End-use performance of alternative fuels in various modes of transportation

D5.5 report

Yuri Kroyan, yuri.kroyan@aalto.fi

Michal Wojcieszyk, michal.wojcieszyk@aalto.fi

Aalto University

Espoo, Finland

www.aalto.fi

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.° 764799.

Deliverable Information	
Grant Agreement Number	764799
Project Acronym	ADVANCEFUEL
Instrument	CSA
Start Date	1 September 2017
Duration	36 months
Website	www.ADVANCEFUEL.eu
Deliverable Number	D5.5
Deliverable Title	Numerical tools accompanied by report on fuel performance analysis
Expected Submission	M33
Actual Submission	M33
Authors	Yuri Kroyan, Michal Wojcieszyk, Martti Larmi, Ossi Kaario, Ayoub Bani
Reviewers	Kristin Sternberg, Philipp von Bothmer (FNR)
Dissemination Level ***Public (PU), Restricted (PP), Confidential (CO)***	*PU*

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

ADVANCEFUEL at a glance

ADVANCEFUEL (www.ADVANCEFUEL.eu) aims to facilitate the commercialisation of renewable transport fuels by providing market stakeholders with new knowledge, tools, standards and recommendations to help remove barriers to their uptake. The project will look into liquid advanced biofuels – defined as liquid fuels produced from lignocellulosic feedstocks from agriculture, forestry and waste – and liquid renewable alternative fuels produced from renewable hydrogen and CO2 streams.

In order to support commercial development of these fuels, the project will firstly develop a framework to monitor the current status, and future perspectives, of renewable fuels in Europe in order to better understand how to overcome barriers to their market roll-out. Following this, it will investigate individual barriers and advance new solutions for overcoming them.

The project will examine the challenges of biomass availability for second-generation biofuels, looking at non-food crops and residues, and how to improve supply chains from providers to converters. New and innovative conversion technologies will also be explored in order to see how they can be integrated into energy infrastructure.

Sustainability is a major concern for renewable fuels and ADVANCEFUEL will look at socio-economic and environmental sustainability across the entire value chain, providing sustainability criteria and policy-recommendations for ensuring that renewable fuels are truly sustainable fuels. A decision support tools will be created for policy-makers to enable a full value chain assessment of renewable fuels, as well as useful scenarios and sensitivity analysis on the future of these fuels.

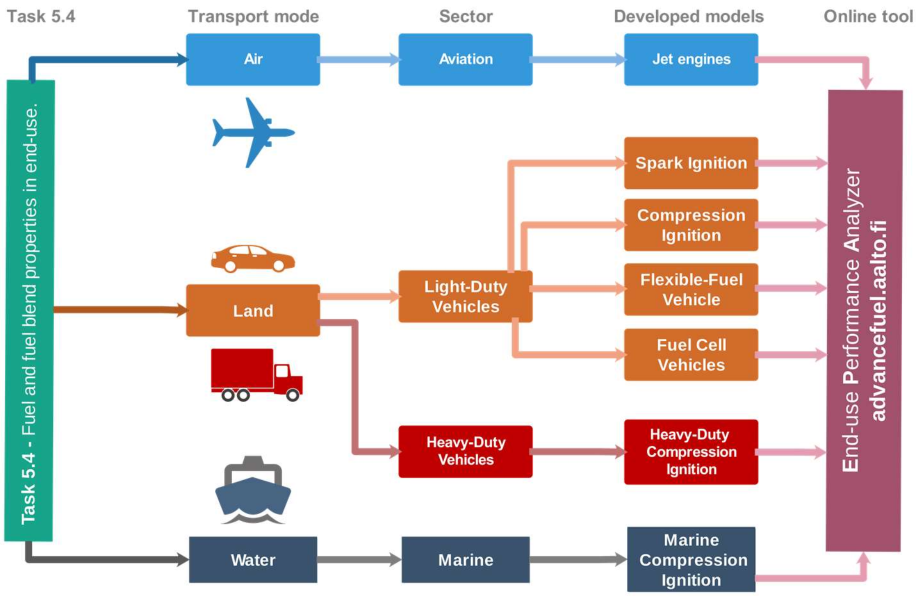
Stakeholders will be addressed throughout the project to involve them in a dialogue on the future of renewable fuels and receive feedback on ADVANCEFUEL developments to ensure applicability to the end audience, validate results and ensure successful transfer and uptake of the project results. In this way, ADVANCEFUEL will contribute to the development of new transport fuel value chains that can contribute to the achievement of the EU's renewable energy targets, and reduce carbon emissions in the transport sector to 2030 and beyond.

To stay up to date with ADVANCEFUEL's stakeholder activities, sign up at: www.ADVANCEFUEL.eu/en/stakeholders

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Executive Summary

This report summarizes the main outcome of the work done by Aalto University during ADVANCEFUEL project under Task 5.4 titled 'Fuel and fuel blend properties in end use'. Through this task, new information focusing on dominant properties of the most prominent RESfuels were gained. The results of this task are essential for the full-chain assessment of RESfuels with respect to the fuel performance and fuel technical acceptance. This report together with the online tool provides outcomes from Task 5.4 activities and constitute Deliverable 5.5. Additionally, the report refers to main publications done under Task 5.4 framework such as master theses ([1], [2]), technical papers ([3], [4]) and journal article ([5]), which were published with open access policy.



This study focused on engine technologies used in various transport sectors presented in the above Figure. Different types of compression ignition engines were considered for heavy-duty and shipping, jet turbines for aviation, whereas light-duty sector was divided into four segments: spark ignition engines of regular passenger cars, compression ignition engines of regular passenger cars, flexi-fuel vehicle's and fuel cells. For all above-mentioned technologies, the end-use performance of RESfuels was investigated in terms of fuel consumption and CO2 emissions. In addition, numerous alternative fuels were analysed in the context of their compatibility with above-mentioned technologies based on their property characteristics. The broad palette of fuel properties was thoroughly analysed and for each transport sector key properties were identified. In that respect, fuels and fuel blends requiring modifications to present day technology or new technologies, were also considered.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

The developed methodology and modelling approach for analysis of alternative fuels are explained in this report. The methods were based on most relevant and recent knowledge, and publications in journals and conferences dealing with fuel conversion and end use of fuels. Numerous transport fuels were analysed based on publicly available literature sources originating from various research institutions. Therefore, to compare results from different measurements, relative change approach was applied, in which fuel properties and end-use performance were always referred to reference fossil-based fuel. Moreover, selections of representative engines and operating conditions depending on the final application in the transport sector were justified. The main aim of the modelling work was to connect set of fuel properties for new fuel blend with its engine performance such as fuel consumption or emissions. It turned out that alternative fuels, including RESfuels, can be analysed in this way when applying black-box modelling. After in-depth data analysis, multilinear regression methods were used for the simulations.

The modelling methodology resulted in the representative models for each transport sector and segment. Those models correlate a set of fuel properties with end-use and provide good estimation of engine performance with high accuracy. Fuel consumption of considered RESfuel can be predicted based on its properties. Heating value proved to be a very important property highly affecting fuel consumption regardless of engine type. However, the final models are always dependent also on other properties, i.e. density is included as well. In case of spark ignition engines, antiknock characteristics needs to be taken into account, while fuel reactivity is important for compression ignition engines.

Finally, based on the developed models, the online tool (End-Use Analyser) was successfully created in the open source format. It has several sections referring to various engine technologies and transport sectors. The main output of the numerical tool is the specific fuel consumption and CO2 emissions while local emissions, like NOx, particulate matter (PM), and unburned hydrocarbon emissions are reported if applicable. The numerical tool is expected to serve project's stakeholders, especially fuel producers, to provide insight in the possibilities of new fuels to be implemented in the market in short or longer term. The description of the End-Use Analyser tool together with guidance is provided at the end of the report. The online tool can be accessed free of charge after registering (link to the End-Use Analyser: **http://advancefuel.aalto.fi/**)

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

Contents

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Abbreviations

2DS	2°C Scenario (Paris agreement)
AF	Animal fat (SVO-type fuel)
AMF	Advanced Motor Fuels
B	Biodiesel (FAME)
BE	Biodiesel (FAME) produced using enzymes
BSFC	Brake specific fuel consumption
BTL	Biomass-to-Liquid fuel
CI	Compression ignition
CN	Cetane Number
CO	Carbon monoxide
CO2	Carbon dioxide
CR	Compression ratio
CSPK	Synthetic Paraffinic Kerosene made from camelina
DF	Dual fuel
DI	Direct injection
DOC	Diesel oxidation catalyst
DPF	Diesel particulate filter
E	Ethanol
ED95	Ethanol 95% and 5% of strong ignition improvers
EGR	Exhaust gas recirculation
EN14214	EU standard for biodiesel, FAME type of fuel
EN15940	EU standard for paraffinic diesel (HVO, GTL)
EN228	EU standard for gasoline fuel
EN590	EU standard for diesel fuel
EU	European Union
EUA	End-Use Analyser
EUDC	Extra Urban Driving Cycle
FAME	Fatty acid methyl ester (traditional biodiesel)
FC	Fuel Consumption
FCV	Fuel Cell Vehicle
FF	Flexi Fuel
FFV	Flexi Fuel Vehicle
GHG	Greenhouse Gases
GPF	Gasoline particulate filter
GTL	Gas-to-liquid

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

H	HVO
HC	Unburned hydrocarbon emissions
HCCI	Homogeneous charge compression ignition
HCK	Hydrocracked diesel fuel
HCKcni	Hydrocracked fossil diesel with cetane improvers
HD	Heavy-duty
HDV	Heavy-duty vehicle
HFO	Heavy Fuel Oil
HoV	Heat of Vaporization
HTL	Hydrothermal Liquefaction
HVO	Hydrotreated Vegetable Oil (Renewable Diesel)
ICAO	International Civil Aviation Organization
ICE	Internal Combustion Engine
ICEV	Internal Combustion Engine Vehicle
IEA	International Energy Agency
Iso-Bu	Iso-butanol
JSPK	Synthetic Paraffinic Kerosene made from Jatropha
LD	Light-duty
LDV	Light-duty vehicle
LNG	Liquefied Natural Gas
LTO	Landing and Take-off Cycle
M	Methanol
MGO	Marine Gas Oil
MON	Motor Octane Number
MPFI	Multiple port fuel injection
N2	Nitrogen
NCVmass	Net calorific value mass based
NCVvol	Net calorific value volume based
NEDC	New European Driving Cycle
NOx	Nitrogen oxides
O2	Oxygen
PFI	Port fuel injection
PM	Particulate matter
PO	Palm oil
RCCI	Reactivity controlled compression ignition
RESfuels	Renewable Energy Source fuels
RME	Rapeseed Methyl Ester
RON	Research Octane Number

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

S	Sensitivity
SAF	Sustainable Aviation Fuels
SBO	Soybean oil
SCR	Selective catalytic reduction
SFC	Specific Fuel Consumption
SI	Spark ignition
SME	Soybean Methyl Ester
SPK	Synthetic Paraffinic Kerosene
SVO	Straight vegetable oil
TFEC	Total Final Energy Consumption
TWC	Three-way catalytic converter
UDC	Urban Driving Cycle
ULSD	Ultra low sulphur diesel
VED	Vehicle Energy Demand
VP	Vapour Pressure

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

1. Introduction

The present-day transport sector is responsible for a large part of global fossil-based greenhouse gas (GHG) emissions. This state of matters, unfortunately, concerns all modes of transportation (land, water, and air), that all together are responsible for 29% [6] of the Total Final Energy Consumption (TFEC) in the world, whereas in Europe it accounts for about 33% [7]. According to the International Energy Agency (IEA), global carbon dioxide emissions resulting from fossil fuel combustion were equal to 32.3Gt of CO2 in 2015, while the transport sector is responsible for 24% of those emissions [8]. Figure 1 compares transport sector's CO2 emissions from 1990 to 2015 [8]. It could be noticed that emissions in 2015 are almost two times higher than those from 1990. Additionally, the diagram contains shares of different modes, where road transport is responsible for a majority of the sector's CO2 emissions. The demand for transport increases continuously every year and it is predicted that the trend will proceed in the future [9]. During the combustion of fossil fuels, global emissions in a form of greenhouse gases (GHG) and other local air pollutions are released to the atmosphere. According to the number of research studies, GHGs have a direct impact on climate change [10], and together with other pollutions coming out of the combustion process, they affect strongly environment and in turn, human health [11]. Unfortunately, in both cases, the impact is clearly negative. Therefore, it is of high interest to mitigate the GHG effect and reduce the use of fossil fuels. World governments have various targets of GHGs reduction [12]. European Union member states have key EU targets for 2020, 2030 and long-term goals.

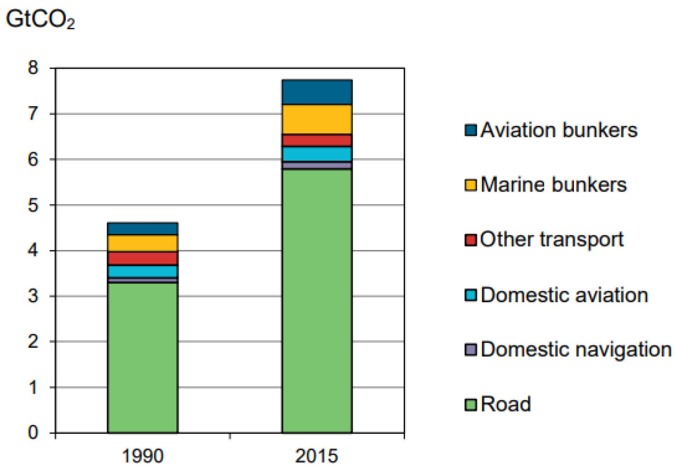


Figure 1 The surge of CO2 emissions in the transport [8].

- Key EU targets for 2020 include a 20% cut in GHG emissions compared to the state from 1990, 20% share of renewable energy in the TFEC and 20% increase in energy effciency.
- Key EU targets for 2030 contain 40% cut in GHG emissions compared to the state from 1990, 27% share of renewable energy in the TFEC and 27% increase in energy effciency.
- Long-term goals are aiming at 2050, the target is 80-95% cut in GHG emissions compared to the state from 1990.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

In order to achieve those targets, research and development that supports the commercialization of sustainable energy solutions become an essential and inseparable part. Biomass represents significant potential among other renewable energy source alternatives, especially when considering economics. Additionally, in many places, biomass is available in large quantities that can satisfy the necessary feedstock demand for fuel production on commercial-scale. According to the IEA, advanced biofuels will dominate the transport sector’s alternatives to fossil-fuels [13]. Synthetic fuels produced from renewable sources and some biofuels can be freely blended with fossil fuels, even in the whole range of the concentrations. Additionally, they can be used directly in the current-fleet of engines and existing refueling systems without any modifications (drop-in fuels). In other cases, there are specified safe limits of blending concentrations, so-called ”blending-walls”, that ensure proper operation of the engines with no modifications. The most promising biofuels represent not only strong environmental benefits but they also have better fuel properties than standard fossil-based fuels. Good examples are ethanol, that has a higher octane number (ON) than gasoline and hydrotreated vegetable oil (HVO) that has a higher cetane number (CN) than standard diesel fuel. Implementing drop-in biofuels into the market brings directly a positive environmental impact. According to IEA: ***”Conventional biofuels are on course to meet 2DS targets for 2025; however, accelerated production of advanced biofuels is necessary to meet 2DS needs for transport sector decarbonization”*** [14]. Thus, biofuels and synthetic fuels produced from renewable sources play an essential role in the transportation-greening process. Therefore, all actions supporting commercialization of transport biofuels increase the chances of meeting EU and global climate targets. Biofuels additionally can be produced from wastes, such as used cooking oil or lignocellulosic wastes, which open an excellent opportunities for sector coupling via waste management and decarbonisation of transport sector.

1.1. The scope and objectives of Task 5.4

This work aims is to support and accelerate the commercialization of renewable energy source fuels (RESfuels) in the transportation sector. Task 5.4 called “Fuel and fuel blend properties in end-use“, provides explanations regarding to how and why RESfuels and fuel blends affect the end use performance (efficiency, fuel consumption, CO2 emission, local emissions) and how they are linked to combustion / fuel oxidation systems and emission mechanisms and aftertreatment technologies. Based on RESfuel tests in various engines, mathematical models were developed, that represent a unique and most significant fuel properties effect on engine performance for a specific fleet of engines. The main sources of data were journal publications, technical papers, public articles and reports. The numerical tool, owns all developed models, and provides the end-use performance assessment for RESfuels in aviation, marine, on-road light duty (LD) and heavy-duty (HD) transportation. Figure 2 represents the scope of Task 5.4, and highlights the achievements; developed models and online tool.

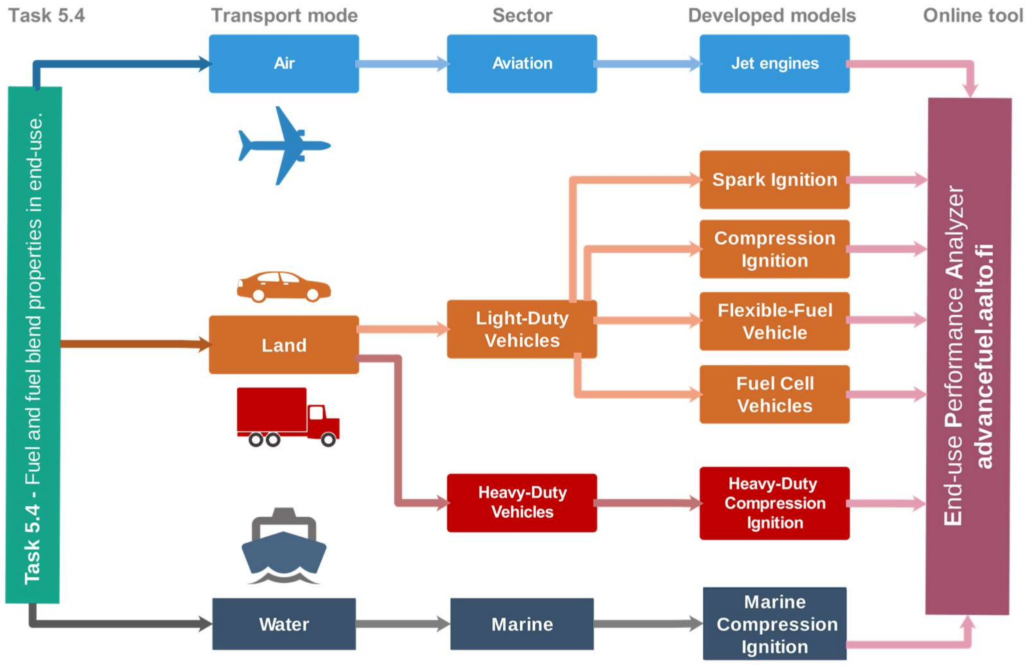


Figure 2 Scope of Task T5.4 with highlighted achievements (developed models and online tool).

The main output of the numerical tool is the specific fuel consumption and the CO2 emission. The numerical tool is called **EUA (End-Use Analyser)** and is located in an online platform, available free of charge to all users. In order to access the tool, one need to type into the internet browser the following link: **http://advancefuel.aalto.fi/**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

2. End-use performance of internal combustion engines (ICE)

This section introduces internal combustion engine (ICE), its operation and suitable fuels with division on spark and compression ignition engines. Moreover, new combustion concepts are briefly considered. Engine performance indicators used in this report are explained, too.

