P-value
LHV	−0.959	0.070	−13.78	0.001
Density	0.534	0.185	2.884	0.007
Cetane number	0.084	0.030	2.754	0.009

Fuel consumption experimental data only from the Braunschweig driving cycle were used for the final model training (Fig. 6). The multilinear regression method was applied and resulted in the model that enables estimation of fuel consumption change for alternative fuel blends compared to reference diesel. Knowing the relative changes of fuel properties referred to fossil diesel, the model expressed by Eq. (7) can estimate the effect of the considered blend on fuel consumption from the heavy-duty fleet perspective. Lower heating value on the mass basis, density and cetane number turned out to be the most significant properties according to the stepwise multilinear regression method. The p-values for coefficients corresponding to those properties were below 1%. This result is in line with the lack of correlations between heating value, density and cetane number. It could be interpreted that selected properties in the final model are independent variables and each provides unique information that is utilized by the model. The results of stepwise multilinear regression are collected in Table 2, which includes obtained coefficients, their standard errors, t-values and p-values.

$$\alpha_{HD} = -0.959 \cdot \beta + 0.543 \cdot \gamma + 0.084 \cdot \eta, \tag{7}$$

where α_{HD} denotes the relative change of fuel consumption for the heavy-duty vehicle, β stands for the relative change of lower heating value on the mass basis, γ - relative change of density and η - relative change of cetane number. For alternative fuel blends, relative changes (in %) are always referred to fossil diesel fuel.

The accuracy of the obtained model was high with a coefficient of determination 0.975. To verify the validity of the model, both internal and external validations were executed. The internal validation illustrated in Fig. 7 represents the response of the model to the training data. The estimation of fuel consumption change resulted in an average absolute error of 0.8%, while the average absolute change of fuel consumption was 3.5%, indicating the significance of the results. In Fig. 8, the predicted versus measured values were plotted together with the histogram of residuals. The distribution of residuals confirms normal distribution with a mean value close to 0. For external validation purposes, a few average fleet data from the Braunschweig cycle were used as well as experimental results from the ADEME cycle. The average absolute error of the estimation is 1.1%. External validation of the model is illustrated in Fig. 9.

3.4. Deployment of the model to the end-use performance simulations for potential diesel blends

In this section, the obtained model served for simulations of end-use performance in the case of promising blends that were considered in the literature (details in Supplementary material) but have not been tested on a regular heavy-duty vehicle according to the specified driving cycle. Poly-oxymethylene dimethyl ethers (OMEs) are potential diesel fuel components recently identified in different studies due to sustainable production pathways (i.e. e-fuel route) and significant reductions in toxicity of tailpipe emissions [68,69]. Also, blends consisting of 10% OMEs oligomers and fossil diesel were concluded to nearly meet EN 590 standard [70]. In another approach [71], OMEs were blended with other renewable components such as HVO, FAME and 2-ethylhexanol (an isomer of n-octanol). Higher aliphatic alcohols could be other potential diesel blending components that have attracted the attention of researchers over the last few years. Due to more favorable properties than methanol or ethanol, heavier alcohols including butanol and pentanol isomers were investigated in multiple studies to partially substitute fossil diesel in CI engines [72–75].

The simulation results for various composition blends of OMEs, butanol and pentanol, as well as neat fuels including HVO and FAME, are presented in Fig. 10. Among all investigated fuels, HVO has a leading performance in terms of gravimetric fuel consumption. On the contrary, the addition of OMEs significantly worsens fuel consumption, even up to 40%–65% increase for neat OME-type of fuel is observed. The increase in fuel consumption is dependent on the length of the carbon chain of a specific OME oligomer, which was observed for 35% volumetric blends with diesel. In the case of a relatively low concentration of OMEs in blends with HVO, the final fuel has a positive effect on gravimetric fuel consumption compared to reference diesel. OMEs addition could increase the density of high-concentration HVO blends to possibly meet EN 590 requirements. Neat FAME increases fuel consumption by around 15%, while 2-ethylhexanol by 10%. Among blends consisting of four renewable components (Mix1-3), the best performance is attributed to the highest HVO concentration whereas the highest fuel consumption is observed for the blend with the highest

