



REDIFUEL

Deliverable report

Deliverable No: D3.7
Dissemination level: Public (PU)
Title: Report on emission and efficiency impact on existing engines

Date: 31/07/2021
Version: FINAL
Author(s): Kai Deppenkemper (FEV); Jaykumar Yadav (RWTH)
Reviewed by: Márton Krár (MOL)
Approved by: Technical Coordinator – Benedikt Heuser (FEV)

Grant Agreement Number: 817612
Project Type: H2020-LC-SC3-RES-21-2018-development of next generation biofuels and alternative renewable fuel technologies for road transport
Project acronym: REDIFUEL
Project title: Robust and Efficient processes and technologies for Drop In renewable FUELS for road transport
Project start date: 01/10/2018
Project website: www.redifuel.eu
Technical coordination: FEV (DE) (www.fev.com)
Project management: Uniresearch (NL) (<http://www.uniresearch.com>)



Executive Summary

The joint project “Robust and Efficient Processes and Technologies for Drop-In Renewable Fuels for Road Transport” (REDIFUEL) aims to produce an ultimate renewable drop-in biofuel, which is compliant with EN590 norms in a sustainable manner. In this project, a holistic fuel characterization is planned to assess the fuel characteristics and engine performance of this new paraffinic biofuel, consisting of about 30 vol% bio-alcohols. This report presents the characterization and engine testing of a surrogate REDIFUEL mixture representative of the expected real end-product. Density, viscosity and CN of different blending proportion of this renewable fuel with diesel are screened, to assess its drop-in capability and the inherent impact on engine performance. With 40 vol% share of REDIFUEL in diesel, both the minimum EN590 requirements for CN and density are met. When this blend is compared against diesel, reduction potential in indicated specific particulate matter, indicated specific carbon monoxide, indicated specific hydrocarbon and CO₂ emissions are respectively observed. Numerical simulations show that blending REDIFUEL with diesel enhances the mixture formation, enabling a higher level of oxygen entrainment in the spray plume.



Contents

Executive Summary	2
Contents	3
1 Introduction	5
2 Methods.....	6
2.1 Heavy duty single cylinder engine	6
2.2 3D-CFD Numerical modelling.....	8
2.3 Fuel composition and properties.....	9
3 Results	11
3.1 HD SCE test bench results	11
3.2 3D-CFD simulation results.....	14
4 Discussion and Conclusions	16
4.1 4.1 Discussion.....	16
4.2 4.2 Conclusions	16
5 Deviations from Annex 1	17
6 References	18
7 Acknowledgement	19
8 Risk register	20
 Figures:	
Figure 1 Explicative engine load map in break mean effective pressure (BMEP) vs engine speed	8
Figure 2 Computational mesh for gas exchange and mixture formation simulations illustrating the fixed embedding (left) and air utilisation (right)	9
Figure 3 HD SCE results at cruise point for base NO _x level, IMEP = 10 bar, n = 1200 min ⁻¹ , p _{inj} = 1280 bar, α _{Q50} = 6.2 °CA a. TDC, T _{boost} = 41 °C, p _{boost} = 1789 mbar, p _{exh} = 1875 mbar, ISNO _x = 5.8 g/kWh	12
Figure 4 Heat release analysis at cruise point IMEP = 10 bar, n = 1200 min ⁻¹ , p _{inj} = 1280 bar, α _{Q50} = 6.2 °CA a. TDC, T _{boost} = 41 °C, p _{boost} = 1789 mbar, p _{exh} = 1875 mbar, ISNO _x = 5.8 g/kWh	12
Figure 5 HD SCE results at best efficiency point for base NO _x level, IMEP = 20.98 bar, n = 1200 min ⁻¹ , p _{inj} = 1658 bar, α _{Q50} = 10.2 °CA a. TDC, T _{boost} = 39 °C, p _{boost} = 2800 mbar, p _{exh} = 2904 mbar, ISNO _x = 6.1 g/kWh.....	13
Figure 6 Heat release analysis at best efficiency point for base NO _x level, IMEP = 20.98 bar, n = 1200 min ⁻¹ , p _{inj} = 1658 bar, α _{Q50} = 10.2 °CA a. TDC, T _{boost} = 39 °C, p _{boost} = 2800 mbar, p _{exh} = 2904 mbar, ISNO _x = 6.1 g/kWh	14
Figure 7 Comparison of air utilization (top), and lambda plots for RFA30P70 and diesel (bottom), at cruise point....	15
Figure 8 Comparison of air utilization (top), and lambda plots for RFA30P70 and diesel (bottom), at rated power operation.....	15



Tables:

Table 1 HD SCE specifications	6
Table 2 Measuring devices for the HD SCE	7
Table 3 HD SCE calibration settings	8
Table 4 Fuels used in simulation and their composition	10
Table 5 Fuel blend properties	10
Table 6 Comparison of OPN for different blends of B0 and RF_{A30P30} at cruise point and rated power point operation	15