2.1. Spark ignition (SI) engines and fuels in brief

The spark ignition (SI) internal combustion engine (ICE) was developed by Nikolaus Otto in 19th century, therefore it is known as Otto Engine. SI engines operate in so-called Otto cycle where the mixture of air and fuel is ignited by the spark from a spark plug. The combustion in spark ignition engines is a known as turbulent premixed combustion that is characterized by the fast heat release and high flame propagation. This, in turn, allow SI engines to operate in higher maximal revolutions per minute (RPM) in comparison to compression ignition engines (CI). Spark ignition engines operate in compression ratios (CR) from around 8 to 12, whereas compression ignition engines from 12 to 24. SI engines are in general lighter than CI engines, their maximum torque is at mid speed range, whereas in CI engines at lower speed range. Older SI engines were equipped with carburetor that was mixing the air and fuel together. Afterwards, the port fuel injection (PFI) systems were installed, and specifically multiple port fuel injection (MPFI). Modern SI engines are equipped with direct injection (DI) similarly to CI engines [2].

The primary fuel for SI engines is a gasoline characterized in European Union (EU) by EN228 standard, which gives safe limits for significant fuel properties that will ensure the proper operation of SI engine. One of the most critical properties stated in the standard is Research Octane Number (RON), and Motor Octane Number (MON). SI engines, are restricted by knocking limits of fuels. When the air-fuel mixture in the end- gas region is sufficiently compressed and reaches high enough pressure and temperature, fuel can automatically ignite (ignition not caused by spark plug). As a result, a shock wave is generated which creates the metallic “pinging” sound, and causes the rapid increase of cylinder pressure. Knocking combustion leads to various damages, for example, piston crown melting, piston ring sticking, cylinder bore scuffing, piston ring-land cracking, cylinder head gasket leakage, and cylinder head erosion. The RON, MON and

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement N.º764799.

sensitivity (the difference between RON and MON) of the fuel define how well the fuel is resistant to auto ignition [15], [16]. More specifically, RON represents mild driving conditions, whereas MON represents severe, high speed and high load driving. The table in 'Appendix A: SI fuels specification.' shows EN228 standard limitations and typical values of gasoline properties from Finnish refineries.

Alternative SI fuels include, alcohols (ethanol, methanol, isopropanol, n-propanol, isobutanol, prenol, fusel alcohol), olefins (e.g. di-isobutylene), furans and ketones (e.g. cyclopentanone) [17]. Some of them can be utilized directly without any retrofitting of engines or refueling systems within the specified blending walls. As an example, the current EN228 standard allows 3% of methanol in the blend. According to EU Fuel Quality Directive gasoline can contain up to 10% volumetric blend of ethanol (E10 fuel), while maximum 5% blend (E5 fuel) should be also available for non-compatible vehicles. In the market, most of the cars are approved by engine manufacturers to use E10 fuel. However, the use of ethanol or other alcohols in higher concentrations requires modifications in current engines. Ethanol has a higher Research Octane Number (RON) than gasoline. Therefore, when using it in a special dedicated engine that has a higher compression ratio, E85 fuel comprising 85% of ethanol and 15% of gasoline can bring a significantly higher thermal efficiency of the energy conversion process compared to the case when used in the regular unmodified Spark Ignition (SI) engine. The same applies to methanol. Heavier alcohols, such as butanol, are significantly more compatible with the present-day internal combustion engine technology and could be used in higher concertation ratios with gasoline compared to ethanol. A very important fact is that alcohols strongly reduce the local emissions such as hydrocarbons (HC) and particulate matters (PM) even in the small portions of blends. It is beneficial especially for the direct injection (DI) SI engines. However, due to the high heat of vaporization of alcohols, in the cold engine conditions, this effect can be disadvantageous, and increase local emissions. Therefore, engine optimization is essential. Gasoline engine emission control is carried out by the three-way catalytic converter (TWC) that oxidizes carbon monoxides (CO) and hydrocarbons (HC) to carbon dioxide (CO2), by reducing nitrous oxides (NOx) to nitrogen (N2). Modern vehicles equipped with DI SI engines are additionally equipped with gasoline particulate filter (GPF), to reduce the PMs [2]. Specification of selected SI fuels can be found in 'Appendix A: SI fuels specification.'

2.2. Compression ignition (CI) engines and fuels in brief

The mechanism of compression ignition (CI) engine (or 'diesel engine' in other words) is based on a diesel process developed already in the late 19th century by Rudolf Diesel. Fundamentally, combustion is controlled by turbulent mixing. In principle, CI engine is characterized by higher

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

thermal efficiency than SI engine. It is a consequence of higher compression ratio of CI engine – only air is compressed by the piston and it is not limited by knocking phenomena as in the case of SI engines. Due to the higher end-gas temperature inside the cylinder, fuel self-ignites after injection. Modern engines are equipped mostly with direct injection system, which is crucial for engine operation and proper combustion. Other modern CI engine's features are turbocharging, charge air cooling, common rail high-pressure injection system, and four valves per cylinder, for instance. Regarding local emissions such as nitrogen oxides (NOx) and particulate matter (PM), advanced aftertreatment measures include exhaust gas recirculation (EGR), diesel oxidation catalyst with particulate filter (DOC+DPF), and selective catalytic reduction (SCR) for NOx. More information about CI engine characteristics and operation can be found in cited master thesis [1].

In diesel process, mixing controlled combustion can be divided in 3 primary stages: mixture formation, ignition and proper combustion. Combustion process itself imposes specific requirements on fuels, which are denoted as diesel fuels. The fuel reactivity is a critical property. In order to enable stable combustion, high reactivity fuels are needed, which is directly related to autoignition process. The primary measure of the fuel's reactivity is cetane number (CN). Other key properties are density, viscosity, volatility and oxygen content, which impact mixture formation and combustion process. Those are only examples but there are plenty of other important properties for diesel fuels, which can be found in fuel standards. In the EU, standard EN590 sets the limits for properties such as CN, density, viscosity, lubricity, oxidation stability, etc. Fuel standards are a guidance towards engine compatibility and complying with them is required by engine manufacturers to accept the engine warranty.

Diesel-like fuels encompass reference diesel and liquid alternatives such as biomass-to-liquid (BTL), hydrotreated vegetable oil (HVO), traditional biodiesel (FAME) or gas-to-liquid (GTL). Fully compatible fuels with modern engines are denoted as drop-in and can be freely blended with reference diesel, here HVO and GTL as good examples. Whereas traditional biodiesel is not fully compatible with modern CI engines when using higher concentrations in blends with reference diesel. In such case, blending-wall is determined – it is 7% volume-based of FAME allowed in EN590 diesel. Higher blends might cause oil dilution or stability problems [18]. Additionally, alcohol blends with ignition improvers or DME can be also used in CI engines but those need dedicated engine technologies and infrastructures, hence, are less attractive then BTL or HVO. Selected properties of CI fuels are presented in 'Appendix B: CI fuels specification.'. Additionally, specification of reference EN590 diesel fuel from Finnish market is presented in the same Appendix.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

2.3. New combustion modes

Besides well-established combustion concepts in SI and CI engines, there are also novel approaches including dual fuel (DF) combustion, mixing controlled combustion of low reactivity fuel, homogenous charge compression ignition (HCCI) or reactivity controlled compression ignition (RCCI) modes. Those new concepts aim to utilize alternative fuels and limit environmental impact from ICE in the transport sector.

2.3.1. Dual fuel combustion

The dual fuel combustion realized in diesel engines with high compression ratio combines the traits of spark ignited and compression ignited combustion processes. In DF combustion, the low reactivity fuel (for ex. methane) is compressed and ignited by the auto-ignition of a small amount of high-reactivity fuel (diesel-pilot) close to the top-dead-center (TDC) [19].

DF engine technology, where the main fuel energy comes from a low-reactivity fuel (i.e. methane, natural gas, biogas, CNG, ethanol, and methanol) and the ignition energy is provided by a high-reactivity fuel (i.e. diesel and HVO), is a well-known technology for robust engine operation with decreased environmental impact. Traditionally, the approach to deliver the low-reactivity fuel is via the intake manifold (port fuel injection, PFI) to create a homogeneous fuel-air mixture. Owing to the small quantity of pilot diesel, the lean premixed combustion of the main fuel yields low NOx and soot emissions [20].

2.3.2. Mixing controlled compression-ignition of low reactivity fuels in CI engines

Mixing controlled compression ignition of low reactivity fuel can be also called as pilot assisted diesel combustion concept. It is characterized by separate high-pressure direct injection (DI) system to deliver both low reactivity main fuel (for ex. Methanol) and high reactivity pilot fuel (for ex. Diesel fuel). Unlike dual fuel PFI configuration where low reactivity fuel is injected to the intake manifold, in this concept, it is directly injected into the combustion chamber. It can be achieved either by special nozzle capable of delivery of both fuels or by special design of cylinder head accommodating two separate injectors. In turn, ignition of low reactivity fuel is provided by diesel pilot, which acts as an efficient spark for the high-pressure low-reactivity fuel sprays yielding a non-premixed combustion. This combustion concept is particularly promising for alcohols as low reactivity fuels. Latest methanol studies [20] revealed that high pressure DI of methanol with diesel pilot seems to be a viable concept, even with high methanol substitution rates – especially good potential in marine applications.

2.3.3. Homogeneous charge compression ignition (HCCI)

Homogeneous charge compression ignition combustion (HCCI) combines the features of SI combustion and CI combustion. The fuel is injected early and it is usually split into multiple times. The premixed air and fuel are compressed to reach the auto-ignition point, which ignites

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

the fuel. HCCI combustion initiates at the different locations in the cylinder, so there is no identifiable flame front. Thus, HCCI combustion does not have local high temperature reaction zone, which significantly reduces NOx and PM emissions. Besides, unlike diesel combustion, the HCCI combustion is faster owing to the premixed diesel. However, due to premixed fuel, knocking of HCCI is a serious problem, which limits its utilization to lean air/fuel mixing conditions [21]. The combustion timing is still a challenge in HCCI.

2.3.4. Reactivity controlled compression ignition (RCCI)

Reactivity controlled compression ignition combustion is a combustion mode in which low reactivity fuel is applied and high reactivity fuel controls the combustion. Therefore, the RCCI utilizes two fuels with different characteristics and its combustion mechanism is similar to HCCI. The RCCI technology is a promising concept that has high efficiency, low NOx and PM emissions, mainly due to the low combustion temperature [21]. Moreover, compared to HCCI mode, it is much easier to control the RCCI combustion due to presence of high reactivity fuel.

2.4. Performance indicators for ICE

Performance of internal combustion engine can be represented by several indicators such as fuel consumption, CO2 emissions or local emissions. When analyzing impact of alternative fuels on end-use, those performance indicators are treated with special attention.

2.4.1. Fuel consumption

Fuel consumption (FC) is an indicator of how much fuel is needed for a considered engine/vehicle at specified operating conditions. Depending on the application, we can distinguish various representations of fuel consumption.

- Brake Specific Fuel Consumption (BSFC) – fuel consumption is referred to delivered power of the engine. BSFC is calculated dividing fuel mass flow by brake power provided by the engine. The unit of BSFC is g/kWh. Usually, BSFC is reported for steady-state measurements on engine dynanometer. This engine indicator shows how efficiently fuel is used in order to deliver brake power. BSFC value can be also compared between various engines. Calculation formula:

  $$b_e = m/P_e$$

  Where, b_e – BSFC, P_e – brake power, m – fuel mass flow.

- Fuel consumption (FC) in driving cycle – fuel consumption is referred to the specific driving cycle (such as NEDC or Braunschweig) for a given vehicle. FC can be volume- or mass- or energy-based and the whole test is done on a chassis dynamometer or during onroad measurements. Usually, the total fuel consumption throughout the driving cycle is divided by the total distance covered by this test. In that case, the unit of FC might be l/100km or kg/100km or MJ/100km, respectively. Calculation formula:

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

$$b = m_T/s$$

where b – FC, s – distance covered by the vehicle during specified driving cycle, m_T – total mass (or volume or energy) of fuel consumed throughout the whole driving cycle.

Alternatively, total fuel consumed can be divided by the energy needed during the whole driving cycle for a specified vehicle – heavy-duty trucks or buses as examples. Then the unit of FC is the same as in case of BSFC.

2.4.2. CO2 emissions

CO2 emissions resulting from the combustion of the fuel in ICE are associated with global emissions of greenhouse gases (GHG). In this report, presented CO2 emissions are referred to tailpipe emissions only. It means that CO2 emitted in various fuel production stages, including raw material collection, refinement and distribution, are not taken into account. Instead, CO2 released during combustion of hydrocarbons is calculated based on volumetric fuel consumption, carbon content of the fuel and its density. To quantify them, CO2 emissions are expressed in g/km or g/kWh.

2.4.3. Local emissions

Local emissions are associated with the local air pollution and should not be in any case confused with global emissions, referred to GHG. Local emissions encompass following compounds:

- nitrogen oxides (NOx),
- sulfur oxides (SOx),
- particulate matter (PM),
- unburned hydrocarbons (HC),
- carbon monoxide (CO),
- unregulated emissions, such as aldehydes.

While HC and CO are handled by diesel oxidation catalyst (DOC), NOx and PM are the main concerns for compression ignition engines. When optimizing diesel engine, trade-off between NOx and PM is a limitation [22]. That is why, there are needed additional measures such as DPF, SCR or NOx trap catalyst making the aftertreatment system quite complex. NOx is not a problem in a case of spark ignition engines while three-way catalyst (TWC) takes care of NOx, HC and CO simultaneously. In former technology of port fuel injection (PFI) in SI engines, PM were not an issue, too. However, in modern direct injection SI engines, increased PM emissions can cause some problems. Possible solution can be found in gasoline particulate filters (GPF) [23]. SOx emissions are not any longer concern in road transport due to compulsory utilization of low sulfur diesel. Instead, nowadays the main SOx emitter is maritime sector despite more stringent regulations coming into force like sulfur cap 2020. Elevated levels of unregulated emissions could be a problem for some alternative fuels, i.e. aldehydes emissions from alcohol blends were investigated in the literature [24], [25].

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

3. Methodology

This section explains approach in analyzing RESfuels from the end-use perspective. Representations of engine performance and fuel properties are justified, too. Modeling techniques resulting in representative models are presented subsequently. The whole procedure in Task T5.4 presented in Figure 3 The whole procedure of RESfuels analysis.included extensive literature studies, which resulted in the collected database necessary for initial analysis and further modeling. For the purpose of this work, methodology development, modeling, and validation were executed in subsequent steps. Developed models were published already in few technical and journal papers ([3], [4], [5]).

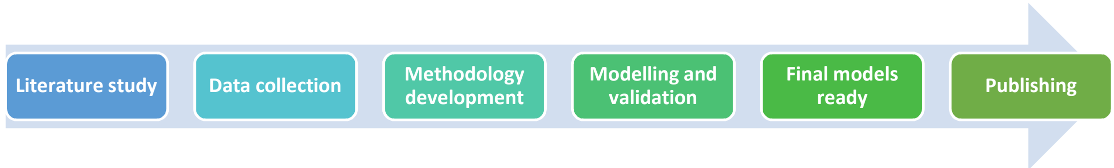


Figure 3 The whole procedure of RESfuels analysis.

3.1. Structure of the modeling task

It is a complex task to examine RESfuels in the context of end-use and draw generic conclusions. In practice, there are always advantages accompanied by challenges related to the final use of the new fuel in the internal combustion engine (ICE). Moreover, selected alternative fuel can be a good solution in one application but not a feasible option in another field. Even for the same engine, while switching towards RESfuel, contrary results might be observed depending on operating conditions, i.e. high-speed & high load versus low-speed & low load. To properly assess RESfuel performance in ICE, it is essential to specify boundary conditions of the task.

Therefore, starting from the boundary conditions, the main focus of this work is put on alternative fuel properties and their impact on engine performance. In other words, alternative fuels are analyzed based on their properties (see Section 3.3). The structure of the task is schematically presented in Figure 4. On the one hand, it is important to specify engine and its operating conditions resulting from the final application in the transport sector. For instance, CI engines of light-duty vehicles are significantly different from marine engines or jet turbines. On the other hand, set of fuel properties related to RESfuel need to be specified as well. The main aim of the modeling work is to connect the set of fuel properties with engine performance for specified engine type and operating conditions. Engine performance can be expressed by fuel consumption, CO_2 emissions or local emissions (see Section 2.4). Alternatively, new fuels can be analyzed in terms of combustion characteristics such as ignition delay or in-cylinder pressure

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

but it is not executed in this study. To sum it up, the modeling results should enable decision makers or fuel producers to predict the engine performance from the fleet point of view (fuel consumption, GHG emissions) based on already available knowledge on renewable fuels expressed by the set of fuel properties.

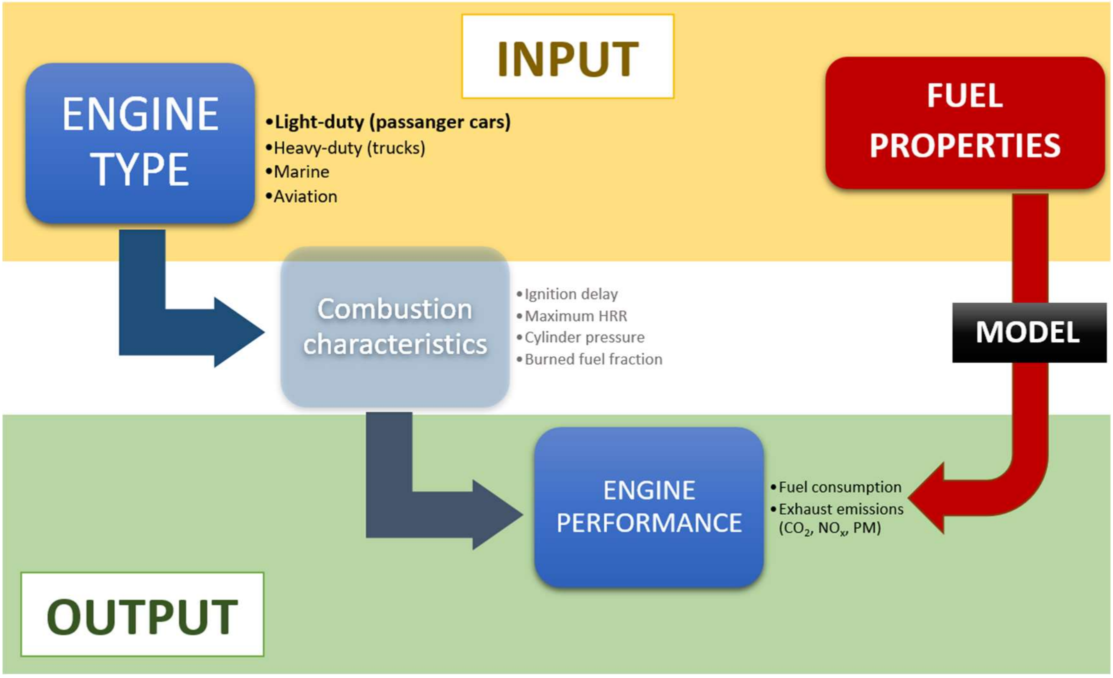


Figure 4 Schematic representation of the approach to modeling task [1].

3.2. Selected representation of engine performance

Depending on the final application in the transport sector, different vehicles/vessels/aircrafts with various engines are selected. It is also important to specify the most representative engines and operating conditions. This section determines vehicles, engines and operating conditions for each transport sector considered in this study.