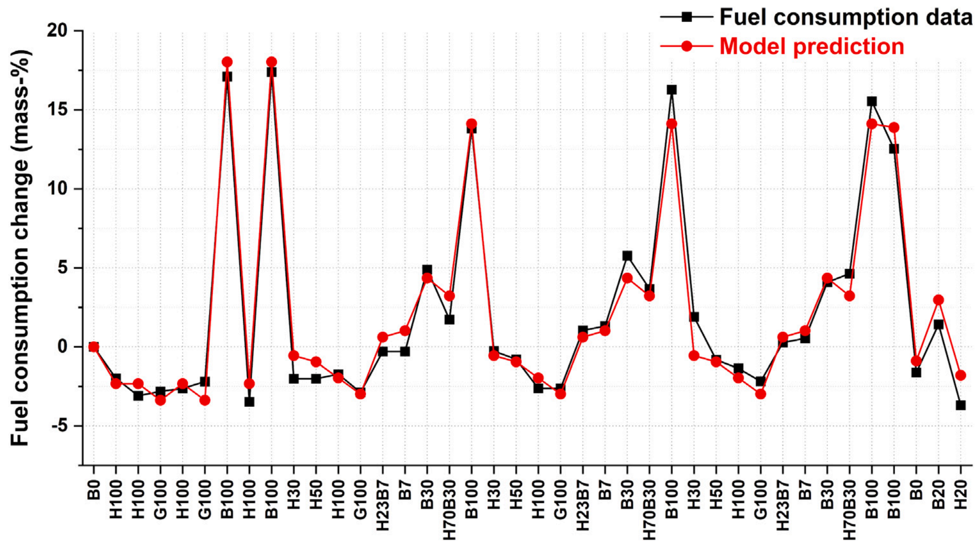

Fig. 7. Internal validation of the modeling results — model prediction vs fuel consumption data from Braunschweig driving cycle. 'B' denotes FAME-type of fuel blend, 'H'-renewable diesel (HVO) blend, 'G' - GTL fuel blend, while the adjacent number stands for the volumetric concentration of that alternative fuel component in the final blend.

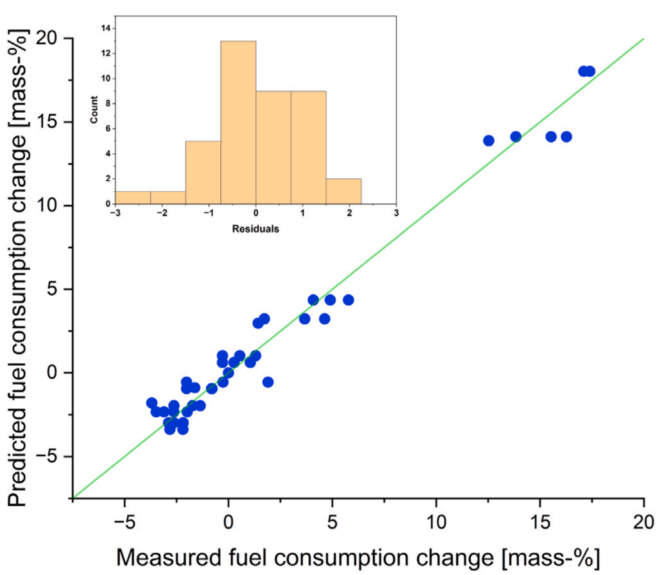

Fig. 8. Residual analysis for the developed model based on data used in Fig. 7.

OMEs concentration. For blends of higher alcohols with concentration not exceeding 40% of volume, the fuel consumption change increases moderately, up to 10% with minor differences between butanol and pentanol.

In general, renewable fuels except HVO are expected to worsen the fuel economy. The exact effect depends on the physicochemical properties of the renewable component, blending ratio, other components used in the blend as well as reference fuel. All aforementioned factors are taken into account by the model proposed in the present study and the effect can be quantified as illustrated in Fig. 10.

3.5. Applicability and limitations of the model

The model represented by Eq. (7) is applicable to liquid renewable fuels and their blends with fossil diesel, especially those with drop-in characteristics that could be used in the current fleet of heavy-duty vehicles. The results indicate the performance change of the considered fuel blend compared to reference diesel. Knowing basic properties such as lower heating value on a mass basis, density and cetane number, the model enables a quick comparison of fuel consumption for various blends. As the model relies on relative percentage changes, the results can be scaled from one vehicle to the whole fleet of vehicles, but also the analysis can be carried out for fuels ranging from single chemical compounds to complex chemistry fuels composed of large numbers of different molecules.

Based on the developed model, fuels considered previously only in the laboratory or bench scale can be assessed from the perspective of the entire fleet of heavy-duty vehicles. The common limitation of end-use testing for new fuels originating from low technology readiness level production pathways is a very low amount of produced fuel in the lab scale. In particular, the driving cycles for heavy-duty vehicles require dozens of liters of fuel while only around half a liter of sample is required by basic fuel analytics including cetane number, heating value and density that serve as direct input to the model. Hence, the introduced model opens groundbreaking possibilities for early insight into the end-use performance of new fuel candidates and significantly supports their development. However, the results should be treated as indicative while there is no validation available for relatively new fuel components that have not been extensively studied in this work.