1 Introduction

This deliverable report is part task 3.4 “Single cylinder combustion and emission optimization” of the work package 3 “Biofuel-fuel system compatibility aspects and engine related evaluation” within the REDIFUEL project. The objective of this task is to gain a deeper understanding of different alcohol/paraffin mixtures with up to 30 % of C₆-C₁₁ bio-alcohols in a pure Gas-to-Liquid (non-additives) and their impact on emission and performance after combustion for existing engines. Therefore, different blends of REDIFUEL in diesel are analysed on a heavy-duty single cylinder research engine and by 3D-CFD simulations. The single cylinder investigations are important to measure all relevant parameter at constant boundary conditions. That enables to analyse the specific fuel impact on combustion by evaluation of their heat release rate. Furthermore, this data is used to calibrate numerical simulation models that are used to investigate the fuel/air mixture formation and air utilization during combustion.

The results of this deliverable are used to give a clear recommendation of most promising fuel blend of REDIFUEL in diesel that are required for any further investigation program in the work package 3.



2

Methods

To be drop-in capable by mixing with diesel a fuel must satisfy the EN590 standard. In the norm, several properties are regulated, such as oxidation stability, viscosity, boiling range, etc.. The research results of this deliverable, mainly two properties were considered: density and Cetane Number (CN). While the density is an indicator of the volumetric energy content of the fuel, ensuring a similar CN as diesel guarantees not major modifications to engine calibration and hardware. The diesel used in this research is a standard B0 diesel without biofuel content. Different blends of a surrogate alcohol mixture (SAM) with GtL and of the RF_{A30P70} (i.e., the surrogate mixture featuring a similar composition of the real end-product) with diesel are screened with regards to their self-ignition tendency and density. This preliminary screening served to identify a drop-in blend compliant with the EN590 regulation. Successively, blends of RF_{A30P70} with diesel were tested in a heavy-duty single cylinder engine (HD SCE), to assess the potential of efficiency gain and emissions reduction. To gain an in-depth combustion analysis of the most promising mixtures, three-dimensional computational fluid dynamic (3D-CFD) simulations were conducted too.

2.1 HEAVY DUTY SINGLE CYLINDER ENGINE

The HD SCE was derived from a six-cylinder heavy duty commercial vehicle engine of N3 class compliant to Euro VI stage C. The engine specifications are listed in Table 1. The engine featured a common rail fuel injector with a built-in pressure intensifier and an in-house developed prototype electronic control unit with a model-based fuel path control. Such a prototype control system provides a wide range of flexibility especially in adjusting relative separation and energizing duration of main injection, pilot injection and pressure intensifier. The exhaust gas recirculation (EGR) rate is derived from the CO₂ concentration in the intake runner. The exhaust back pressure (p_{exh}) is regulated with two flow control butterfly valves: one valve for a faster control and the other for a finer control of p_{exh} . The regulated emissions are measured at the engine exhaust. The measurement line for the unburned hydrocarbon (HC), carbon monoxide (CO) and nitrogen oxides (NO_x) is pre-heated to a temperature of 200 °C to avoid condensation. The measurement devices used are listed in Table 2.

Table 1 HD SCE specifications



Parameter	Unit	Value
Displacement	liters	2.13
Stroke	mm	156
Bore	mm	132
Compression ratio	-	18.3
Max. cylinder pressure	bar	250
Max. injection pressure	bar	2700
Max. rail pressure	bar	1200
EGR	-	Cooled high pressure EGR
Injection system	-	CRIN 4.2 Bosch
Injection nozzle	cm ³ /30s @ 100 bar	850
Number of holes	-	8
Injection nozzle cone angle	°	142

Table 2 Measuring devices for the HD SCE

Parameter	Device	Range
CO, CO ₂ , NO _x , HC	FEVER NDIR, CLD, FID	CO ~ 0 – 5000 ppm CO ₂ ~ 0 – 20 %-vol NO / NO _x ~ 0 – 3000 ppm THC ~ 0 – 3000 ppm C3
Filter Smoke Number (FSN)	AVL 415S	0 – 10 FSN
Fuel flow	Emerson CMF010 Coriolis	0 – 120 kg/h
Combustion pressure sensor	Kistler 6044 A	0 – 300 bar

The combustion and emission behaviour of the fuels under consideration are assessed by testing these fuels at a given load for different EGR rates. Among that four load points have been selected ranging from low part loads up to rated power operation, see Figure 1. Furthermore, the selected load points are preferred because those are relevant for both the world harmonized stationary cycle (WHSC) and world harmonized transient cycle (WHTC) for emission regulation, see Figure 1. At engine part load, the in-cylinder thermodynamic conditions like temperature, pressure and turbulence are expected to be high enough to permit the assessment of the ignition behaviour of the fuels based on engine operation.