3.2.1. Light-duty vehicles (SI, CI, FFV, FCV)

In case of LDV fleet, the engine performance could be measured on the steady-state tests, where alternative fuels are tested on the specific load and speed points of engine. This option applies to SI, CI and FFV internal combustion engines. However, it has been proven in the master thesis of Yuri Kroyan [2] and Michal Wojcieszyk [1], that steady state performance, does not preserve the trends, and emerges a high data inconsistency in LDV engines. Another limiting factor of steady-state approach is a lack of transient engine operation, which is very significant

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

in a real driving. Due to that finding, the steady-state option, was rejected from methodology. The other possibility are analysis of combustion characteristics via supercomputers. However, in that approach, there are thousands of highly influencing parameters, and the scope of the project would need to be much wider to include such detail level analysis. The most convenient, and representative option turned out to be driving cycles specific fuel consumption. Figure 5 summarizes three possible approaches.

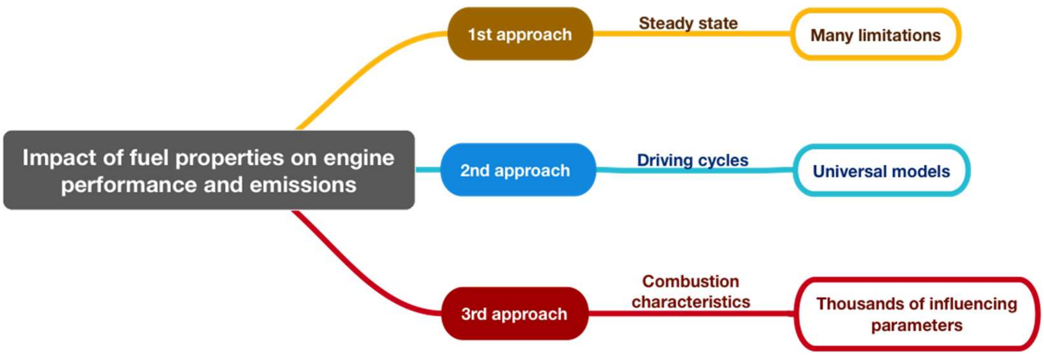


Figure 5 Possible approaches for measuring engine performance [2].

The second considered approach is based on the driving cycles that are a compilation of many steady-state points with additionally transient operating conditions. Driving cycles were introduced to measure average fuel consumption and emissions during real driving conditions in a more reliable way. Therefore, the driving cycle based engine performance represents the most accurately the effect of alternative fuel from the end-user perspective. The New European Driving Cycle (NEDC) was introduced in 1990s, it includes, four repetitions of Urban Driving Cycle - UDC also known as an ECE-15, and one Extra-Urban Driving Cycle - EUDC (Max. speed 120km/h during 11 seconds). Figure 6 shows NEDC velocity profile.

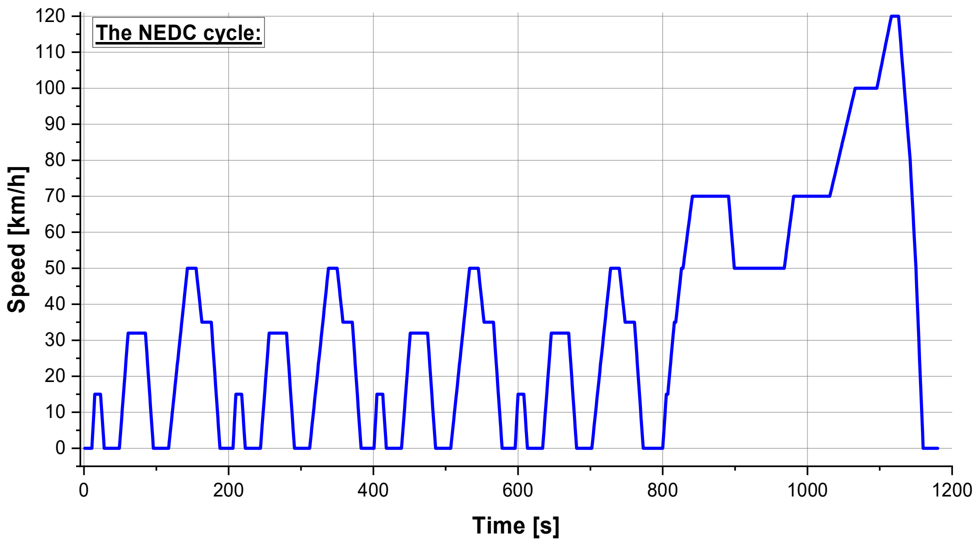


Figure 6 NEDC velocity profile.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

3.2.2. Heavy-duty vehicles

The selection of CI engines in heavy-duty sector is much broader than in LDV case. The engine's parameters can vary significantly, especially when comparing different displacement of the engine. In this work, average bus engine (8.0L displacement volume) was selected for modeling purposes. When searching for representative driving conditions, it was decided to choose Braunschweig cycle presented in Figure 7. This driving cycle approximates bus operation in the urban area. After extensive literature review, measurement data were collected from various literature sources. Those data correspond to the experimental results of buses run on alternative fuels and tested on chassis dynamometer according to the Braunschweig velocity profile. Results can be associated with vehicle of 15 tons on average and energy demand of 11kWh over the whole test cycle [26].

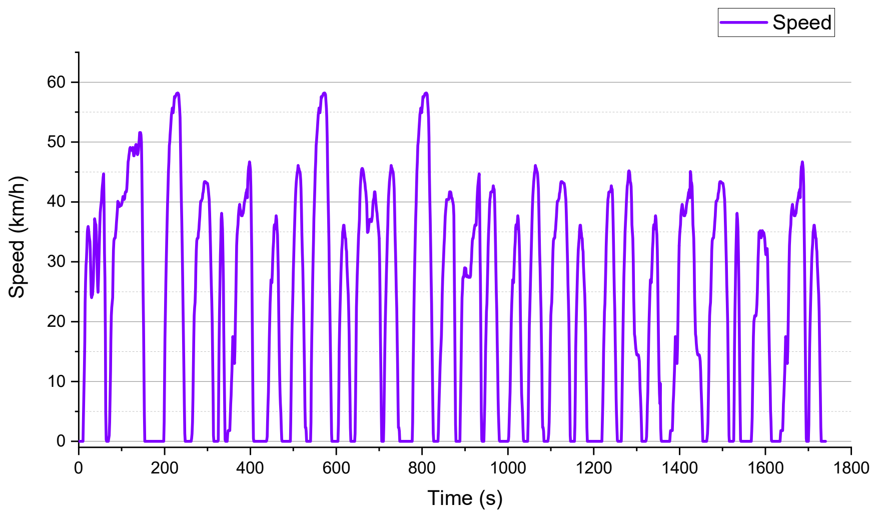


Figure 7 The Braunschweig cycle's velocity profile.

3.2.3. Marine engine

When trying to obtain a descriptive model for alternative fuels and their impact on marine engine performance, it is essential to select appropriate data, similarly to other transport sectors. The existing marine engine and its operation on various fuels was concluded as the most suitable source for acquiring the data. However, it is important to note that marine engine tests are very expensive. It is a consequence of high investment and maintenance costs of the engine, and fuel costs related to the high fuel consumption in experiments. In that respect, only results from one publically available study were identified [27] – the research focused on alternative fuels and their performance in medium-speed marine engine with the power output of 400 kW at engine speed of 750 revolutions per minute (rpm). For modeling purposes, steady-state measurements were selected: 75% load at nominal engine speed. Usually, those conditions are representing the most efficient engine operation and mimic vessel's conditions at the overseas freight [27]. Engine specification is presented in Table 1.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Table 1 Test engine specification and operational conditions [4].

Engine type	Medium-speed marine CI
Number of cylinders	1
Bore x Stroke	320 x 440 mm
Displacement volume	35.4 l
Compression ratio	16.2
Nominal power	400 kW
Selected engine's operational conditions	
Applied test load	75%
Applied test speed	750 rpm

3.2.4. Aviation

In aviation, there could be distinguished few stages of aircraft operation, taxi-in, take-off, climb-out, cruise, approach, landing and taxi-out. International Civil Aviation Organization (ICAO) introduced the simplified flight cycle, called the landing and take-off cycle (LTO) [28]. The LTO is a standardized procedure for testing jet fuels, engines and emissions in aviation. Aircrafts spend most of their time while cruising. Therefore, in the methodology, the effect of sustainable aviation fuels (SAF) on performance of jet engine is selected over cruise conditions. The performance of jet engine is represented as cruise specific fuel consumption (SFC) the units of SFC is kg/N*hr.

3.3. Key properties of transport fuels

Fuel, regardless of its origin, is characterized by set of physical and chemical properties. Depending on the engine technology and final application in the transport sector, fuel needs to fulfill specific criteria. The critical fuel properties are specified and limited in fuel standards like EN228 or EN590 for SI and CI road fuels, respectively. Jet fuels need to meet the most stringent regulations whereas marine sector has the highest flexibility. Physico-chemical properties indicate the end-use applicability of the fuel and its compatibility with the current fleet of engines. Therefore, alternative fuels, including RESfules, can be analyzed from the perspective of fuel properties. Important properties of transport fuels are described and analyzed below (based on both [1] and [2]).

3.3.1. Octane number

Octane number is a measure that describes antiknocking behavior of the fuel – it is an antiknock indicator. Therefore, it is a critical property for SI engines. Octane number is measured in CFR engine while tested fuel is compared to Primary Reference Fuels (PFR) mixture of iso-octane with excellent antiknock characteristics and n-heptane with poor antiknock behavior.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

- Research Octane Number (RON) – represents mild driving conditions. RON is a better indicator for SI engines operating at full throttle and low engine speed.
- Motor Octane Number (MON) – represents severe, high-speed and high-load driving. MON is a better indicator for engines operating at full throttle and high speeds or part throttle with low and high engine speeds.
- Octane sensitivity (S) – a difference between RON and MON.

3.3.2. Cetane number (CN)

Cetane number is a measure of fuel reactivity. In CI engines, fuels with good auto-ignition properties are preferred, whereas in SI case, low reactivity fuels are needed. Mixture of reference fuels tested in CFR engine determines the CN value: cetane (n-hexadecane) has excellent ignition properties and CN equals 100, while alfa-methylnaphthalene is characterized by poor ignition and its CN is 0.

3.3.3. Heating value

Heating value or calorific content informs about energy content of the fuel and is related to energy released during combustion. In ICE applications, lower heating value (LHV) is commonly used. LHV volume-based (LHVvol) denotes energy gathered in a unit of volume (MJ/l) and LHV mass-based (LHVmass) determines available energy per unit of mass (MJ/kg). Higher calorific content means better energy density and it is beneficial from the fuel storage perspective. For fossil-based fuels like diesel and gasoline the LHV is high and roughly 44 MJ/kg – in turn, it is challenging for alternative fuels to compete in that respect.

3.3.4. Density

Density specifies the mass of a fuel in a certain volume in specific conditions. For transport fuels, usually density at 15ºC is measured. Density of reference diesel should be in the range of 820-845 kg/m3 while for gasoline it is lower, 720-775 kg/m3. Density plays a major role in fuel injection by influencing spray formation and mixing.

3.3.5. Viscosity

Generally, the viscosity of the fuel is highly temperature dependent – the higher the temperature, the lower the viscosity. It is a critical fuel property for injection system as it affects spray formation and mixing. Hence, it is one of the most important CI fuel properties. In EN590 standard, kinematic viscosity of the diesel fuel should be in the range of 2.00−4.50 mm2/s at 40ºC. Viscosity of gasoline is an order of magnitude lower than for diesel. Additionally, EN228 does not specify viscosity limits – SI fuels are generally low-viscous. Besides injection system, viscosity has an impact on selection of the whole fuel delivery system, i.e. fuel pump etc.

3.3.6. Lubricity

Lubricity of the fuel is an important property, especially when considering high-pressure injection system including pumps and injectors. Unless fuel owns good lubricating properties, the wear of such elements can be faced. Therefore, sometimes it is necessary to enrich the fuel by

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

lubricating additives. Good lubricity is particularly wanted in CI fuels and EN590 standard specifies minimum limits.

3.3.7. Distillation characteristics

Distillation characteristic is determined by evaporated fraction of the mixture in the given temperature. Typical temperature range of boiling temperature is approximately 50-170 ºC for gasoline and 170-380ºC for diesel. It is one of the fuel volatility measures indicating how easily fuel evaporates, which is particularly important for a proper operation of SI engine.

3.3.8. Vapor pressure

Vapor pressure determines the pressure [kPa] of fuel vapors over the liquid at the given temperature. In gasoline standard, vapor pressure is measured at the temperature of 37.8 °C (100 °F). It is important property for SI fuels indicating fuel volatility.

3.3.9. Vapor Lock Index (VLI)

Vapor-Lock Index (VLI) defines the tendency of the fuel to form vapor-bubbles in the fuel injection systems. VLI describes better the properties of fuel in terms of vapor-lock, hot-starting and hot-running performance than vapor pressure and boiling characteristic alone. It is valid when vapor pressure exceeds system pressure of injectors, which appears especially in fuels that contain high concentrations of alcohols. VLI is calculated based on vapor pressure and evaporated fraction at 70°C, and the normal range is between 800 and 1250. The lower the values, the better anti-vapor-lock properties of SI fuel.

3.3.10. Heat of vaporization

Heat of vaporization (HoV), known also as heat of evaporation or enthalpy of vaporization, represents the amount of energy that has to be added to fuel in a liquid state to transform given mass of that fuel into a gas. The unit of HoV is kJ/kg, and it is a very significant fuel property, especially in SI engines. High HoV of the fuel can bring a beneficial cooling effect in the combustion chamber during evaporation by absorbing part of the released energy in combustion process. This, in turn, allows increasing the compression ratio or effective compression ratio of the SI engine, which improves the thermal efficiency. In general, alcohols have much higher HoV than reference EN228 gasoline.

3.3.11. Cold flow properties

Cold flow properties of fuel are important for CI and jet fuels but have no special meaning for SI fuels (consequence of high volatility of SI fuels).

- Cold Filter Plugging Point (CFPP) – represents lowest temperature at which fuel flow and filtration is unimpeded. CFPP is a good indicator of fuel reliability in low temperatures for modern engines engines with advanced filtering systems, which can handle precipitated cristals to some extent. Fuels with additives tend to have significantly lower CFPP than cloud point [29]. In EN590 standard, climate-dependent fuel grades are just distinguished by CFPP.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

- Cloud point – is a temperature at which fuel starts to crystallize (paraffin waxes).
- Pour point – suggests theoretical lowest temperature, at which fuel can be pumped from the fuel tank.
- Freezing point – very important property for jet fuels due to extremly cold conditions at higher altitudes.

3.3.12. Flash point

Flash point is a safety-related property not influencing combustion behavior. The flash point temperature determines the lowest temperature under normal pressure at which fuel vapors mixed with the air can ignite in a closed vessel. In general, SI fuels are low-flashpoint while EN590 standard for diesel fuel sets 55°C as a minimum flash point temperature, which, in turn, limits low boiling compounds in a fuel mixture. Therefore, the risk of ignition during storage is significantly lower for diesel than for gasoline fuel.

3.3.13. Oxidation stability

Stability is an important property affecting storage. It determines the resistance of the fuel to undergo unwanted chemical reactions in contact with the environment. Oxidation process of the fuel and later polymerization can lead to decreased quality and eventually, the clogging of filters or fuel lines might occur.

3.3.14. Purity of the fuel

Purity of the fuel indicates its quality and concentration of unwanted molecules in the fuel mixture. Road and jet fuels have very low limits of contaminants whereas marine fuels can have higher levels of impurities. Contaminants such as sulfur, ash or total sediment adversely affect emissions, aftertreatment systems, fuel lines, injection, etc.

- Sulfur – formes corrosive SOx during combustion; an adverse effect on human health.
- Lead – formely used as octane booster but has also harmful effect on human health.
- Vanadium – element which can be sometimes found in marine heavy fuel oils.
- Water content – solubility of water in fuel should be highly limited due to storage.
- Gum content – possible effect of oxidation of SI fuel, adverse effect on fuel system.
- Carbon residue – carbon residue in the highest boiling fraction, precursor for deposits.
- Ash - inorganic compounds in the fuel.
- Total contaminants/sediment – all undissolved materials present in the fuel, i.e. sand particles or rust. Might lead to filter clogging, wear of injectors etc. Very important property for lower grade marine fuels.

3.3.15. Acidity

Too high acidity can lead to corrosion when fuel has the contact with metal elements like supply lines and injectors, resulting in adverse rust formation and final destruction. Copper strip corrosion test is specified in EN590 standard for diesel fuel. Additionally, it is very important property for marine fuels, especially those of lower quality.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

3.3.16. Conductivity

Conductivity is a very important fuel property when it comes to safety of fuel storage in tanks. In refinery terminals, at the filling stations or during vehicle/aircraft refueling, fuel can accumulate the static electricity. This raises the danger of static discharges that are proven to be a fire hazard. The improvement of electrical conductivity, is mainly done by blending with conductivity improvers (fuel additives). They help the fuel to constantly discharge the electricity and prevent the electrical charge to be accumulated in the fuel. Fuel conductivity is especially important in aviation.

3.3.17. Summary of significant fuel properties for specific engines

When considering alternative fuels for specific application, the attention should be put on the properties marked in Table 2.

Table 2 Summary of significant fuel properties for specific engine application.

Properties	SI	CI	Jet	Fuel-cell	Marine
RON	x				
MON	x				
Octane sensitivity	x				
CN		x			x
Heating value	x	x	x	x	x
Density	x	x	x	x	x
Viscosity		x	x		x
Lubricity		x	x		x
Distillation characteristics	x	x	x		
Vapor pressure	x				
Vapor Lock Index	x				
Heat of Evaporation	x				
CFPP		x			x
Cloud point		x			x
Pour point					x
Freezing point			x		
Flash point		x	x		x
Oxidation stability	x	x			x
Purity of the fuel	x	x	x	x	x
Acidity and copper corrosion	x	x	x		x
Conductivity	x	x	x		

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

3.4. Relative changes approach

Experimental data representing performance of alternative fuels were collected from different literature sources coming from research institutions located around the world. Therefore, to create uniform alternative fuel database from various experimental set-ups, it was decided to express all numerical values by relative changes referred to the reference fuel. Each transport sector was assigned with reference fuel, i.e. CI LDV fleet with diesel, SI LDV fleet with gasoline or marine engines with HFO. It is important to note that even for selected transport sector, there is no universal reference fuel. For instance, reference diesel in US has different properties than reference diesel in Europe. That is why, baseline fossil-fuel used in the given experiment was considered always as a reference fuel, while alternative fuels were always referred to this reference fuel. The formula used to convert absolute numerical values into relative changes is as follows:

$$\% X = \frac{X_{alternative} - X_{reference}}{X_{reference}} * 100\%$$

Where:

X – is fuel property or engine performance indicator (i.e. density or FC)

$\% X$ – is relative change of X for alternative fuel

$X_{alternative}$ – is absolute value of X for alternative fuel

$X_{reference}$ – is absolute value of X for reference fuel

Note: This calculation was executed for every engine performance indicator and each fuel property of tested alternative fuel. The exception was done for all elemental components such as carbon, hydrogen, and oxygen, where absolute values were used instead.

Following guidelines were used while creating numerical matrix necessary for modeling purposes:

- Fuel properties of alternative fuels and their blends were expressed in terms of relative changes. It means that fuel property of alternative fuel was always compared with the same property of reference fuel for the same experiment.
- Engine performance indicators represented by fuel consumption or CO2 emissions were also expressed by relative changes. It means that FC of alternative fuel was always compared with FC of reference fuel for the same experimental set-up.
- Created models were expected to predict relative change in FC or CO2 emissions for considered new fuel blend (refered to reference fuel).