In practice, diesel fuel blending can be accomplished by fuel producers and distributors of diesel products. The addition of renewable components can be implemented at refinery sites but also at terminals or retail stations. In all those cases, the model can be applied by fuel producers and distributors to estimate the end-use performance of their planned blends with respect to fuel economy and tailpipe CO_2 emissions for heavy-duty fleet. In particular cases, end-users can do the blending by themselves, i.e. blending HVO with EN590 diesel. This can be done for instance in Nordic countries where the driver has the possibility to refuel neat HVO at many retail stations. The model provided by this study helps to understand the effect of renewable component addition on fuel consumption, which is an important parameter for fleet operators.

When considering the limitations of the model, it is important to note that the prediction represents a generalized result for the average heavy-duty fleet. Therefore, the result is showing trends in fuel consumption change based on selected experimental data corresponding to heavy-duty vehicles available in the market. In the future, due to the development of engine technology, optimized engines could better exploit the potential of renewable fuels. Paraffinic diesel with very good autoignition characteristics and high cetane number can be an example

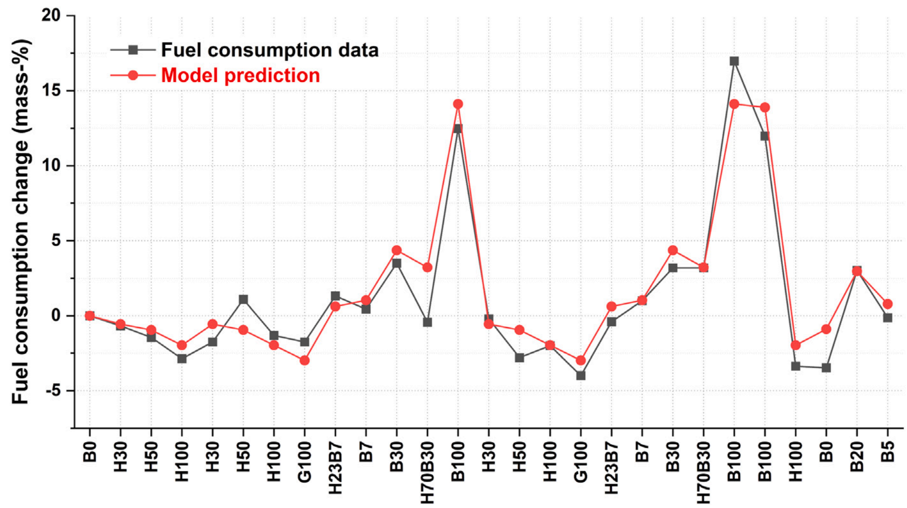

Fig. 9. External validation of the modeling results by experimental data from Braunschweig and ADEME driving cycles. 'B' denotes FAME-type of fuel blend, 'H'- renewable diesel (HVO) blend, 'G' - GTL fuel blend, while the adjacent number stands for the volumetric concentration of that alternative fuel component in the final blend.