The given fuels are analysed at a Euro VI stage C base indicated specific nitrogen oxides (ISNO_x) level of around 6 g/kWh. While performing the EGR sweeps, a constant centre of combustion ($\alpha_{0.50}$) is kept in order to avoid impact on emission of retarded combustion. The fuels are compared at the same engine indicated mean effective pressure (IMEP) as shown in Figure 1 and the relevant engine calibration parameters like, injection pressure (p_{inj}), boost pressure (p_{boost}) and temperature (T_{boost}) defined in Table 3.



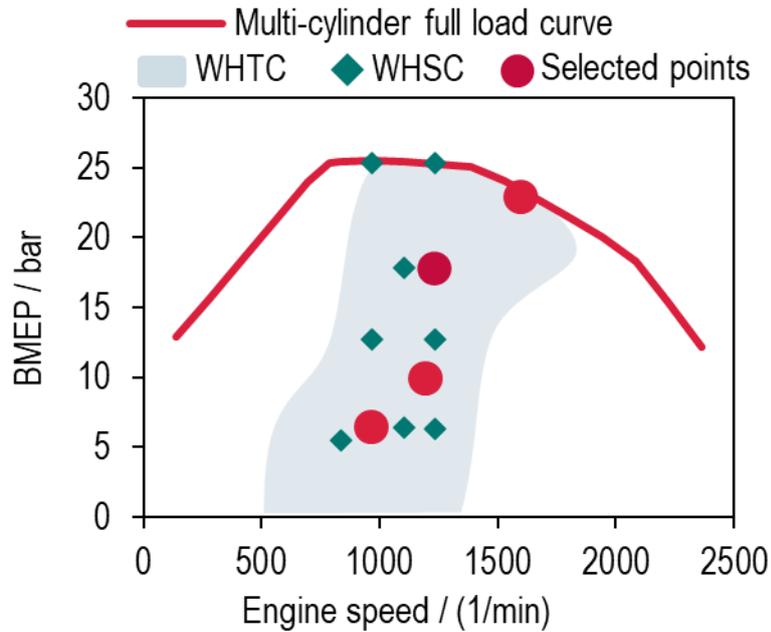


Figure 1 Explicative engine load map in break mean effective pressure (BMEP) vs engine speed

Table 3 HD SCE calibration settings

Engine speed / min ⁻¹	BMEP / bar	IMEP / bar	α_{Q50} / °CA ATDC	p_{inj} / bar	T_{boost} / °C	p_{boost} / mbar	p_{exh} / mbar
1600	22.8	24.9	15.1	2612	54	3500	3623
1200	19.6	21.0	10.2	1680	39	2800	2904
1200	9.8	10.3	6.2	1280	41	1790	1825
900	5.9	6.4	6.5	1037	41	1280	1325

2.2 3D-CFD NUMERICAL MODELLING

Reynolds-averaged Navier–Stokes numerical simulations are performed using the CFD code provided by CONVERGE. CONVERGE is a general-purpose CFD tool that automates the mesh generation process and the adaptive mesh refinement (AMR) algorithm [1]. In particular, the AMR delivers small grid size where high temperature and velocity gradients are calculated without significantly increasing the total number of computational cells. A full mesh is adopted during the 3D-CFD gas exchange simulations, while a sector mesh is used for the mixture formation simulations, as shown in Figure 2 (left). The mixture formation cases simulated here featured a base grid of 1.4 mm and an additional mesh refinement yielding a local grid of minimum 0.35 mm.

The Renormalization Group $k-\epsilon$ equations are chosen to model the turbulence. The Kelvin-Helmholtz and Rayleigh-Taylor model is used to capture the fuel spray break-up [2]. The mass, momentum, and energy are calculated at each node of the grid using the unsteady Navier-Stokes equations, which are implicitly discretized based on a finite volume method over the Cartesian grid [3]. For the analysis of the droplet evaporation, the FROSSLING model is selected [4]. The droplet collision is analysed by using the no time counter collision model [4] and the blob injection model is used to inject liquid parcels inside the computational domain [4]. For solving the pressure-velocity coupling the pressure

implicit for the splitting of operator algorithm is used [3]. The O'Rourke and Amsden model is set for the wall heat transfer calculations [4]. For the analysis of the spray wall interactions, the rebound/slide model is adopted [4]. To assess the quality of the mixture formation process the characteristic numbers air utilisation (AU) and oxidation potential number (OPN) are used. The AU indicates the volumetric fraction of air inside the combustion chamber, sorted per air/fuel equivalence ratios (λ) ranges [5]. The AU is evaluated at a given engine operating condition, from starting of injection (SOI) to exhaust valve opening (EVO). The OPN is a number based on the AU. It represents the share of lean mixture (i.e. air utilization between $1 < \lambda < 2$) divided by the rich one ($\lambda < 1$) and by the unused air ($\lambda > 2$) [6] as shown in Figure 2 (right). The higher the OPN, the better the expected soot oxidation potential.