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

3.5. Black-box modeling

Modeling methodology is thoroughly described in released scientific publications ([3]–[5]). In principle, data from various sources were collected in the form of the matrix. Relative change approach was applied, see explanation in Section 0. After initial data analysis, the multilinear regression was selected as an appropriate mathematical methodology. It was concluded that fuel properties are treated as an input while end-use performance indicator was conceived as single output. Therefore, the multilinear regression enabled analysis of such a matrix of data with multiple input and single output. In the scope of this work, various alternative fuels and their blends were analyzed in this way. In general, set of fuel properties (A,B,C,D) is a direct consequence of fuel blend composition (%X+%Y). This set of fuel properties corresponds to the end-use performance such as fuel consumption (FC) in the specific transport application. Model between fuel properties and fuel consumption is based on black-box methodology, while multilinear regression correlates input and output data. Additionally, knowing carbon content of the fuel and its density, it was possible to calculate CO2 emissions based on volumetric fuel consumption (FC). Summary of black box modeling applied in this study is presented in Figure 8. The modeling was executed stepwise with the control of fitting quality parameters such as R-square and significance level of coefficients resulting from multilinear regression. Finally, all models were validated.

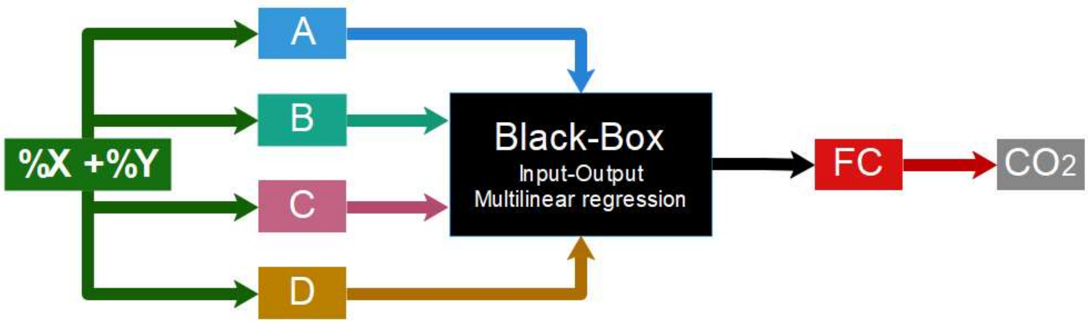


Figure 8 Structure of the variables and modeling [3].

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

4. Results and recommendations

This section presents results focused on end-use of RESfuels in various transport sectors and engine types. Recommendations are given for selected fuel options in each transport sector/segment. Additionally, alternative fuels are analyzed in the context of their properties. Finally, modeling is performed to correlate those properties with end-use performance.

4.1. Light-duty fleet

Light-duty fleet was divided into 4 various segments: regular passenger SI vehicles, regular passenger CI vehicles, flexi-fuel vehicles, and fuel cell vehicles. The reason behind such a division is significant difference in engine technologies in each above-mentioned LDV segment.

4.1.1. Regular passenger SI vehicles

The main outcomes of regular passenger SI vehicles analysis were published in technical paper [3] and journal article [5].

Considered fuels and recommendations

- **Reference EN228 gasoline**

Gasoline is a complex mixture of hydrocarbons with typical boiling range of temperature between 50 and 170ºC. Despite EN228 standard, the quality of the reference gasoline can vary significantly between batches depending on refinery fractions used to obtain the final fuel.

- **Methanol**

Methanol (CH3OH) is a colorless liquid which belongs to alcohol group and contains only one atom of carbon. Because of that, methanol combustion is characterized by the lowest emissions of CO2 compared to other alcohols. Methanol could be successfully produced from renewable feedstock such as wood waste, grass, algae and black liquor. Methanol has higher octane number, (RON and MON) than EN228 gasoline. Density and heat of vaporization are also higher in the case of methanol. Which would lead to potential performance benefits, if the engines are methanol-optimized (higher effective CR). What follows, the net vapor pressure of methanol is roughly a half of gasoline. Characteristic is oxygen content, that reaches half of the total mass of fuel. Methanol has a significantly lower boiling point compared to gasoline. Freezing point for methanol is −97, 6°C, which is much lower than for petrol (−40°C). Net calorific value of methanol is slightly lower than half of gasoline’s, which means that over two times more fuel (methanol) would be utilized in the engine in order to maintain even torque like in the case when running on gasoline.

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement N.º764799.

- **Ethanol**

Ethanol ($C2H5OH$) is an alcohol, which is nowadays commercially blended with gasoline. Where maximal permitted ethanol content specified in EN228 standard is just 10%. Similarly, to methanol, ethanol can be also produced from first, second and third generation biomass, when additionally it predominates over methanol with lack of toxicity. Ethanol is more compatible with a current fleet of SI vehicles than methanol. However, the use of ethanol bends in high concentrations such as E85, require several engine modifications. The modifications, mainly aim to mitigate the corrosive effect of ethanol by implementing corrosion resistant engine components. Additionally, optimizations include the adjustable spark timing according to concentration of ethanol in order to utilize the high RON of E85, which increases the thermal efficiency of such SI ICEV. Vehicles that have such optimizations are commonly known as flexible fuel vehicles (FFV). Using of ethanol requires also increased duration of fuel injection, which is straightforward related to 37,2% lower calorific content of ethanol compared to gasoline (volume base). This in consequence means that the range of vehicle powered by ethanol will be shorter in comparison to gasoline, given that the tank volume is constant. Pure ethanol has much higher RON than gasoline, which is very beneficial for fuel producers, especially when talking about utilization of lower quality petrol. Ethanol has around 6% higher density than gasoline, however as mentioned before significantly lower calorific content. Carbon content is 38% lower in ethanol. Ethanol will freeze below −114°C which is very beneficial for end-use in cold climate countries. However, during cold start, increased emissions might be problematic [25].

- **Propanol**

Propanol is a liquid alcohol with colorless appearance, which has three atoms of carbon in the structure. There are two isomers of propanol, isopropanol, and n- propanol. Propanol can be produced from biomass feedstock as aforementioned alcohols. However, it is rarely considered to be used as a fuel, because of high production costs comparing with other alcohols. Propyl alcohol is sometimes called "rubbing alcohol" or "gas dryer" because of it has drying properties. Although n-propanol keeps water in solution with gasoline, it prevents water from freezing in gas lines. From the properties point of view, both isomers represent high octane number (above 108). N-propanol has a higher density than isopropanol, where at the same time both values are bigger than gasoline's density. Propanol (included both isomers) has just around 16% higher calorific value than ethanol, which is still 25% lower than gasoline's NCV (volume base). Additionally, taking into account high production costs of propanol, one can say that ethanol is a cheaper option for an alternative fuel. Freezing temperature for n-propanol is the lowest among alcohols and is equal −127°C, where for isopropanol is −90ºC.

- **Butanol**

Butanol as all alcohols is in a form of colorless liquid. Butyl alcohol contains four atoms of carbon in the molecular structure. There are four isomers of butanol: isobutanol, n-butanol, 2-

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

butanol, and tetr-butanol. Butanol compared to other alcohols such as propanol ethanol or methanol is the most similar to gasoline from the properties perspective. Which in turn allows butanol to be used in regular SI engines at significantly higher concentrations than methanol or ethanol. Among isomers of butanol, the highest octane number 103,5 has isobutanol, where the lowest occurs in n-butanol. If it comes to density, the highest has n-butanol and the lowest tetr-butanol. Butanol has significantly higher heat of vaporization, over 520 kJ/kg, and much lower net vapor pressure compared to gasoline. Where the lowest value is observed for sec-butanol 1,67 kPa at 37, 8°C and the highest 12kPa for tetr-butanol (which is still around six times lower than gasoline's NVP). Butanol's net calorific value is around 20% lower compared to gasoline, but it is the highest number of aforementioned alcohols. If it comes to the production of butanol, biomass feedstocks could be utilized (included first and second generation). However, challenging part is related to the traditional fermentation process, where small concentrations of butanol are toxic to microorganisms. The comforting fact is that butanol can be produced in a cost-effective manner from ethanol. Additionally, infrastructure for ethanol production could be successfully upgraded to butanol production with minor investment.

Modeling outcome

The final model could be presented in the following form [3]:

$$\boldsymbol{\alpha = -0.47 \cdot A + 2.75 \cdot B - 2.39 \cdot C - 1.0 \cdot D}$$

Where:

α – fuel consumption (FC),

A – RON,

B – Density,

C – LHV volume-based,

D – Oxygen content.

Note: All units are represented as percentage changes relative to standard gasoline, (except oxygen, which is given in mass-based content).

When checking the model quality, validation was executed. Figure 9 presents both predicted by model values and source values. In addition, CO2 relative change is presented in the same Figure.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

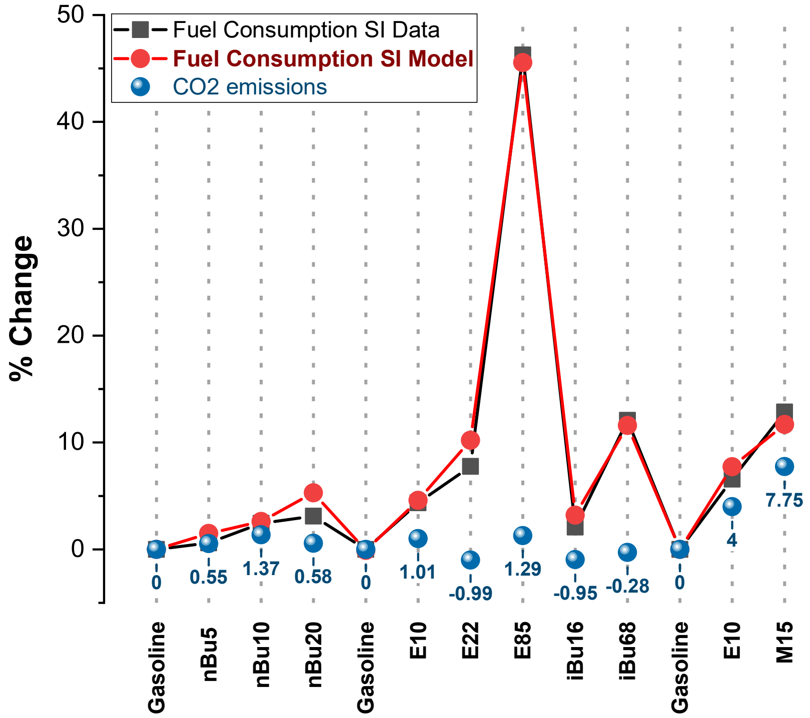


Figure 9 SI LDV modeling results and validation [3].

Key findings from the modeling work:

- Visible trends and good consistency of data from various journal articles.
- In the prediction of FC, it turned out that RON, density, LHV volume-based, and oxygen content are the most significant properties with statistical significane (p-value< 0.05).
- R-square value being over 0.99 proves very high model's accuracy.
- Model is mainly applicable for various alcohol fuels and their blends with reference gasoline but also other SI fuels can be tested.
- LHV and density have the biggest impact on FC.
- Higher octane number fuels tend to exhibit slightly lower fuel consumption.
- Higher blends of iso-butanol with gasoline reduce tailpipe emissions of CO2 due to higher octane number and similar to gasoline LHV.
- E22 fuel (22% ethanol blend) represents good thermal efficiency. Despite 8% increased volumetric fuel consumption, tailpipe CO2 emissions are reduced by 1%.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

4.1.2. Regular passenger CI vehicles

In this segment, reference diesel and liquid alternatives such as biomass-to-liquid (BTL), hydrotreated vegetable oil (HVO), traditional biodiesel (FAME), and gas-to-liquid (GTL) were considered as CI fuels. In the first step, drop-in applicability of those fuels was analyzed. Then, important CI fuel properties were classified and selected for modeling purposes. Afterwards, relative changes of key fuel properties were examined and their impact on fuel consumption change was analyzed. Multilinear regression, which correlated change in fuel properties with fuel consumption change for alternative fuels, was executed for key properties. Finally, the results were validated. The main outcomes of regular passenger CI vehicles analysis were published in technical paper [3] and journal article [5].

Considered fuels and recommendations

- **Reference diesel**

Despite EN590 standard, significant differences can be noticed when comparing fossil-based diesels from various geographic regions or distribution lines. The final properties of reference diesel depend on the origin of crude oil, refinery and blending practices.

- **BTL**

BTL or biomass-to-liquid diesel is classified as paraffinic diesel with high cetane number. This advanced biofuel can be produced from the cellulosic feedstock using Fischer-Tropsch synthesis. Physico-chemical properties of BTL and HVO are close to each other due to the similar chemical composition – both fuels are mixtures of straight chain and branched paraffinic hydrocarbons. BTL is considered as high quality drop-in CI fuel with very good engine performance in terms of emissions [30]–[33]. Its properties are determined by EN15940 standard for paraffinic fuels. Comparing to EN590 standard, the main difference is a consequence of lower density for BTL – in EN15940 standard the density range is 765-800 kg/m3.

- **HVO**

HVO is produced from vegetable oils, waste cooking oil or animal fats in the process of hydrotreating in the presence of catalyst. It is classified as high cetane number paraffinic diesel with numerous advantages including excellent ignition characteristics, higher HC ratio, good stability and reduced PM emissions due to lower sooting tendency [22], [34], [35]. The final end-use applicability is reported to be better than for reference diesel, while engine optimization can bring further performance gains [36], [37], [38]. Standard EN15940 for paraffinic fuels is valid also for HVO because of the lower density compared to the reference diesel. In all cases CN of HVO exceeds 70, meaning very good autoignition characteristic.

- **FAME**

FAME or traditional biodiesel consists of fatty acid methyl esters. It is the first generation biofuel produced by transesterification process from edible oils such as rapeseed, sunflower or palm, usually competing with food crops. Properties of FAME fuel depend on the feedstock, while mass-based oxygen content of pure biodiesel can exceed 10% [39]. Better lubricity and lower

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

PM emissions are main advantages [40], [41]. Worse stability and poor low temperature properties are drawbacks making FAME less attractive than HVO [42]. In addition, oil dilution can be observed for higher biodiesel blends [18]. EN14214 is a separate standard for FAME-type of fuel with higher density and viscosity compared to EN590 diesel. The limits are 860-900 kg/m3 and 3.5-5.0 mm2/s for density and viscosity, respectively. In the current market of EU and according to EN590, FAME blending is limited to 7% volume-based content (B7 fuel). However, Fuel Quality Directive in EU permits usage of higher FAME blends, i.e. 10% blends can be encountered in France but only few engine manufacturers approve higher than B7 blends, especially in CI light-duty fleet [43]. Whereas B20 and B30 blends need engine modifications and calibration [40].

- **GTL**

GTL or gas-to-liquid fuel is also a paraffinic diesel with high cetane number. However, it might be either fossil-based or produced from renewable sources. It exhibits similar properties as BTL or HVO and performs well in CI engines while reducing emissions [35]. Standard EN15940 is valid also for GTL.

Fuel property classification

Fuel properties were analyzed in the context of their impact on end-use applicability. There are several important end-use aspects such as characteristics of ignition, injection system, mixing and combustion, fuel supply system, safety and storage, and impact on exhaust emissions. For each of those aspects, various properties are treated with different priority. Figure 10 classifies how properties affect various aspects of engine operability [1].

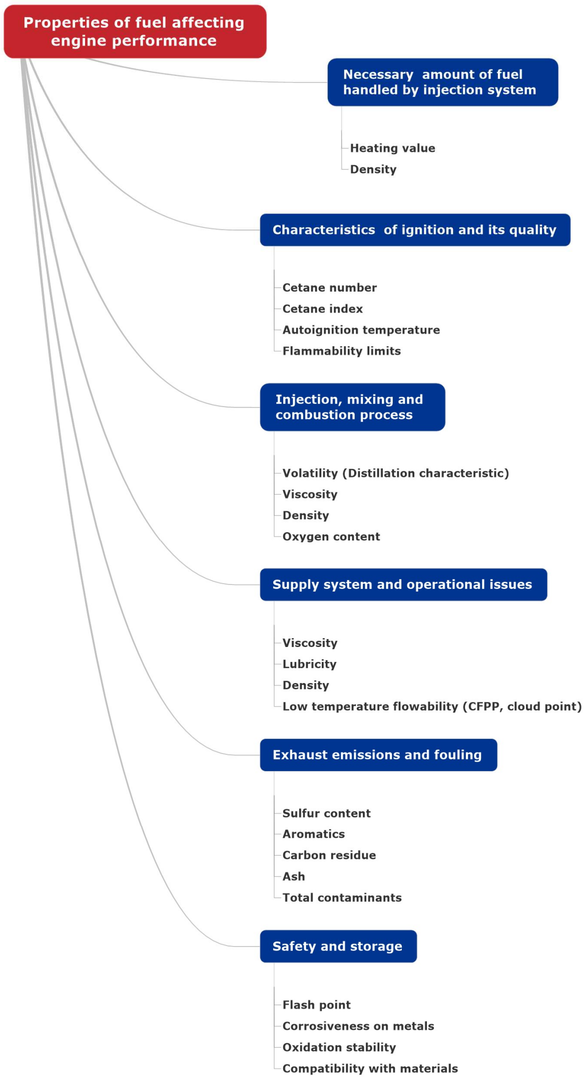


Figure 10 Classification of important properties for CI engine operation [1].

Analysis of key fuel properties and their impact on fuel consumption change

Changes of key CI fuel properties were analyzed in the context of fuel consumption change for alternative fuels. Those properties, namely CN, density, viscosity, LHV mass- and volume-based, and oxygen content together with fuel consumption of the regular vehicle over the NEDC test cycle, were reported for alternative fuel blends in various literature sources. Main findings of this work ([3], [5]) are presented as follows.

- Fuels with higher CN have usually lower FC.
- Lower LHV (both mass and volume-based) results in increased FC.
- However, not a straightforward relation between LHV and FC can be observed – other properties such as CN or density also affect FC.
- Growing density encompasses slight increase in FC.
- High viscosity fuels represent higher FC.
- Oxygen content proportional to FAME content in blend; no oxygen in paraffinic diesel.

Modeling outcome

After stepwise multilinear regression approach, the final model for CI fuels can be presented in the following form [3]:

$$\boldsymbol{\alpha = -0.076 \cdot A - 1.075 \cdot B - 1.110 \cdot C}$$

Where:

α – fuel consumption (FC),

A – CN,

B – Density,

C – LHV mass-based.

Note: All units are represented as a percentage changes relative to reference diesel.