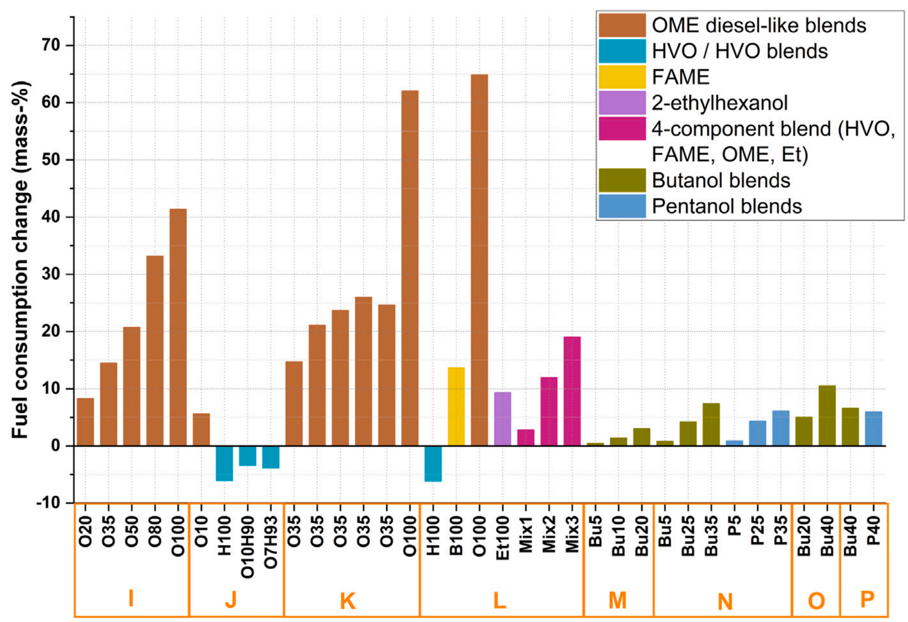

Fig. 10. Simulation results of heavy-duty vehicle's fuel consumption change over Braunschweig cycle for various renewable components considered in the literature: I [68], J [70], K [69], L [71], M [72], N [73], O [74], P [75]. 'B' denotes FAME-type of fuel blend, 'H'- renewable diesel (HVO) blend, 'O' - OMEs fuel blend, 'Et' - 2-ethylhexanol, 'Bu' - butanol blend, 'P' - pentanol blend, while adjacent number stands for volumetric concentration of alternative fuel component in the final blend. Mix1-3 denote fuels consisting of four components (HVO, OME, FAME, Et) specified in Supplementary material.

of renewable fuel with the potential to further improve fuel economy as shown in previous studies [56,76]. Also, the use of additives might improve the fuel economy of heavy-duty vehicles as presented in the previous study [77] but these phenomena might not be fully captured by the present model. Finally, the model was developed on experimental data from the Braunschweig driving cycle, hence, the fuel consumption change is primarily valid for transient driving conditions and might not fully reflect driving with high constant speed over an extended period of time. Despite the above-mentioned limitations, the model should properly represent the fuel economy change and tailpipe CO_2 emissions over the average heavy-duty fleet for renewable fuel blends including HVO, BTL and FAME components.

4. Conclusions

The current work investigated the effects of renewable fuels on the end-use performance in the fleet of heavy-duty vehicles. Based on the literature data, a state-of-the-art mathematical model has been developed representing the collective impact of the most significant fuel properties on fuel consumption in heavy-duty compression-ignition engines. In the current study, retrieved fuel consumption results from driving cycles were represented as relative changes in reference to standard diesel fuel used in each separate experimental campaign. Such a unique approach helped to reveal strong trends when compiling data originating from various sources. The developed model with high accuracy estimates fuel consumption changes for alternative fuels and their blends with standard diesel based on fuel properties exclusively. The main results from the present study are listed below.

1. The developed fuel consumption model for heavy-duty vehicles highlights the importance of fuel properties and their effect on end-use performance. Based on multilinear regression and utilizing fuel properties as input parameters, the current approach proved to be an efficient method to predict fuel consumption

change for renewable fuels and their blends. The accuracy of prediction is verified by a high coefficient of determination (R-square 0.975) and low average absolute error in both internal and external validations, 0.8% and 1.1% respectively.

2. In the final model, lower heating value, density and cetane number turned out to be the most relevant properties with statistical significance confirmed by p-values of coefficients being below 1%. The observed collective impact of fuel properties is represented by Eq. (7).
3. The model serves for the assessment of commercial fuel blends considered for use in the current fleet of heavy-duty vehicles. The high accuracy of the fuel consumption prediction is anticipated for variable composition blends of HVO, FAME and BTL as well as e-fuels and reference fossil diesel compliant with EN 590 standard.
4. The model can be also applied to the analysis of a wide range of alternative fuels, from simple chemistry fuels (few molecules) to complex fuel products composed of a wide range of chemical species. Hence, the model could be utilized for studies across the entire range of technology readiness levels from laboratory to commercial scale.
5. In the current work, the model enabled the assessment of selected new blending components researched on the bench or laboratory scale. Simulations were done for blends of polyoxymethylene dimethyl ethers (OMEs), and higher alcohols including butanol and pentanol. At the expense of improved well-to-wheel GHG emission characteristics, the addition of renewable components is usually associated with worse gravimetric fuel consumption compared to reference diesel. An interesting option is blending OME with HVO featuring improved engine performance while keeping density within EN 590 limits.
6. The obtained model aims to support decision-makers, fuel producers and researchers in the development of renewable fuels and accelerate their market uptake.

CRediT authorship contribution statement

Michał Wojcieszyk: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data curation, Writing – original draft, Writing – review & editing, Visualization. **Yuri Kroyan:** 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, 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

Data used in analysis and modeling are provided in Supplementary material file attached at the submission process.

Acknowledgments

This work was part of the ADVANCEFUEL project, European Union's Horizon 2020 project under grant agreement $N.^{\circ}764799$. The authors would like to also acknowledge support from Fortum and Neste Foundation, Teknologiateollisuus, Merenkulun Säätiö, Henry Fordin Säätiö, and Tekniikan Edistämissäätiö.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.energy.2023.129494.

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