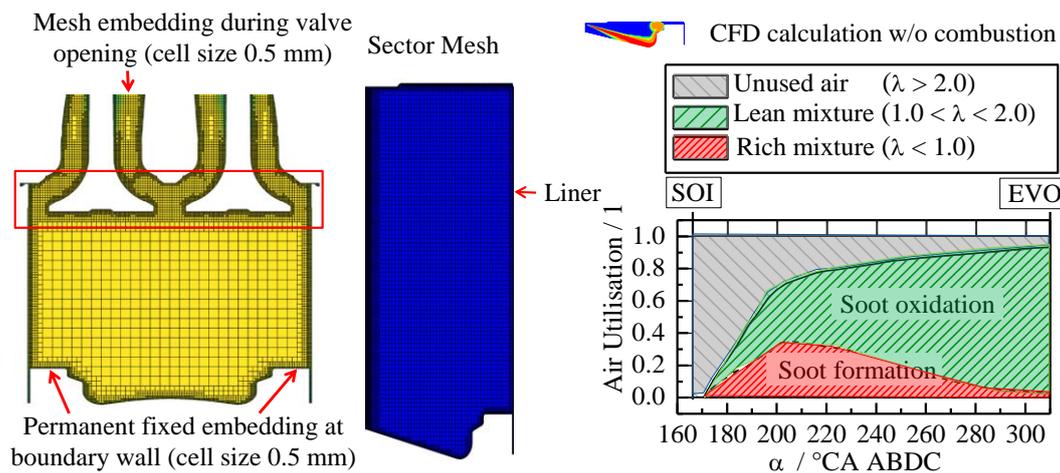


Figure 2 Computational mesh for gas exchange and mixture formation simulations illustrating the fixed embedding (left) and air utilisation (right)

2.3 FUEL COMPOSITION AND PROPERTIES

To evaluate the mixture formation and emission reduction potential of diesel (B0) and different blend of REDIFUEL with diesel (B0) numerical 3D-CFD simulations are performed. At the beginning of the project the real end-product is available only on lab-scale quantities, so a surrogate REDIFUEL mixture consisting of 30 vol% alcohols mixed with paraffinic diesel (RF_{A30P70}) is adopted for this study. The oxygenated fraction of RF_{A30P70}, termed from now on surrogate alcohol mixture (SAM), consists of C₆ – 21 wt%, C₇ – 20 wt%, C₈ – 18.5 wt%, C₉ – 16 wt%, C₁₀ – 13.5 wt% and C₁₁ – 11 wt% linear alcohols. The paraffinic part is represented with a pure Gas-to-Liquid (GtL, non-additives) mixture, consisting of carbon 84.6 wt% and hydrogen 15.4 wt%. The mixture composition and properties of the different fuel blends simulated here are shown in Table 4. The mixture formation during the high-pressure cycle under the cold evaporative condition (without combustion) is analyzed due to unavailability of chemical mechanism for the blend of REDIFUEL with diesel (B0).

The density of the blends decreased gradually with an increasing volume fraction of the paraffinic part since the paraffinic part is a mixture of normal and iso-paraffins which have the lowest density of all hydrocarbons. The lowered density makes the fuel lighter and enhances the air-fuel mixing resulting in better mixture formation [3]. The lower distillation temperature of the paraffinic part makes it easier for the blends to evaporate and form into a more combustible air-fuel mixture [4]. The higher Cetane Number of the paraffinic part indicates a shorter ignition delay and premixed combustion period, which leads to a lower maximum temperature, hindering the formation of the NO_x emission [4]. The lower heating values (LHV) of the blends are lowered with the increase in RF_{A30P70} composition as B0 is replaced with the oxygenated fraction of RF_{A30P70}. Further, the increase of RF_{A30P70} composition in the blend increases the fuel bone oxygen content, the higher oxygen content in the blend will improve the mixture formation and result in the higher OPN.

Table 4 Fuels used in simulation and their composition

Diesel / REDIFUEL Vol %	Overall mixture composition vol%				Density kg/cm ³	LHV MJ/Kg	Oxygen / %	ICN 1
	Diesel	SAM	GTL	UCOME				
100 % B0 Diesel	100.00 %	0.00 %	0.00 %	0.00 %	839.0	42.90	0	52.10
60 % B0 + 40 % RF_{A30P70}	60.00 %	12.00 %	28.00 %	0.00 %	820.30	42.45	1.47	53.60
93%RF_{A30P70} + with 7% UCOME	0.00 %	27.90 %	65.10 %	7.00 %	800.22	41.38	4.17	57.90