When checking the model quality, validation was executed. Figure 11 presents both predicted by model values and source values. In addition, CO2 relative changes are presented in the same Figure.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

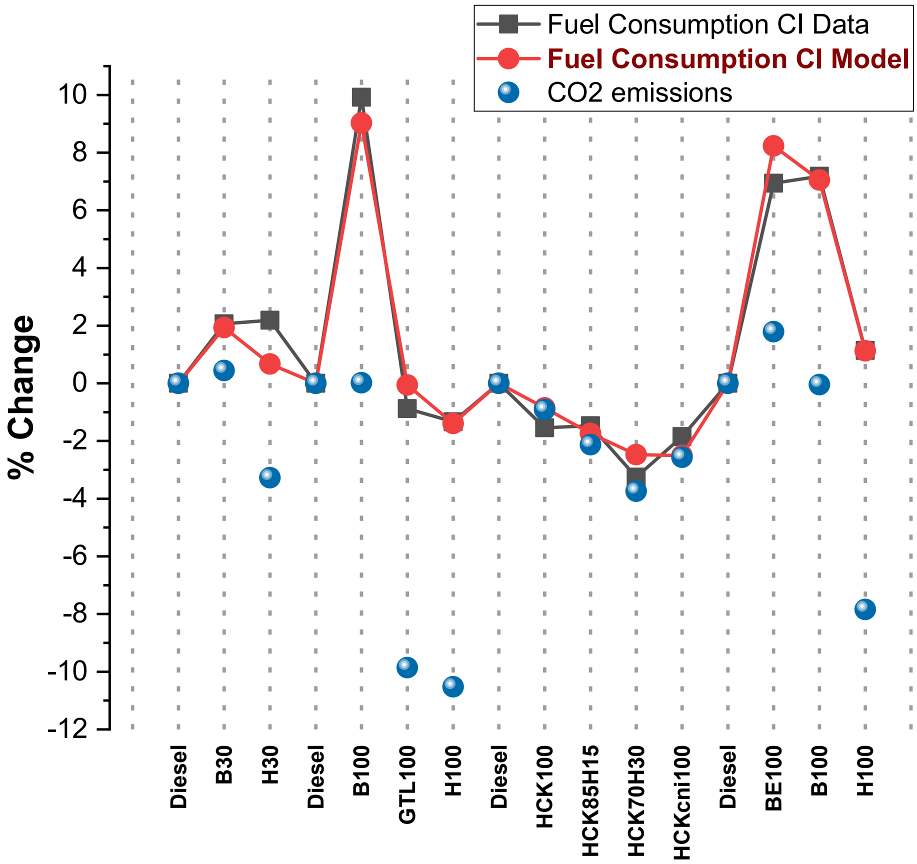


Figure 11 CI LDV modeling results and validation [3].

Key findings from the modeling work

- Consistent data from various literature sources enabled observation of trends between fuel properties and fuel consumption change for alternative fuels.
- Density, CN and LHV mass-based turned out to be the most significant properties treated as independent input parameters. All properties passed the t-test of significance level (p-value < 0.05).
- The accuracy of the model is high with R-square over 0.96, which ensures reliable outcomes.
- Model is applicable for paraffinic diesels (BTL, HVO, GTL), FAME fuels and blends of those with reference diesel in freely chosen concentrations.
- The biggest impacts on fuel consumption exhibit density and heating value.
- Tailpipe CO2 emissions for biodiesel are in similar range as for reference diesel, whereas paraffinic fuels tend to decrease CO2 emissions up to 10% for neat HVO.
- Knowing relative changes of fuel properties (density, LHV and CN), it is possible to estimate fuel consumption change for alternative fuels and their blends over NEDC driving cycle for an average CI passenger car engine.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

4.1.3. Flexi-fuel SI vehicles

Flexi-fuel vehicles are light-duty spark ignition vehicles that are optimized to more than one fuel (gasoline). Their engines can safely handle the higher concentrations of alternative fuels at high concentrations. They appeared in the largest number in the US market, however they were also popular in EU member states. Dependent of the producer of FFVs and model, there are different optimizations. However, the most common upgrades include:

- Corrosion resistant materials
- Higher effective CR
    - Advanced ignition timing
    - Variable Valve Timing VVT
    - Boosting the intake pressure
    - Feedback control in FFV adjusts fuel delivery and ignition timing
- Injectors designed to higher fuel flows
- Fuel heating systems

Due to following optimizations, FFV can operate not only more reliable with alternative fuels such as alcohols, but also more efficiently, and utilize more from their potential such as high RON.

Considered fuels and recommendations

In general FFVs, are designed to alcohol-gasoline blends, most commonly: methanol-gasoline, ethanol-gasoline and butanol-gasoline blends. Based on the sources used for modelling, there were blends of methanol as high as 85% with 15% of gasoline (M85), ethanol also at 85% concentration (E85) and isobutanol as high as 55% (Iso-Bu55).

Modeling outcome

The created FFVs model can be presented in the following form:

$$\boldsymbol{\alpha = -0,418 \cdot A - 1,223 \cdot B - 1,674 \cdot C}$$

Where:

α – Fuel Consumption [% Change of L/100km relative to EN228 gasoline]

A – RON,

B – Density,

C – LHV volume-based.

Note: All units are represented as a percentage changes relative to reference gasoline.

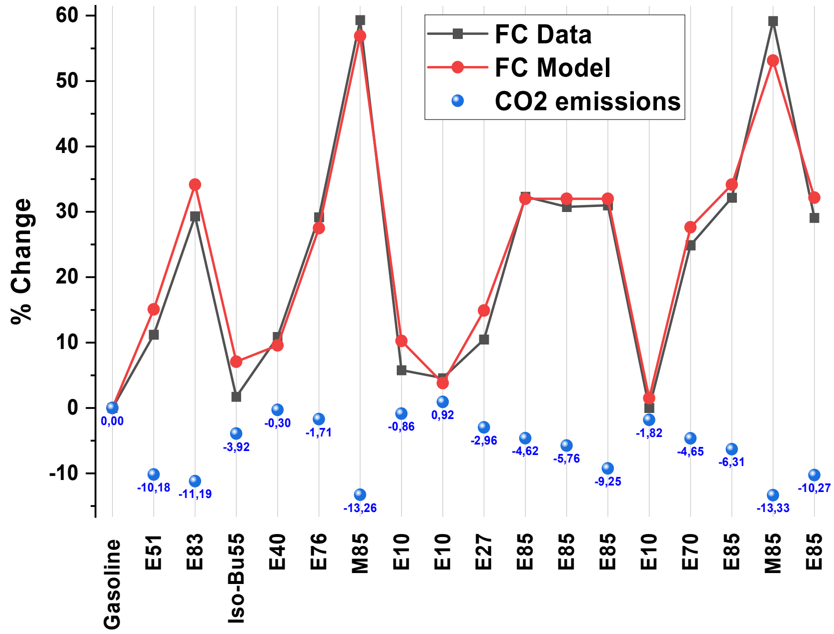


Figure 12 FFV modeling results and validation.

Key findings from the modeling work

- Multilinear regression was executed for all selected properties like density, lower heating value mass-based, lower heating value volume-based, research octane number, motor octane number, sensitivity, vapour pressure, carbon content, hydrogen content, oxygen content, and carbon to hydrogen ratio.
- As a result three properties were selected as significant input to the model: RON, density, LHV volume-based.
- Model has good accuracy of the engine performance prediction: R-square equals 0.98 and all parameters passed significance test, p-value < 5%.
- Meaning: model indicates relative change in fuel consumption for alternative fuel compared to reference gasoline, while input is represented by relative changes of key fuel properties, such as RON, density, calorific content.
- Applicability: Model can be applied to predict the fuel consumption from the end-user perspective. The performance can be estimated for alcohols (methanol, ethanol, butanol) at any given concentration ratios with a high accuracy.
- All alcohols, applied in FFVs represent lower tailpipe CO2 emissions compared to regular gasoline, even despite much higher volumetric fuel consumption (such as in a case of M85 or E85).

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

4.1.4. Fuel cells vehicles

Fuel cell vehicles are combining the benefits of electrical and internal combustion vehicles. They are equipped with electric motors, therefore they behave like EVs when driving (instantly maximal torque available), they are quiet, but at the same time, they have a range similar to ICEVs. FCVs are not burning the fuel in a conventional way as it occurs in spark-ignition or compression ignition ICE. Instead, a fuel cell unit, as an electrochemical cell, oxidizes the fuel with oxidizing agent (oxygen), in so-called redox reactions. In that process, electrons are released, creating electricity that powers the electrical motors and produces propulsion. Therefore, there is no combustion involved, with expansion of gases that produce the work, which subsequently drives the vehicle like in the case of ICEVs. In fuel cells, chemical energy of a fuel is directly converted into electricity. The majority of current fuel cell technology utilized commercially for passenger vehicles is based on proton exchange membrane (PEM).

Considered fuels and recommendations

Fuel cell vehicles are mostly designed to hydrogen that is kept in tanks at very high pressures (around 700 bar). The reason for such high compression is that hydrogen has a very low density equal to 0.0899 g/L at standard temperature and pressure (STP), after compression to 700 Bars, the density increased to about 40 g/L. In comparison, the density of gasoline is about 740 g/L. When it comes to mass based calorific content, the situation is reverse; hydrogen has 120 MJ/kg, whereas gasoline has around 44 MJ/kg. Therefore, compression of hydrogen increases significantly the range of FCVs. Despite direct use of hydrogen, novel compact fuel processors are able to reform hydrocarbons, such as methanol, ethanol, butanol or even gasoline into hydrogen-reach gas to power fuel cells.

Modeling outcome

The created FCV model can be presented in the following form:

$$\boldsymbol{\alpha = -6{,}361 \cdot A - 1{,}969 \cdot B}$$

Where:

α – *Fuel Consumption [% Change of L/100km relative to reference gasoline],*

A – Density,

B – LHV mass-based.

Note: All units are represented as a percentage changes relative to reference gasoline.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

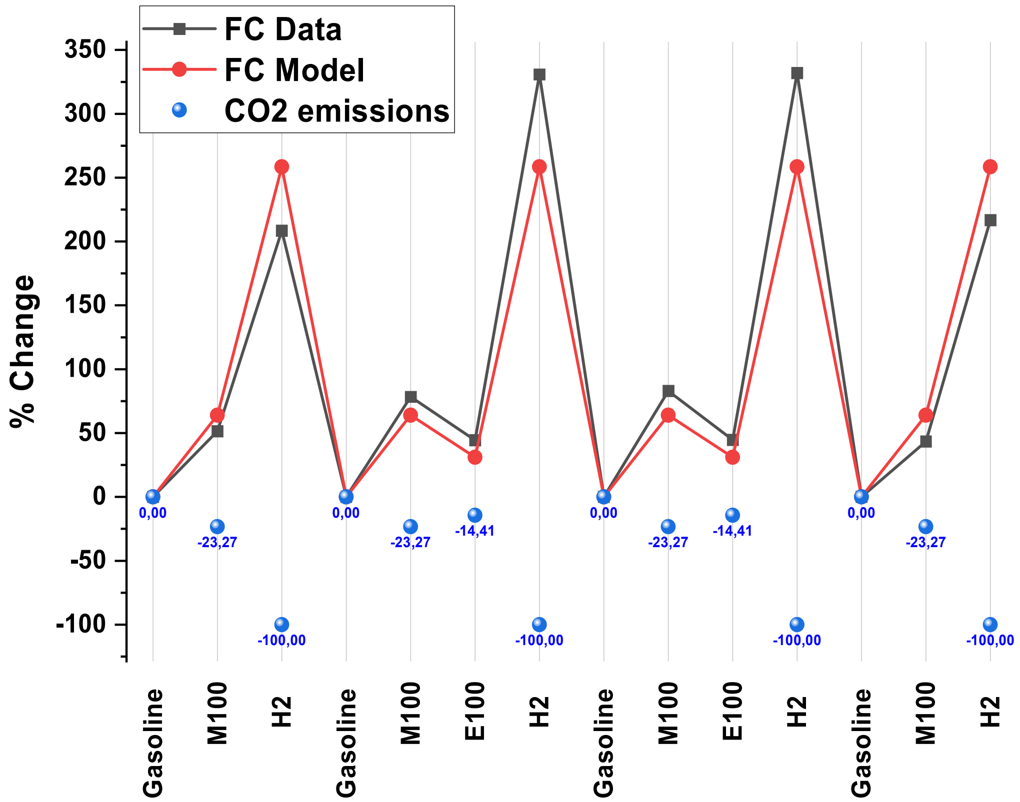


Figure 13 FCV LDV modeling results and validation.

Key findings from the modeling work

- Multilinear regression was executed for all selected properties like density, lower heating value mass-based, lower heating value volume-based, vapour pressure, carbon content, hydrogen content, oxygen content, carbon to hydrogen ratio, and molar mass.
- As a result three properties were selected as significant input to the model: density, LHV mass-based.
- Model has good accuracy of the engine performance prediction: R-square equals 0.96 and all parameters passed significance test p-value < 5%.
- Meaning: model indicates relative change in fuel consumption for alternative fuel compared to reference gasoline, while input is represented by relative changes of key fuel properties, such as density, calorific content.
- From the practical perspective, FCVs, would use about 4.5 times more liters of compressed to 700 bars hydrogen than gasoline to provide the same power for vehicle. However, when looking into energy consumption, FCVs would use arround 35% less MJ/km when running on hydrogen instead of gasoline. This means that FCVs, would operate much more efficient with hydrogen than with gasoline through reformer. When it comes to methanol and ethanol, the volumetric fuel consumption would be two times

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

higher and 1.5 times higher respectively, compared to gasoline. Whereas energy consumption will be for methanol and enthanol, ten times and five times lower respectively, compared to gasoline. Therefore, FCVs, would operate in the scale from most efficient to least efficient in the following order, hydrogen, methanol, ethanol, gasoline.

- Applicability: Model can be applied to predict the fuel consumption from the end-user perspective. The performance can be estimated for alternative fuels with a high accuracy.
- All alcohols, applied in FCVs represent lower tailpipe CO2 emissions compared to regular gasoline, even despite much higher volumetric fuel consumption. Additionally, hydrogen has absolutely zero tailpipe CO2 emissions, due to the the lack of carbon in the fuel.

4.2. Heavy-duty transport

Majority of heavy-duty engines in the market are compression-ignition with various displacement depending on the vehicle category (buses, medium or heavy-duty trucks, etc.). Therefore, combustion process, engine operation and fuels are similar like in CI LDV passenger car segment. In this work, heavy-duty engines were analyzed on the example of bus engines, which were tested over Braunschweig driving cycle. Fuel selection and modeling were executed accordingly.

Considered fuels

Due to the same diesel engine concept, all CI fuels used in LDV fleet can be also utilized in HDV fleet. Study done by Advanced Motor Fuels, division of International Energy Agency, presented possible fuel options for heavy-duty application [44], see Table 3. The most prominent solutions in heavy-duty trucks are foreseen in drop-in diesel fuels, ethanol compression ignition engines, DME powertrains or gas engines. Under the scope of ADVANCEFUEL project, drop-in diesel fuels and ethanol are considered with special attention. For drop-in diesel fuels like BTL or HVO, the same fuel property classification applies as in LDV fleet. However, ethanol requires dedicated engine technology resulting in very high compression ratio. In addition to ethanol, ED95 fuel contains roughly 5% of strong ignition improvers to enable operation according to CI combustion concept. There is only one engine manufacturer, Scania, who commercialized this technology that have not fully succeeded so far. In contrary to HVO, which gained higher market acceptance due to its fully drop-in characteristics.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Table 3 Availability of technology for commercial vehicles [44] (++ common, + available, - not available, 0 plausible, D under development).

	Light commercial vehicles	Medium-duty trucks	Heavy-duty trucks	Long haul heavy-duty trucks with trailers
Petrol	++	0	-	-
Diesel	++	++	++	++
Hybrids	0	+	+	0
Electricity	+	0	-	-
Ethanol SI	+			
CNG SI	+	+	+	-
CNG DDF	-	-	+	-
LNG SI	-	-	0	+
LNG DDF	-	-	D*)	D*)
DME	-	-	D	D
Ethanol CI	-	-	+	0

*) refers to direct-injection DDF technology meeting the most stringent emission regulations

Modeling outcome

After stepwise multilinear regression approach, the final model for CI diesel fuels can be presented in the following form:

$$\boldsymbol{\alpha} = \mathbf{0.075} \cdot \boldsymbol{A} + \mathbf{0.415} \cdot \boldsymbol{B} - \mathbf{0.881} \cdot \boldsymbol{C}$$

Where:

α – fuel consumption (FC),

A – CN,

B – Density,

C – LHV volume-based.

Note: All units are represented as a percentage changes relative to reference diesel.

When checking the model quality, validation was executed. Figure 14 presents both predicted by model values and source values together with estimated CO2 emissions.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

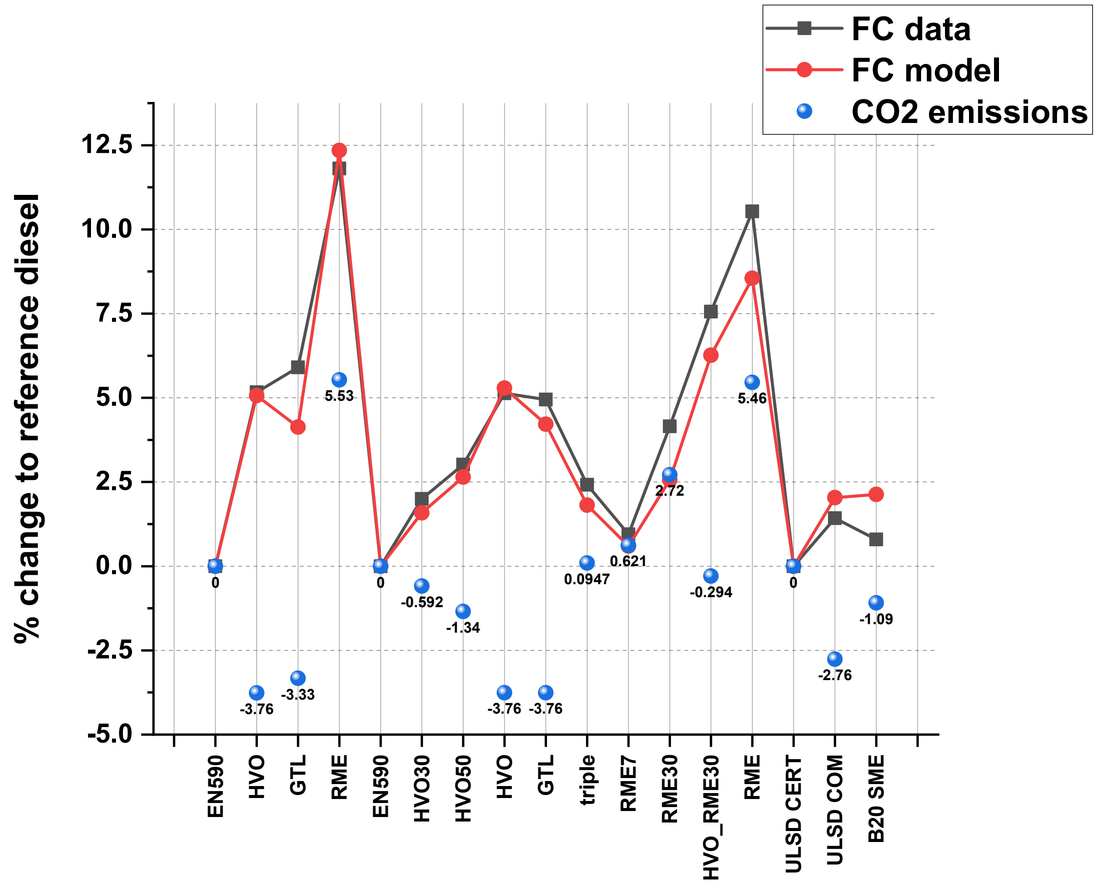


Figure 14 CI HDV modeling results and validation.