The surrogate fuel approach is adopted for simulating different blend of REDIFUEL with diesel. For diesel fuel, DF-2 (surrogate for diesel) is taken as a liquid phase surrogate, which is widely used [5]. As the measured and modeled properties of 1-Octanol are found to be in very good agreement with that of SAM, it is chosen as its liquid surrogate [6]. The paraffinic part is modeled as 45 vol% cyclo-octane, 51 vol% iso-cetane and 4 vol% n-decane, a mixture of cyclo-octane, iso-cetane, and n-decane are used as a surrogate for the paraffinic part of the fuel [7]. Two different blends of RF_{A30P70} with diesel (B0) are studied here. The first blend of 60 vol% B0 and 40 vol% RF_{A30P70} is selected, owing to its CN and delivers a density of around 820 kg/m³ satisfies within the EN590 regulation and the second blend 93 vol% RF_{A30P70} and 7 vol% UCOME is selected, owing to its CN and delivers a density of around 800 kg/m³ for artic grade. Furthermore, a second blend, having fully renewable fuel 93 vol% RF_{A30P70}, is simulated to derive trends for fully renewable substitution share in the fuel mixture.

In Table 5, the relevant fuel properties of the blends that are tested on the HD SCE are mentioned, as the CN and oxygen content increase, the carbon content and the calorific value decrease with an increase in the RF_{A30P70} share. Besides that, the fully renewable fuel blend of 93 vol% RF_{A30P70} and 7 vol% UCOME is investigated.

Table 5 Fuel blend properties

Fuel	Density at 15 °C / kg/m ³	Carbon mass fraction / %	Hydrogen mass fraction / %	Oxygen mass fraction / %	Calorific value / MJ/kg	Cetane number / 1
100 % B0 diesel	839.0	86.5	13.8	0.0	42.9	52.1
80 % B0 + 20 % RF_{A30P70}	829.8	85.46	14.03	0.74	42.7	52.5
60 % B0 + 40 % RF_{A30P70}	820.3	84.42	14.26	1.47	42.5	53.6
50 % B0 + 50 % RF_{A30P70}	815.2	83.90	14.37	1.82	42.3	54.1
20 % B0 + 80 % RF_{A30P70}	798.9	82.34	14.71	1.83	42.0	56.7
93 % RF_{A30P70} + 7 % UCOME	800.2	81.01	14.74	4.17	41.4	57.9



3 Results

In this section, the experimental and numerical results are discussed. First, the results of ignition delay and density measurements are discussed. Based on these results the most promising blends are tested at the HD SCE.

3.1 HD SCE TEST BENCH RESULTS

In the following section, the results from the screening of the fuel blends on the HD SCE are discussed. The presented results are obtained at an engine speed of 1200 min⁻¹ and two different load level.

Cruise point

In Figure 3, the results for the cruise point operation at the base ISNO_x of 5.8 g/kWh are presented. The different fuel blends are displayed in bar charts and distinguished by colour style. The indicated specific particulate matter emissions (ISPM) are presented in the top-left plot in Figure 3. Generally, adding the RF_{A30P70} to diesel reduces the ISPM emission.

This can be attributed to the presence of oxygen and paraffinic molecules in the RF_{A30P70}. Less soot precursors are generally formed when diluting diesel with a straight-chained oxygenated mixture, as shown in the literature [8, 9]. Moreover, this renewable drop-in fuel might positively affect also soot oxidation, due to its fast ignition chemistry and enhanced mixture formation properties [9]. As the 40 vol% RF_{A30P70} in diesel is compliant with EN590 in accordance with previous discussions, in this result section the relative changes with reference to diesel in performance and emissions are presented for this blend only. A relative reduction of ISPM by up to 12 % is achieved with a blending proportion of 40 vol% RF_{A30P70} in diesel.

The indicated specific carbon monoxide (ISCO) emissions are shown in the middle-left corner of Figure 3. With an increase in RF_{A30P70} substitution in diesel, lower ISCO emissions are observed. This could be attributed to the faster ignition, which would prevent over-leaning in air/fuel mixture and to the inherent oxygen moieties included in the renewable fuel. Moreover, an enhanced mixture formation (due to better atomization owing to the paraffinic content) is also beneficial to ensure a proper oxygen entrainment [10]. The indicated specific hydrocarbon (ISHC) emissions, shown in the lower-left bar plot in Figure 3, reduce with increasing RF_{A30P70} share. Similarly to ISCO emissions, an improved mixture formation might be the reason for the observed trend [10]. Due to reduced ISCO and ISHC emissions, a marginal rise in the indicated thermal efficiency (ITE) by 0.6 %-points was noticed for the blend with 40 vol% RF_{A30P70} in diesel, as shown in top-right diagram of Figure 3. A relative reduction in ISCO and ISHC by up to 6 % and 18 % is respectively noticed for the blend under consideration.