Key findings from the modeling work

- Multilinear regression was executed for all selected properties like density, lower heating value mass-based, lower heating value volume-based, cetane number, viscosity, carbon content, hydrogen content, oxygen content, and carbon to hydrogen ratio.
- As a result three properties were selected as significant input to the model: density, LHV volume-based and CN.
- Model has good accuracy of the engine performance prediction: R-square equals 0.96 and all parameters passed significance test.
- Meaning: model indicates relative change in fuel consumption for alternative fuel compared to reference diesel, while input is represented by relative changes of key fuel properties, such as density, calorific content and cetane number.
- Applicability: Model can be applied to predict fuel consumption over Braunschweig driving cycle for average bus equipped with CI engine. The performance can be estimated for alternative fuels such as paraffinic diesel, traditional biodiesel and blends of those with reference diesel.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

4.3. Maritime sector

Maritime sector has a very big 'inertia' meaning that visible changes are observed over extended period of time. Ships together with engines are usually expected to serve for few decades. Therefore, in order to decarbonize shipping in a faster pace, alternative drop-in fuels or retrofit solutions are needed. In this work, possible marine fuel alternatives were analyzed and assessed based on their properties, commercialization stage, possible benefits, and main bottlenecks in the market. Eventually, the attempt to model medium-speed marine engine performance was executed. Due to limited availability of data, the model is only demonstrative and attempts to predict CO2 emissions and fuel consumption (FC) for straight vegetable oil (SVO) fuels and their blends with heavy fuel oil (HFO). The main outcomes of the marine sector analysis were published in the technical paper [4].

Considered fuels and recommendations

Compression ignition engines are dominant in the marine market. For propulsion of bigger vessels, which consume majority of the sector's energy, medium and low-speed engines are used. Those engines resemble smaller units from CI LDV fleet but all components are significantly bigger and the engine provides very high power output per cylinder. It means that all CI fuels considered in Section 4.1.2 could be theoretically used in the shipping. However, the primary driver in the maritime sector is fuel price rather than its quality. Premium alternative fuels, used already in aviation and road sectors, cannot compete at the moment with cheap residual oils or marine gas oil (MGO). Good example is HVO, which is ready solution but not probable to enter the marine market. Instead, the solution should be searched in lower quality alternative biofuels. Upgraded pyrolysis oil or biocrude from hydrothermal liquefaction (HTL) are good examples. Another promising solution is methanol with demonstrated retrofit and new-built solutions. Main advantages and drawbacks of potential marine biofuels are summarized in Table 1.

Analysis of key fuel properties and their impact on fuel consumption change

Changes of key marine fuel properties were analyzed in the context of CO2 changes for alternative fuels. Those properties, namely density, viscosity, heating value mass- and volume-based, and oxygen content together with fuel consumption of medium-speed marine engine at steady-state conditions, were reported for HFO, MGO, and SVO-type alternative fuels. Main findings of this work [4] are presented as follows:

- In principle, the higher is the heating value, the lower CO2 emissions are observed.
- However, there is no straightforward correation between LHV and CO2 emissions – other properties also matter.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

- Higher density results in increased CO2 emissions. The same stands for viscosity but the trend is not so apparent.

Table 4 Main advantages and disadvantages of selected marine biofuels [4].

Fuel	Advantages	Disadvantages
SVO	+Reduction of GHG +Improved lubrication properties +Low SO_x emission +Lower PM emissions	-Long-term storage and water separation challenges -Lower energy content of approximately 10% -Microbiological growth increased -Higher acidity and risk of damage to certain rubber materials
FAME	+Reduction of GHG +Improved lubrication properties +Possibility of blending with MDO or HFO	-Long-term storage and water separation challenges -Lower energy content of approximately 10% -Microbiological growth increased
HVO	+High quality paraffinic fuel +No blending wall, easily mixable with MDO +Commercially available	-Higher price than fossil diesel -Limited feedstock when using only vegetable oils
Methanol	+Can be produced from lignocellulosic feedstock (TRL reaches 8th level) +Feasible in dual fuel concept	-Major production from natural gas (currently) -Low flashpoint -Toxicity
Pyrolysis oil & HTL biocrude	+Potential substitute for HFO and also as a blending component (no need for retrofit is expected) +Abundant feedstock	-Not yet certified for use -Fuel stability not known completely -Relatively low TRL (5/6), first commercial plant expected after 2025

Modeling outcome

The created marine demonstration model can be presented in the following form [4]:

$$\boldsymbol{\alpha = -0.19 \cdot A + 2.09 \cdot B + 0.97 \cdot C}$$

Where:

α – CO_2 emissions,

A – viscosity,

B – density,

C – LHV mass-based.

Note: All units are represented as a percentage changes relative to reference fuel – heavy fuel oil (HFO).

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Assessment of the model quality was based on the residual analysis – high value of R-square ensures good quality of the fitting. Validation of the model is presented in Figure 15.

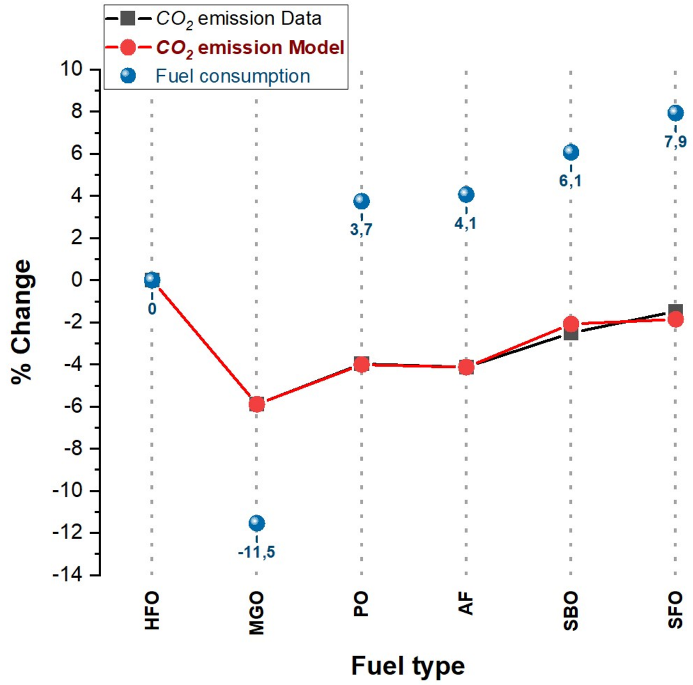


Figure 15 CI marine modeling results and validation [4].

Key findings from the modeling work

- The model has good accuracy with the coefficient of determination over 0.98 and all parameters reaching satisfactory significance level (p-value below 5%).
- Three properties turned out to be significant in prediction of CO2 emissions.: density, LHV mass-based and viscosity. As a consequence, those properties impact highly FC, too.
- Model can be used in estimation of medium-speed marine engine performance under steady-state conditions (75% load at nomianl engine speed) for SVO-type fuels and their blends with HFO. Despite high quality of fitting, the results should be treated with caution due to the limited availability of input data. More experimental data would be needed to analyze broader pallete of the fuels.
- Density highly impacts CO2 emissions – lower density followed by lower CO2 emissions.
- Among all tested fuels, MGO has lowest tailpipe CO2 emissions and FC. It is a consequence of highest energy content of MGO combined with the lowest density and viscosity.
- For SVO-type fuels, tailpipe CO2 emissions are slightly lower than for reference HFO.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

4.4. Aviation sector

Jet engines applied in aviation, belong to the group of internal combustion engines, however, they differ significantly from reciprocating engines used in road and marine transportation. In reciprocating engines, combustion is intermittent like in the case of four-stroke or two-stroke, piston engines. In contrast, jet engines are characterized by continuous combustion. Similarly, to reciprocating engines, the thermal efficiency of jet engines is a function of the compression ratio. Modern jet engines have a compression ratio that oscillates between 30:1 to 40:1, which allows achieving as high thermal efficiencies as 50%. Jet engines are gas turbines, that have 5 main designs; turbojet (pioneer design), turboprop (turbine engine that drives an aircraft propeller), turboshaft (electric generation), high-bypass turbofan (applied in the most of the present-day commercial aircrafts), low-bypass afterburning turbofan (mostly used for military supersonic aircrafts).

Considered fuels and recommendations

There are five types of sustainable aviation fuels (SAF) applied commercially:

- **Fischer Tropsch (FT-SPK),** fuels such as Biomass-to-Liquid (BtL). BtL can be blended up to 50% with fossil-based jet fuel.
- **Hydrotreated Esters and Fatty Acids (HEFA),** also could be blended up to 50% with fossil kerosene.
- **Renewable Synthesized Iso-Paraffinic (SIP),** fuel and could be blended with fossil kerosene up to 10%.
- **Synthetic paraffinic kerosene with aromatics via Fisher Tropsch (FT-SKP/A),** with 50% of blending with fossil kerosene.
- **Alcohol-to-jet (ATJ),** from isobutanol (certified in 2016) and ethanol (certified in 2018). ATJ could be blended with the fossil kerosene up to 50%.

SAF that complies with D7566 is automatically recognized as meeting the ASTM D1655 specification for conventional jet fuel (i.e. can be used as jet fuel without restrictions within the given blending walls).

Modeling outcome

The created jet model can be presented in the following form:

$$\boldsymbol{\alpha = 0.021 \cdot A - 0.993 \cdot B}$$

Where:

*α – Fuel Consumption [% Change of kg/N*hr relative to Jet A1],*

A – Viscosity,

B – LHV mass-based.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

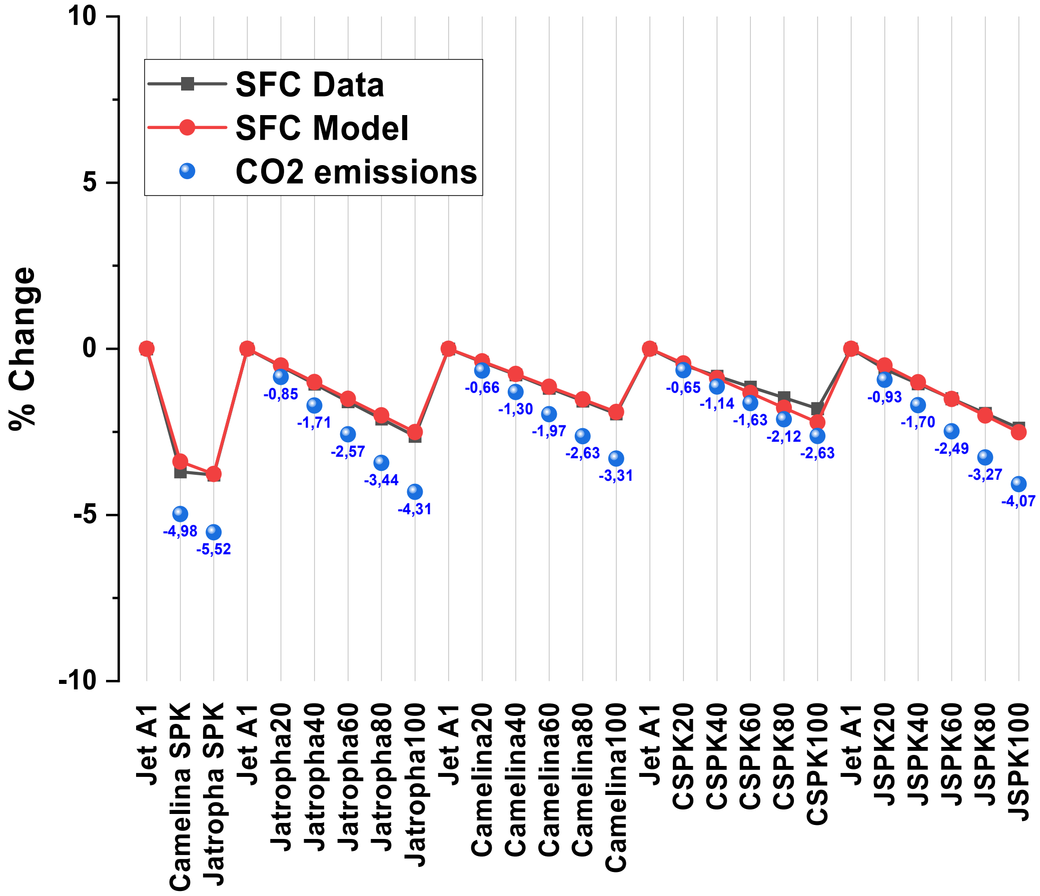


Figure 16 Jet engines (aviation) modeling results and validation.

Key findings from the modeling work

- The model has good accuracy with the coefficient of determination over 0.997 and all parameters reaching a satisfactory significance level (p-value below 5%).
- Two properties turned out to be significant in the prediction of SFC: viscosity and LHV mass-based.
- The model can be used in the estimation of the end-use performance of SAF in terms of mass-based fuel consumption over cruising conditions of the aircraft. When comparing Synthetic Paraffinic Kerosene (SPK) made from various bio feedstocks, one can conclude that there are no big changes in terms of fuel consumption. However, it could be noticed that both SFC and CO2 emissions are decreasing with increasing concentration of SPK, reaching over 2% lower mass-based SFC for pure SPK, and over 3% lower CO2 emissions.
- Among all tested fuels, SPK made from Jatropha operates more efficiently and reduces the most CO2 emissions.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

5. End-Use Analyser (EUA) tool

This section provides guidelines for users and explanation of various models included in the online application called End-Use Analyser. The online tool can be accessed free of charge after registering. The website, where the tool is deployed, contains following sections:

- Home – general description of the tool,
- Team – lists personnel involved in the modelling work and design of the tool,
- Tool – the main calculation interface for regular user (front-end),
- My Simulations – history of registered listing user's previous calculations,
- Contact – provides contact to the Authors from Aalto University,
- Logout – user can log out at any time.

The link to the End-Use Analyser tool: http://advancefuel.aalto.fi/. The front page of EUA tool is presented in Appendix C. The tool is designed in a way that all input required from the user is explained on step-by-step basis. The panel of the tool available for the user looks like presented below.

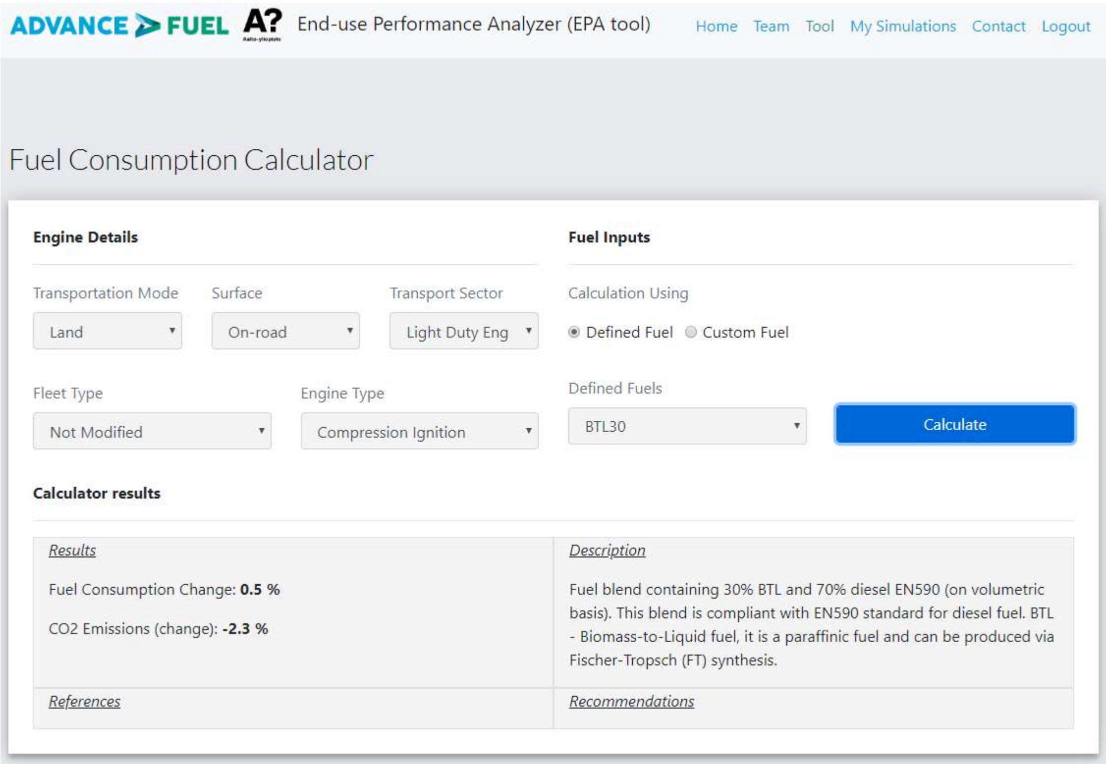


Figure 17 User front panel of the online EUA tool.

In the first step, user can select transport sector and engine technology. Engine specification is located on the left hand side of the input panel. Here, transportation mode (i.e. land, air, water), surface (i.e. on-road, off-road), transport segment (i.e. light-duty, heavy-duty), fleet type (regular passenger cars or flexi fuel vehicles), and engine type (SI or CI) should be specified.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

In the next step, user can specify the fuel of the interest by 4 possible options (on the right hand side of the input panel):

- Defined fuels – selection of proposed fuels from the list.
- Raw inputs – user can define fuel properties of both reference fuel and considered alternative fuel by typing absolute values of key fuel properties.
- Relative inputs – user gives the percentage changes of properties for alternative fuel referring to the reference fuel.
- Fuel blend – user specifies the alternative fuel and its concentration in blend with reference fossil fuel.

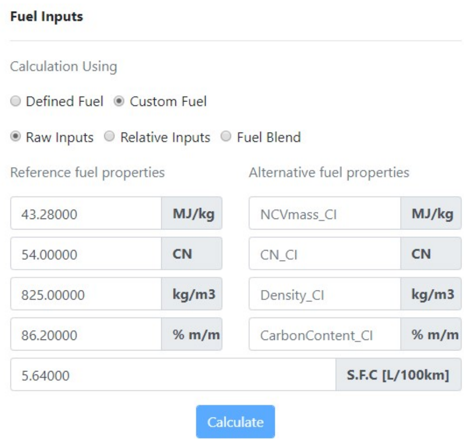


Figure 18 User input regarding fuel specification.

Note: It is important to provide all necessary input to the program and then click on Calculate button. The tool gives a result of end-use performance for new fuels including fuel consumption change and CO2 emission change. Additionally, the output provides short description of used model, recommendations, and references. The most accurate results are represented by 'Raw inputs' and 'Relative inputs' options, where user can define reference fuel, whereas 'Defined fuels' and Fuel blend' options give indicative results. The tool performs calculation based on the models developed during Task 5.4 of ADVANCEFUEL project. The methodology as well as results are presented in Sections 2, 3, 4 of this report. To clarify the basis of the operation of the tool, summary of the used models, their meaning and applicability are described below.

Table 5 Summary of all developed models for various transport sectors.

Sector	Engine	Model	R-Square
Light-Duty	SI	$FC = -0{,}47 \cdot RON + 2{,}75 \cdot Density - 2{,}39 \cdot LHV_{vol} - 1.0 \cdot O_2$	0,988
	CI	$FC = -0{,}076 \cdot CN - 1{,}075 \cdot Density - 1{,}110 \cdot LHV_{mass}$	0,966
	FFV-SI	$FC = -0{,}418 \cdot RON - 1{,}233 \cdot Density - 1{,}674 \cdot LHV_{vol}$	0,978
	FCV	$FC = -6{,}361 \cdot Density - 1{,}969 \cdot LHV_{mass}$	0,959
Heavy-duty	CI	$FC = 0{,}075 \cdot CN + 0.415 \cdot Density - 0{,}881 \cdot LHV_{vol}$	0.964
Marine	CI	$CO_2 = -0{,}19 \cdot Viscosity + 2{,}09 \cdot Density - 0{,}97 \cdot LHV_{mass}$	0.985
Aviation	Jet	$SFC = 0{,}021 \cdot Viscosity - 0{,}993 \cdot LHV_{mass}$	0,997

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

Table 6 Regular passenger SI vehicles (LDV fleet).