Generally, an increase in RF_{A30P70} share leads to a direct reduction in indicated specific carbon dioxide (ISCO₂) emissions. A relative reduction in ISCO₂ by up to 2.6 % is seen for the blend with 40 vol% RF_{A30P70} in diesel, refer middle-right diagram of Figure 3. To explain this ISCO₂ reduction, a parameter named as theoretical fuel carbon flow rate (TFCFR) is introduced. The TFCFR is defined as the fuel carbon mass fraction times the fuel mass flow rate. It represents the theoretical carbon mass flow rate that is available for a complete combustion of the fuel at a given engine load, accounting for variations in injected fuel mass due to changes in calorific fuel content and ITE. The lower-right corner of Figure 3 shows a TFCFR reduction by 2.3 % for the blend with 40 vol% RF_{A30P70} in diesel, which nearly agrees with the aforementioned relative ISCO₂ reduction.

In addition to that, the blend with 93 vol% RF_{A30P70} and 7 vol% UCOME provides some further potential due to its high content of paraffinic hydrocarbons and increased share of molecular oxygen. Both lead to an improved mixture formation and fasten combustion. The results show a relative reduction in ISCO and ISHC by more than 20 % and 32 % while ISPM emission are lowered by around 15 %.

The improved mixture formation and fasten combustion result in a better combustion efficiency and show a ITE rise by around 0.9 %-points. The TFCTR is reduced by more than 5 %.



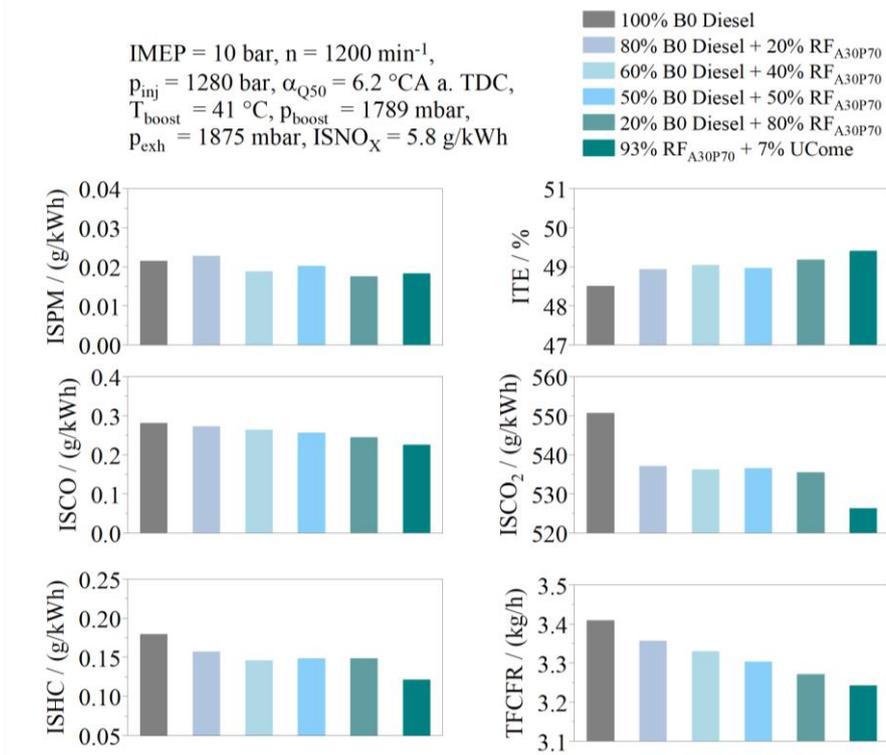


Figure 3 HD SCE results at cruise point for base NO_x level, IMEP = 10 bar, $n = 1200 \text{ min}^{-1}$, $p_{inj} = 1280 \text{ bar}$, $\alpha_{Q50} = 6.2 \text{ }^\circ\text{CA a. TDC}$, $T_{boost} = 41 \text{ }^\circ\text{C}$, $p_{boost} = 1789 \text{ mbar}$, $p_{exh} = 1875 \text{ mbar}$, $ISNO_x = 5.8 \text{ g/kWh}$