Model recommendation	Applicable for alcohol fuels and blends of those with reference gasoline; other fuels can be tested, too.
Reference fuel	Reference EN228 gasoline
Defined fuels	Ethanol, methanol, iso-butanol, etc.
Representative operating engine conditions	New European Driving Cycle (NEDC)
Representative engine or vehicle (only for indicative purposes)	SI engine, displacement from 1L to 3L, DI or MPFI, Euro 4,5 or 6. Default FC=6.22 L/100km, average mass=1354kg, Vehicle Energy Demand (VED)=10.9kWh/100km for NEDC.
Model input	LHVmass, density, RON, O2
Model output (results)	%change of volumetric FC and CO2 emissions; indication of local emission trends

Table 7 Model for Flexible-Fuel Vehicles (SI LDV).

Model recommendation	Applicable for alcohol fuels and blends of those with reference gasoline; other fuels can be tested, too.
Reference fuel	Reference EN228 gasoline
Defined fuels	Ethanol, methanol, iso-butanol, etc.
Representative operating engine conditions	New European Driving Cycle (NEDC)
Representative engine or vehicle (only for indicative purposes)	SI engine, displacement from 1L to 3L, DI or MPFI, Euro 4,5 or 6. Default FC=6.22 L/100km, average mass=1354kg, Vehicle Energy Demand (VED)=10.9kWh/100km for NEDC.
Model input	LHVvol, density, RON
Model output (results)	%change of volumetric FC and CO2 emissions; indication of local emission trends

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Table 8 Model for regular passenger CI vehicles (LDV fleet).

Model recommendation	Applicable for paraffinic diesels (BTL, HVO, GTL), traditional FAME biodiesel and blends of those with reference diesel fuel
Reference fuel	Reference EN590 diesel
Defined fuels	BTL, HVO, GTL, FAME in various concentrations
Representative operating engine conditions	New European Driving Cycle (NEDC)
Representative engine or vehicle (only for indicative purposes)	CI engine, 2.0L, turbocharged, common rail, DI, 4-cylinders / 16-valves, emission class: Euro 5/6. Default FC=5.6L/100km, average mass=1617kg; vehicle energy demand=13kWh/100km for NEDC.
Model input	LHVmass, density, CN
Model output (results)	%change of volumetric FC and CO2 emissions; indication of local emission trends

Table 9 Model for HDV engines.

Model recommendation	Applicable for paraffinic diesels (BTL, HVO, GTL), traditional FAME biodiesel and blends of those with reference diesel fuel
Reference fuel	Reference EN590 diesel
Defined fuels	BTL, HVO, GTL, FAME in various concentrations
Representative operating engine conditions	Braunschweig driving cycle
Representative engine or vehicle (only for indicative purposes)	CI engine of bus, 8.0L, emission class: EEV. Default FC=40L/100km, average vehicle mass=14 000kg; vehicle energy demand (VED) over cycle=100kWh/100km (for Braunschweig driving cycle)
Model input	LHVmass, density, CN
Model output (results)	%change of volumetric FC and CO2 emissions; indication of local emission trends

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Table 10 Model for marine engines.

Model recommendation	Applicable for SVO-type fuels and blends of those with reference fuel; also applicable for FAME fuels
Reference fuel	Heavy Fuel Oil (HFO)
Defined fuels	SVO of various origin
Representative operating engine conditions	Steady-state conditions at nominal engine speed (750rpm) and 75% engine load
Representative engine (only indicative)	Medium-speed CI engine, around 400kW/cylinder,
Model input	LHVmass, density, viscosity
Model output (results)	%change of CO2 emissions and volumetric FC

Table 11 Model for aviation, jet engines.

Model recommendation	Applicable for SAF such as; FT-SPK, HEFA, SIP, FT-SKP/A, ATJ
Reference fuel	Jet A1
Defined fuels	Cruise conditions; altitude of 10000 – 14000m, speed 0.8 Mach
Representative engine (only indicative)	High-bypass turbofan
Model input	Viscosity, LHV mass-based
Model output (results)	% Change of cruise specific volumetric FC relative to Jet A1

Important: Models are constantly under development with continuously growing amount of data. Therefore, the tool will be respectively updated and include the most recent and the best versions of models for each transport sector. In Table 5, are gathered all recent models presented in Section 4.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

5.1. Technical background of the tool

The EUA web application is a react application that relies on backend API built with Django a high-level framework. Django is integrated with an admin panel that is used to manage all the tool's data. For example, the admin can add a newly developed model and specify all its features. The frontend will automatically update and use the new model. Django consists of an object-relational mapper (ORM) that allows interacting easily with the database using querysets. For this application, we used a Postgres database that has many features and interacts well with Django.

To create a clean and well designed RESTful API we used a powerful library called Django Rest Framework (D.R.F). The API can serve any client that can consume a RESTful API. Every access to an endpoint in the API requires user authentication.

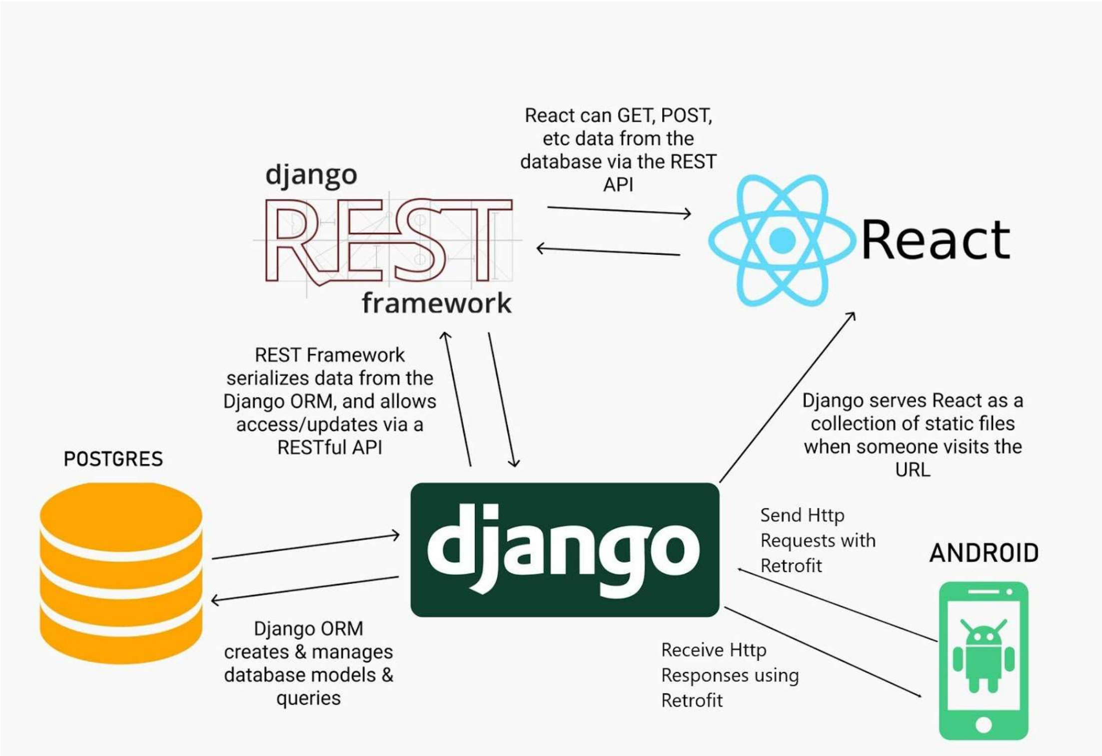


Figure 19 Architecture of the web-based numerical tool (EUA online tool back-end).

The web application consumes the API and manages all the application state with Redux. Bootstrap was used for styling. And there was some load testing done with k6.

For this project, we implemented CI/CD pipeline practice (Continuous integration and continuous delivery). This also allows us to continuously improve the application from continuous deployments.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

6. Conclusion

The task 5.4 from WP5 of ADVANCEFUEL, was focusing on 'Fuel and fuel blend properties in end-use'. This work presented very clearly that fuel properties affect significantly the performance of engines in various modes of transportation. In general, properties that were investigated were: density, heating value, viscosity, vapor pressure, chemical composition, the heat of evaporation, molar mass, and various measures of reactivity such as RON, MON, S, and CN. The end-use performance was modeled for aviation, marine, on-road light-duty and heavy-duty transportation using black-box stepwise multiple linear regression with statistical elimination of variables according to their significance level (variable rejected when the p-value exceeded 5%). In all cases, the effects were investigated from the end-user perspective, by taking the most realistic way of the fuel consumption representation for the given fleet of engines. In the case of on-road transportation, there were driving cycles (NEDC/FTP-75, Braunschweig cycle), in case of aviation, aircraft cruise conditions, and in the case of marine sector, steady-state operation of CI engine. In all developed models, inputs (multiple independent variables) represent fuel properties and outputs (single dependent variable) represent fuel consumption or CO2 emissions. All variables are given as changes relative to standard fossil fuel. In the case of SI, FFV, FCV LDV engines, the reference fuel was gasoline, in the case of CI LDV and HDV engines it was diesel fuel. In the case of aviation the reference fuel was Jet A1, and in case of marine, the reference was HFO.

In light-duty transportation, powertrains such as SI and CI engines from the regular fleet of vehicles, FFV SI engines, and FCVs were investigated and the impact of fuel properties on fuel consumption was modeled. In all cases the accuracy of models in terms of coefficient of determination (R-square) was over 0.96, where the highest was for FFVs SI, reaching 0.99. For regular LDV SI engines, examined fuels were alcohols including methanol, ethanol, iso-butanol, and n-butanol in various concentrations with gasoline. From the modeling, the most significant fuel properties turned out to be RON, density, LHV volume-based, and oxygen content. An interesting outcome was that for some blends such as E22, iBu16, and iBu68, despite the higher volumetric fuel consumption, the tailpipe carbon dioxide emissions were lower compared to gasoline. When it comes to compression ignition LDV engines, the impact of CN, density, and mass-based LHV on volumetric FC were the most significant properties. In the sources taken for modeling fuels such as FAME (biodiesel), HVO (renewable diesel), GTL, and hydrocracked diesel fuel were tested over the NEDC. The CI LDV model turned out to be a very accurate with R-square over 0.96. An interesting observation was that HVO and GTL blends had the volumetric FC very similar to fossil diesel. However, their CO2 emissions were lower than for diesel, reaching tailpipe CO2 reductions of 10% for pure HVO. On the contrary, FAME type of blends, yielded in greater volumetric FC compared to fossil diesel, gaining values nearly 10% higher, while the

CO_2 emissions of FAME are very similar to reference diesel. The FFV SI engine performance turned out to be the most sensitive for RON, density, and volume-based LHV. The developed model, similarly to the previous cases, predicts well the end-use performance, with R-square of 0.98. In the case of FFVs, the similar blends of alcohols were tested as for regular SI LDVs. However, it turned out that those blends in all cases operate more efficiently in FFVs than in regular SI engines, meaning lower FC and CO_2 emissions. The FCVs model represents the effect of density and mass-based LHV on volumetric FC. The R-square was 0.96, which confirms the high accuracy of the model. When it comes to FCVs, the shorter the chains of hydrocarbons, the better the performance, where the best results are for pure hydrogen (the lowest energy consumption per km). However, despite significantly higher mass-based LHV of hydrogen 120 MJ/kg, the density is very low (about 40 g/L when compressed to 700 Bars). Therefore, FCVs use about 4.5 times more liters of hydrogen than reference gasoline. When it comes to emissions, in case of hydrogen there is no tailpipe CO_2 emission. The second-best option for fuel cells is methanol, which in addition to good performance, is an easier and safer option than hydrogen when it comes to fuel storage and refueling.

In heavy-duty on-road transport (buses, trucks, etc.), compression ignition engines dominate the sector. The model for CI HDVs represents the impact of CN, density, and LHV volume-based on volumetric FC, with high accuracy and R-square 0.96. Similarly to CI LDVs, the sources used for modeling were examining the FAME type fuels (such as RME, SME), HVO, BTL, and GTL. Based on the results, pure paraffinic types of diesel such as BTL, HVO and GTL had about 5% higher volumetric FC, however, their tailpipe CO_2 emissions were lower over 3% compared to reference diesel. When it comes to FAME type fuels, both tailpipe CO_2 emissions and FC were higher, reaching values as high as 5.3% and 12.5% respectively. Therefore, renewable diesel is a better option for heavy-duty transportation than biodiesel.

In the marine sector, also compression ignition engines represent the vast majority of the fleet. The developed model represents the impact of viscosity, density, and mass-based LHV on CO_2 emissions with high accuracy (R-square equals 0.98). The reference fuel in the marine sector is HFO, and the source used for modeling was investigating the effect of PO, AF, SBO, and SFO. Within all tested fuels, MGO reveals the lowest tailpipe CO_2 emissions and FC. When it comes to SVO type of fuels, they show slightly lower tailpipe CO_2 emissions and slightly higher FC compared to HFO.

Commercial aviation is powered by jet engines, fueled with kerosene, known in the industry as Jet-A or Jet-A1. The model representing the impact of viscosity and mass-based LHV on mass-based SFC at cruising conditions was developed. The accuracy of the jet model is very high (R-square 0.997). In the aviation industry, RESfuels are called SAF (Sustainable Aviation Fuels), and currently, there are five certified SAF: FT-SPK, HEFA, SIP, FT SKP/A, and ATJ. When it comes to the end-use performance of commercial SAF, only slight changes could be observed in fuel consumption and CO_2 emissions, as SAF standards and requirements are very strict. Based on the tested fuels one can conclude that both SFC and CO_2 emissions are decreasing with increasing concentration of SAF, reaching over 2% lower mass-based SFC and 3% lower CO2 emissions for pure SPK.

As presented in this work, only LHV is not enough for a precise estimation of end-use performance. In the modeling procedure, it turned out that in all engines there were also other significant properties rather than calorific content only. Additionally, fuel properties are inter-related, therefore, this study presented combinations that proved to be significant in the quantitative analysis.

All presented models are built into the user-friendly web-based tool with free public access. The web application is called End-Use Analyser (EUA) and is available under the following link http://advancefuel.aalto.fi/. All models are constantly developing with a growing amount of data, and the models in the tool will be upgraded accordingly, to provide all users with always the best available version of each model.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

7. References

[1] M. Wojcieszyk, "Modeling the impact of fuel properties on compression ignition engine performance," Aalto University, 2018.

[2] Y. Kroyan, "Modeling the impact of fuel properties on spark ignition engine performance," Aalto University, 2018.

[3] Y. Kroyan, M. Wojcieszyk, M. Larmi, O. Kaario, and K. Zenger, "Modeling the Impact of Alternative Fuel Properties on Light Vehicle Engine Performance and Greenhouse Gases Emissions," in *SAE Technical Paper Series*, 2019, doi: 10.4271/2019-01-2308.

[4] M. Wojcieszyk, Y. Kroyan, M. Larmi, O. Kaario, and K. Zenger, "Effect of alternative fuels on marine engine performance," in *SAE Technical Paper Series*, 2019, doi: 10.4271/2019-01-2230.

[5] Y. Kroyan, M. Wojcieszyk, M. Larmi, O. Kaario, and K. Zenger, "Modeling the end-use performance of alternative fuels in light-duty vehicles," *Energy*, vol. Accepted, 2020.

[6] OECD/IEA, "World energy balances :Overview 2017," *IEA Publ.*, 2017, doi: 10.1787/9789264263116-en.

[7] EU, "EU Transport in Figures - Statistical Pocketbook 2017," *Eur. Comm. Publ. Off. Eur. Union*, 2017, doi: 10.2832/147440.

[8] International Energy Agency, "CO_2 Emissions from fuel combustion 2017 - Highlights," *International Energy Agency*, 2017.

[9] ITF, *ITF Transport Outlook 2017*. 2017.

[10] D. A. Lashof and D. R. Ahuja, "Relative contributions of greenhouse gas emissions to global warming," *Nature*, 1990, doi: 10.1038/344529a0.

[11] A. Haines, R. S. Kovats, D. Campbell-Lendrum, and C. Corvalan, "Climate change and human health: Impacts, vulnerability and public health," *Public Health*, 2006, doi: 10.1016/j.puhe.2006.01.002.

[12] I. Energy Agency, "Energy and Climate Change. World Energy Outlook Special Report," *World Energy Outlook Spec. Rep.*, 2015, doi: 10.1038/479267b.

[13] International Energy Agency (IEA), "Renewables 2017 : Key Findings," *Iea*, 2018. .

[14] International Energy Agency, "Tracking Clean Energy Progress," *Technology*, 2017, doi: 10.1787/energy_tech-2014-en.

[15] S. Correa Gonzalez and others, "Modeling the effect of blending multiple components on gasoline properties," Aalto University, 2019.

[16] K. Ronn, "Low-speed Pre-ignition and Super-knock in Spark-ignition Engines," Aalto University, 2020.

[17] D. J. Gaspar *et al.*, "Top Ten Blendstocks Derived From Biomass For Turbocharged Spark Ignition Engines: Bio-blendstocks With Potential for Highest Engine Efficiency," 2019.

[18] A. Tilli, T. Hulkkonen, O. Kaario, M. Larmi, T. Sarjovaara, and K. Lehto, "Biofuel blend late post-injection effects on oil dilution and diesel oxidation catalyst performance," *Int. J. Engine Res.*, 2018, doi: 10.1177/1468087417736466.

[19] Z. Ahmad, J. Aryal, O. Ranta, O. Kaario, V. Vuorinen, and M. Larmi, "An Optical Characterization of Dual-Fuel Combustion in a Heavy-Duty Diesel Engine," in *SAE Technical Papers*, 2018, doi: 10.4271/2018-01-0252.

[20] Y. Dong, O. Kaario, H. Ghulam, O. Ranta, M. Larmi, and B. Johansson, "High-pressure direct injection of methanol and pilot diesel: a non-premixed dual-fuel engine concept," *Fuel*, vol. Accepted, 2020.