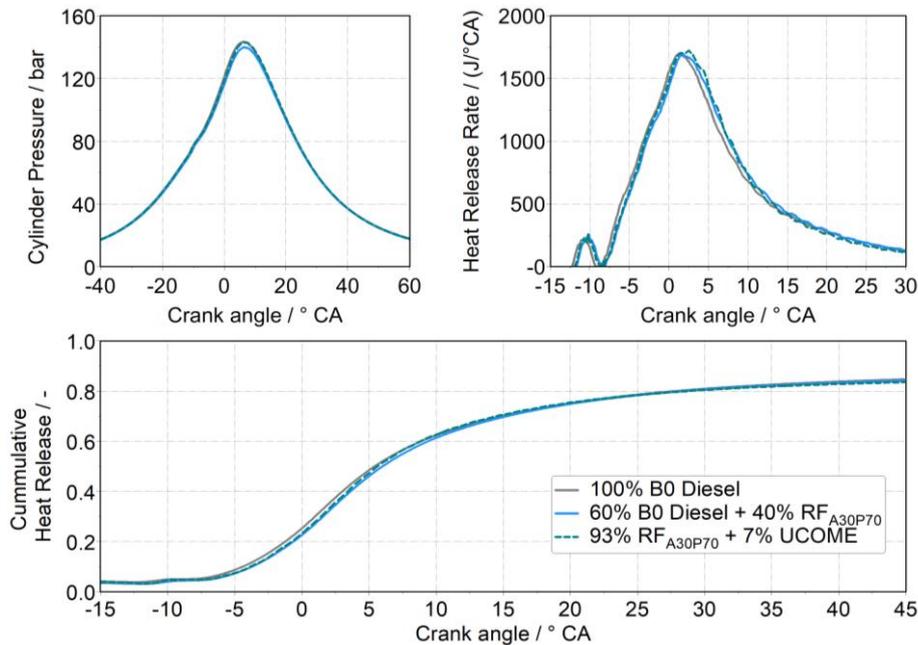


Figure 4 Heat release analysis at cruise point IMEP = 10 bar, $n = 1200 \text{ min}^{-1}$, $p_{inj} = 1280 \text{ bar}$, $\alpha_{Q50} = 6.2 \text{ }^\circ\text{CA a. TDC}$, $T_{boost} = 41 \text{ }^\circ\text{C}$, $p_{boost} = 1789 \text{ mbar}$, $p_{exh} = 1875 \text{ mbar}$, $ISNO_x = 5.8 \text{ g/kWh}$

The heat release analysis for the cruise point at the base ISNO_x level is shown in Figure 4. For the sake of clarity, the Figure 4 presents the heat release analysis for diesel and blends of RF_{A30P70} with 40 vol% / 60 vol% in diesel and the fully renewable blend of 93 vol% RF_{A30P70} / 7 vol% UCOME. Due to a slightly lower ignition delay time (i.e. slightly higher CN) of the RF_{A30P70} blends with diesel, the injection timing is slightly retarded to maintain a constant α_{Q50} . This can be seen in the cumulative heat release plot at a value of around 0.5, refer lower diagram of Figure 4. The heat



release rate (HRR) of the RF_{A30P70} blends, depicted on the upper-right side in Figure 4, is similar to that of diesel. The crank angle position corresponding to the maximum heat released during combustion is slightly retarded for the RF_{A30P70} blends. This can be attributed to an increased injector energizing time - necessary to achieve the load matching (i.e. increased injected mass to compensate the reduced fuel calorific value) - and to the retarded injection timing. Increased injected fuel mass causes a relatively later end of combustion and a subsequent shift in heat release.

Best efficiency point

The results at the higher engine load point of best efficiency show in principle the same tendency, see Figure 5. It can be seen that blends of RF_{A30P70} in diesel behave very similar to pure diesel with respect to their pollutant and CO₂ emission impact. The low emission potential of RF_{A30P70} in diesel can be explained with the predominating high combustion temperature. Thus, excellent boundary conditions for an improved mixture formation and fast combustion are existed already for pure diesel.

The fully renewable blend of 93 vol% RF_{A30P70} with 7 vol% UCOME provides overall improvements also at high load. The ISCO emissions are reduced by more than 20 % while the particulate emissions are lowered by more than 50 %. The ISHC emissions slightly increased of 30 %, but they remain on a significant low level. Again, the high content of paraffinic hydrocarbons and increased share of molecular oxygen are led to a fast combustion that improves the engine efficiency by around 1 %-point. The TFCTR is also been reduced in the manner of 4 %.