[21] Y. Dong, "Reactivity controlled compression ignition (RCCI) combustion using

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

methanol and diesel in a single cylinder research engine," Aalto University, 2018.
[22] H. Aatola, M. Larmi, T. Sarjovaara, and S. Mikkonen, "Hydrotreated vegetable Oil (HVO) as a renewable diesel fuel: Trade-off between NOx, particulate emission, and fuel consumption of a heavy duty engine," *SAE Int. J. Engines*, 2009, doi: 10.4271/2008-01-2500.
[23] B. Liang *et al.*, "Comparison of PM emissions from a gasoline direct injected (GDI) vehicle and a port fuel injected (PFI) vehicle measured by electrical low pressure impactor (ELPI) with two fuels: Gasoline and M15 methanol gasoline," *J. Aerosol Sci.*, 2013, doi: 10.1016/j.jaerosci.2012.11.008.
[24] P. Bielaczyc, J. Woodburn, D. Klimkiewicz, P. Pajdowski, and A. Szczotka, "An examination of the effect of ethanol-gasoline blends' physicochemical properties on emissions from a light-duty spark ignition engine," *Fuel Process. Technol.*, 2013, doi: 10.1016/j.fuproc.2012.07.030.
[25] Z. Fan and T. Donglian, "IEA AMF ANNEX 44: Research on unregulated emissions from alcohol fuelled vehicles," 2016.
[26] N.-O. Nylund and K. Koponen, "Fuel and technology alternatives for buses: Overall Energy Efficiency and Emission Performance. Report VTT Technology 46.," *VTT Technol. 46*, 2012.
[27] A. Petzold *et al.*, "Operation of marine diesel engines on biogenic fuels: Modification of emissions and resulting climate effects," *Environ. Sci. Technol.*, 2011, doi: 10.1021/es2021439.
[28] ICAO, "ICAO Environmental Report 2013," *ICAO Environ. Rep. 2013*, 2013.
[29] K. Mollenhauer and H. Tschoke, *Handbook of Diesel Engines*. Berlin: Springer, 2010.
[30] S. S. Gill, A. Tsolakis, K. D. Dearn, and J. Rodríguez-Fernández, "Combustion characteristics and emissions of Fischer-Tropsch diesel fuels in IC engines," *Progress in Energy and Combustion Science*. 2011, doi: 10.1016/j.pecs.2010.09.001.
[31] N. Mizushima, D. Kawano, H. Ishii, Y. Takada, and S. Sato, "Evaluation of Real- World Emissions from Heavy-Duty Diesel Vehicle Fueled with FAME, HVO and BTL using PEMS," in *SAE Technical Papers*, 2014, doi: 10.4271/2014-01-2823.
[32] D. Ogunkoya and T. Fang, "Engine performance, combustion, and emissions study of biomass to liquid fuel in a compression-ignition engine," *Energy Convers. Manag.*, 2015, doi: 10.1016/j.enconman.2015.02.041.
[33] A. Rimkus, J. Žaglinskis, P. Rapalis, and P. Skačkauskas, "Research on the combustion, energy and emission parameters of diesel fuel and a biomass-to-liquid (BTL) fuel blend in a compression-ignition engine," *Energy Convers. Manag.*, 2015, doi: 10.1016/j.enconman.2015.10.047.
[34] M. Kuronen, S. Mikkonen, P. Aakko, and T. Murtonen, "Hydrotreated vegetable oil as fuel for heavy duty diesel engines," in *SAE Technical Papers*, 2007, doi: 10.4271/2007-01-4031.
[35] T. Murtonen, P. Aakko-Saksa, M. Kuronen, S. Mikkonen, and K. Lehtoranta, "Emissions with heavy-duty diesel engines and vehicles using FAME, HVO and GTL fuels with and without DOC+POC aftertreatment," *SAE Int. J. Fuels Lubr.*, 2010, doi: 10.4271/2009-01-2693.
[36] K. Erkkilä *et al.*, "Emission performance of paraffinic HVO diesel fuel in heavy duty vehicles," in *SAE Technical Papers*, 2011, doi: 10.4271/2011-01-1966.
[37] A. Omari, S. Pischinger, O. P. Bhardwaj, B. Holderbaum, J. Nuottimäki, and M. Honkanen, "Improving Engine Efficiency and Emission Reduction Potential of HVO by Fuel-Specific Engine Calibration in Modern Passenger Car Diesel Applications," *SAE Int. J. Fuels Lubr.*, 2017, doi: 10.4271/2017-01-2295.
[38] J. Heikkilä *et al.*, "Study of Miller timing on exhaust emissions of a hydrotreated

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

vegetable oil (HVO)-fueled diesel engine," *J. Air Waste Manag. Assoc.*, 2012, doi: 10.1080/10962247.2012.708383.

[39] E. G. Giakoumis, "A statistical investigation of biodiesel physical and chemical properties, and their correlation with the degree of unsaturation," *Renewable Energy*. 2013, doi: 10.1016/j.renene.2012.07.040.

[40] P. Bielaczyc, A. Szczotka, P. Gizynski, and I. Bedyk, "The effect of pure RME and biodiesel blends with high RME content on exhaust emissions from a light duty diesel engine," in *SAE Technical Papers*, 2009, doi: 10.4271/2009-01-2653.

[41] D. P. Geller and J. W. Goodrum, "Effects of specific fatty acid methyl esters on diesel fuel lubricity," *Fuel*, 2004, doi: 10.1016/j.fuel.2004.06.004.

[42] A. Engman *et al.*, "Hydrotreated vegetable oil (HVO)-premium renewable biofuel for diesel engines," *Espoo Neste Oil Propr. Publ.*, 2014.

[43] "B10 diesel fuel: vehicle compatibility list," *European Autombile Manufacturers Association*, 2018. https://www.acea.be/publications/article/b10-diesel-fuel-vehicle-compatibility-list.

[44] N.-O. Nylund, "IEA AMF ANNEX 49: Fuel and technology alternatives for commercial vehicles," Espoo, 2016.

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

8. APPENDICIES

8.1. Appendix A: SI fuels specification.

Table 12 Alternative SI fuels with summary of main properties [2].

Property		Unit	Gasoline	Methanol	Ethanol	Isopropanol	n-propanol	2-Butanol	Tert-Butanol	Isobutanol	n-butanol	MTBE	ETBE	TAME	TAEE	DIPE
				Alcohol alternatives		Propanol		Butanol				Ether alternatives				
Chemical Formula			C4-C12	CH3OH	C2H5OH	C3H7OH	C3H7OH	C4H9OH	C4H9OH	C4H9OH	C4H9OH	C5H12O	OC(CH3)3	C6H14O	C7H16O	C6H14O
Appearance			Clear and bright liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid	Colorless liquid
Octane number ON		(RON+MON)/2	90,60	116,00	99,15	108,00	109,50	96,00	100,00	103,50	87,00	107,00	111,00	105,00	100,00	100,00
	RON		96,00	130,00	108,60	118,00	121,00	101,00	105,00	113,00	96,00	115,00	119,00	112,00	105,00	105,00
	MON		85,20	102,00	89,70	98,00	98,00	91,00	95,00	94,00	78,00	99,00	103,00	98,00	95,00	95,00
Density at 15°C		kg/m3	750,00	796,00	794,00	789,00	805,30	806,00	791,00	802,00	810,00	740,00	770,00	766,00	730,00	750,00
Neat vapor pressure 37,8°C		kPa	70,00	32,00	16,00	12,00	2,00	1,67	12,00	3,90	2,40	55,00	28,00	17	7	35
Molar mass		g/mol	108,40	32,00	46,10	60,00	60,00	74,10	74,10	74,10	74,10	88,20	102,20	102,2	116,20	102,20
Content	Carbon	%m/m	84,31	37,50	52,10	60,00	60,00	64,80	64,80	64,80	64,80	68,10	70,50	70,70	72,40	70,50
	Hydrogen		13,09	12,50	13,20	13,33	13,33	13,60	13,60	13,60	13,60	13,70	13,80	13,8	13,80	13,80
	Oxygen		2,60	49,90	34,70	26,67	26,67	21,62	21,62	21,62	21,62	18,20	15,70	15,70	13,80	15,70
Distillation, evaporated	70 summer	% v/v	46,00													
	70 winter		48,00	100,00								100,00				100,00
	100		53,00		100,00	100,00	100,00	100,00	100,00				100,00	100,00		
	150		88,00							100,00	100,00				100,00	
Boiling point		°C	188,00	64,60	78,00	83,00	97,20	99,50	82,40	108,00	117,70	55,00	73,00	86	101,00	68,00
Freezing ←→ melting point		°C	-40,00	-97,60	-114,00	-90,00	-127,00	-114,70	25,70	-108,00	-89,50	-109,00	-94,00	-80		-86,80
Net calorific value NCV		MJ/kg	44,40	20,00	27,00	30,68	30,68		33,00	33,00	33,00	35,10	36,50	36,50		37,00
		MJ/l	32,90	15,90	21,30	24,65	24,65		26,10	26,50	26,70	26,00	27,00	28,10		27,00
Gross Calorific Value GCV		MJ/kg	47,30	23,00	29,70	33,60	33,60						39,00			
Heat of vaporization		kJ/kg	275-365	1160	839,00	756,5	790,833	551	527	556	582	356,00	344,00	354,00		340,00
Auto-ignition temperature		°C	257	464	423,00	456	371	406,1	477,8	415,6	343	435,00	304,00	460		443,00
Flammability limits	Lower	vol-%	1,40	7,00	4,00	2,00	2,00	1,70	2,40	1,20	1,40	1,60	1,00	1,00		1,40
	Higher		7,60	36,00	19,00	12,70	12,00	9,80	8,00	10,90	11,20	8,40	6,80	7,10		7,90
Stoichiometric air fuel ratio			14,7	6,4	9,00	10,3	2,964		11,1	11,2	11,2	11,70	12,20	12,1		12,10
Soulubility at 20C°C	fuel in water	vol-%	not miscible	fully miscible	fully miscible	fully miscible	miscible	37	miscible	8,5	7,7	4,80	2,30	1,4	0,5	1,10
	water in fuel		not miscible			fully miscible	miscible					1,50	0,50	0,6		0,60
Flash point		°C	40	11	13	11,7	23	31	16	28	34	-28,10	-19,00	-11	-5,15	-28,00
Viscosity at 20°C	Dynamic	mPa*s or cP		0,554		2,038	2,256	3,096		4,312	2,544	0,36	0,4		0,48	0,273
	Kinematic	mm2/s	0,83	0,000000737	1,525		1,4-2,8			4,9	3,6	0,47	0,45 - 0,55			
Surface tension at 32°C		mN/m		20,07	1,204	22,11	23,75		20,7	23	24,7	18,30	21,5			17,7
Odour detection in water		ug/l					9					15,00	49,00	194		
Taste detection in water		ug/l										40,00	47,00	128		
Odor threshold		ppm		160	10-84		30					0,053	0,013			

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.°764799.

Table 13 Standard EN228 and typical values of gasoline properties from the Finnish retail market [2].

Property	Unit	EN228		Fuel			
		Min.	Max.	NESTE Futura 1.1.2017		ST1 and ABC	
				95E10	98E5	95E10	98E5
Octane number	RON	95.0	-	96.0	98.7	95.2	98.5
	MON	85.0	-	85.2	87.4	85.7	87.7
Lead content	mg/l	-	5	<2	<2	0	0
Density at 15°C	kg/m^3	720.0	775.0	750	752	750	745
Sulphur content	mg/kg	-	10	7	7	3	5
Oxidation stability	min	360	-	600	500	600	600
Existent gum content	$mg/100ml$	-	5	1	1	1	1
Copper strip corrosion	$rating$	-	1	1	1	1	1
Evaporated at 70°C (E70) - summer	% V/V	22.0	50.0	42.0	32.0	49.0	46.0
Vapour pressure (summer)	kPa	45.0	70.0	67.0	67.0	69.0	69.0
Vapour pressure (winter)	kPa	60.0	90.0	88.0	88.0	88.0	89.0
Vapour lock index	-	-	1250	1094	1011	1135	1250
Evaporated at 70°C (E70) - winter	% V/V	24.0	52.0	44	35	51	48
Evaporated at 100°C (E100)	% V/V	46.0	72	55	51	57	53
Evaporated at 150°C (E150)	% V/V	75.0	-	88	88	88	88
Final boiling point	°C	-	210	187	188	185	188
Olefin content	% V/V	-	18.0	11	11	5	5
Benzene content	% V/V	-	1.0	0.7	0.6	0.8	0.7
Oxygen content	% m/m	-	3.7	3.6	2.6	3.6	2.6
Ethanol content	% V/V	-	10	-	-	9	4.5
Ethers min. 5 carbon atoms	% V/V	-	22	-	-	1	5.5
Aromatic content	% V/V	-	35	31	33	32	33

8.2. Appendix B: CI fuels specification.

Table 14 Alternative CI fuels with summary of main properties [1].

Compression Ignition Engine fuels			Property	CN	Density	LHV	LHV vol	Viscosity	C	H	O
			Unit	-	kg/m3 @15 C	MJ/kg	MJ/l	mm2/s @40 C	% m/m	% m/m	% m/m
Standard diesel		Germany	Typical diesel	53,5	830,0	42,80	35,52	2,6	85,8	13,49	0,72 (5-7% FAME)
		USA	Chevron	44,7	843,8	42,60	35,95	2,24	87,14	12,86	0
		Finland	Neste Futura (-5/-15)	54,0	825,0	43,28	35,71	3,00	86,2	13,8	0 (0% FAME)
			Neste Pro (15% v/v HVO)	60,0	826,0	43,28	35,75	3,00	86,2	13,8	0 (0% FAME)
			St1 Diesel plus -20	63,0	805,0	43,28	34,84	3,10	n.d.	n.d.	0,2 (1,5% FAME)
FAME	Animal		Beef tallow	60,9	874,3	37,22	32,54	4,83	76,09	12,60	11,35
			Fish	51,0	887,3	38,80	34,43	4,30	77,40	11,85	10,75
			Palm	61,2	874,7	37,08	32,43	4,61	76,09	12,44	11,27
		EU	Rapeseed	54,1	882,2	37,63	33,20	4,63	77,07	11,84	10,93
		US	Soybean	51,8	882,8	37,75	33,33	4,29	77,03	11,90	10,95
	Waste		WCO	56,2	880,6	37,88	33,36	4,75	76,90	12,02	10,77
HVO			Neste Renewable Diesel (I)	88,0	780,0	44,10	34,40	2,87	84,61	14,67	0,00
			Neste HVO (II)	80,0	780,3	43,60	34,02	2,87	84,61	14,67	0,00
			Neste HVO (III)	94,8	780,0	43,95	34,28	2,99	84,68	14,52	0,00
			HVO - Universal Oil Products	81,8	775,8	43,86	34,03	2,65	84,84	15,16	0,00
GTL/BTL			SunDiesel BTL CHOREN 2005	80,0	761,2	44,58	33,93	1,55	85,79	12,54	1,67
			FT fuel as GTL	81,2	770,0	43,70	33,65	2,79	84,94	15,06	0,00
			Shell GTL (I) - FT from NG	80,0	784,6	43,90	34,44	3,50	85,00	15,00	0,00
			Shell GTL (II)	75,4	777,0	43,58	33,86	3,13	85,85	14,15	0,00
			Shell GTL (III)	75,0	776,9	43,25	33,60	2,53	85,83	14,17	0,00
			Shell GTL (IV)	75,0	779,0	43,60	33,96	2,74	84,90	15,10	0,00
			SASOL GTL FT diesel	89,2	774,0	44,03	34,08	2,34	84,82	15,18	0,00
DME			IEA AMF data collected	57,5	660,0	28,00	18,48	below 1	52,00	13,00	35,00
SVO			Neat rapeseed oil	39,0	920,0	37,10	34,13	35,00	78,00	13,50	8,90
Ethanol			Pure ethanol	8,0	788,0	26,80	21,12	1,20	52,17	13,04	34,78

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

Table 15 Typical values of properties for EN590 diesel from the Finnish retail market [1].

Property	Unit	Fuel		
		Neste Pro Diesel 2017	Neste Futura Diesel 2017	ST1 Diesel Plus 2017
Cetane number	-	60	54	63
Cetane index	-	55	55	63
Density at 15^oC	kg/m^3	826	825	805
PAH content	$\%m/m$	1	2	1
Sulfur content	mg/kg	3	5	5
Flash point	^oC	74	63	65
Carbon residue	$\%m/m$	$<$ 0,01	<0,02	$<$ 0,02
Ash content	$\%m/m$	$<$ 0,001	$<$ 0,001	$<$ 0,001
Water content	mg/kg	40	53	70
Total contamination	mg/kg	2	3	4
Copper strip corrosion	class	1a	1	1
FAME content	$\%V/V$	0	0	1,5
Oxidation stability	g/m^3	3	2	2
Lubricity	μm	380	300	350
Viscosity at 40^oC	mm^2/s	3	3	3,1
Distillation at 250^oC	$\%V/V$	24	32	25
Distillation at 350^oC	$\%V/V$	97	94	95
Distillation temperature of 95% fraction	^oC	338	351	351
Cloud point	^oC	-14	-5	-12
CFPP	^oC	-26	-15	-22

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N.º764799.

8.3. Appendix C: EUA tool frontpage.

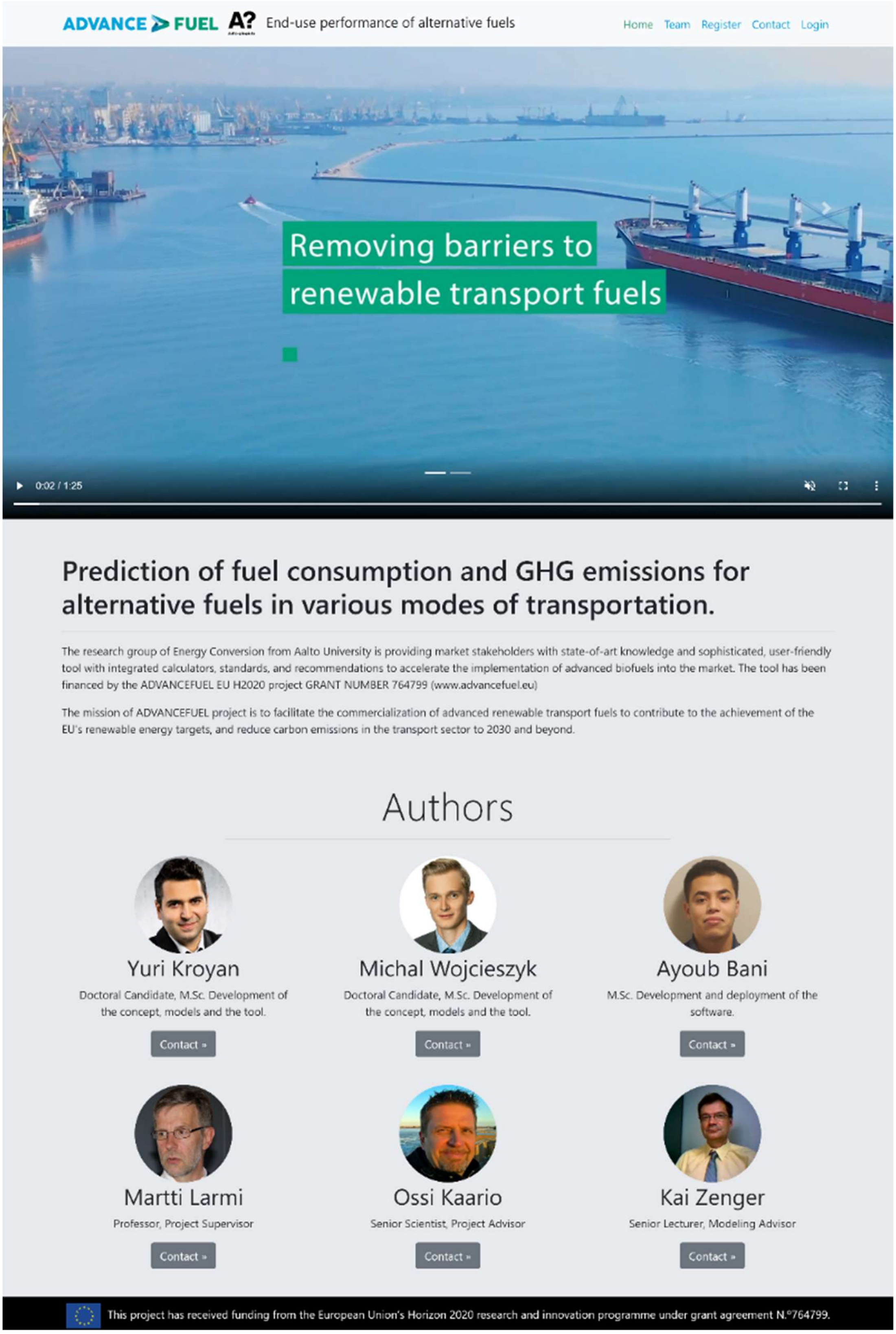


Figure 20 Front page of the web-page, where EUA online tool is deployed (Authors presented, too).