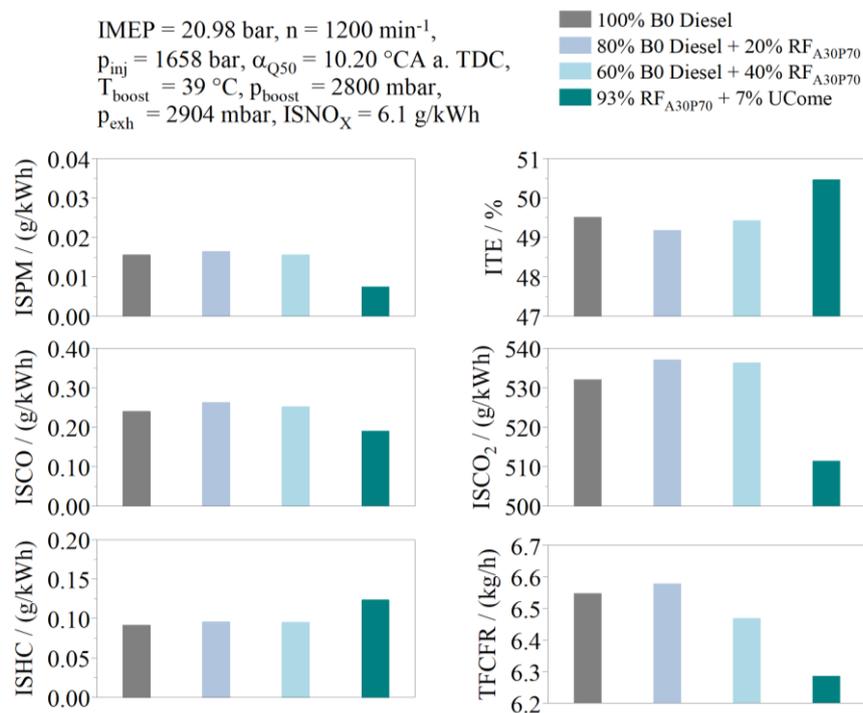


Figure 5 HD SCE results at best efficiency point for base NO_x level, IMEP = 20.98 bar, n = 1200 min⁻¹, p_{inj} = 1658 bar, α_{Q50} = 10.2 °CA a. TDC, T_{boost} = 39 °C, p_{boost} = 2800 mbar, p_{exh} = 2904 mbar, ISNO_x = 6.1 g/kWh

Figure 6 shows the results of the heat release rate analysis. As anticipated from the above shown results, the cumulated heat release of 40 vol% RF_{A30P70} in diesel shows a similar combustion behaviour then pure diesel. Only 93 vol% RF_{A30P70} with 7 vol% UCOME delivers an improved burn-out of the diffusive phase due its molecular oxygen content with the mentioned benefit in efficiency and emissions.



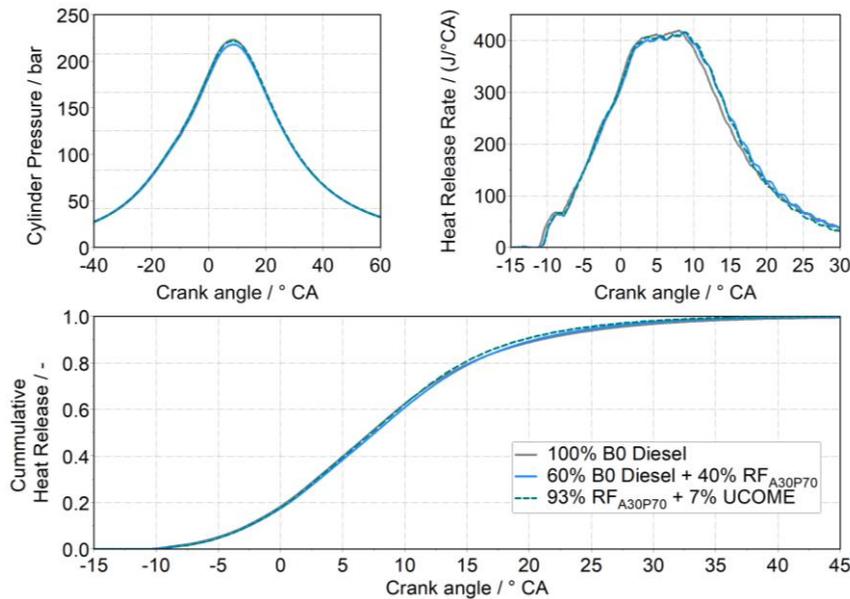


Figure 6 Heat release analysis at best efficiency point for base NO_x level, IMEP = 20.98 bar, n = 1200 min⁻¹, p_{inj} = 1658 bar, α_{Q50} = 10.2 °CA a. TDC, T_{boost} = 39 °C, p_{boost} = 2800 mbar, p_{exh} = 2904 mbar, ISNO_x = 6.1 g/kWh

3.2 3D-CFD SIMULATION RESULTS

In this section, the numerical results are discussed. Firstly, an overview of the surrogate fuel properties estimations for the numerical simulation is provided. Secondly, the 3D-CFD simulations results for the most promising blends of RF_{A30P70} with diesel are presented.

Screening of drop-in biofuels using 3D-CFD

To evaluate the mixture formation and emission reduction potential of the fuels under consideration, numerical 3D-CFD simulations are performed. Herein, the mixture formation during the high-pressure cycle under inert mixing condition is analysed. To model the mixture formation of RF_{A30P70} blends with B0 with a good confidence level, firstly the CFD model is calibrated using diesel experimental data from the HD SCE at cruise point operation. Here, the same ISNO_x level as shown in the test bench results section (i.e. 5.8 g/kWh) is chosen. Successively, the physicochemical properties of diesel are exchanged with those of the blends of RF_{A30P70} and B0 diesel. Two different blends of RF_{A30P70} with B0 are studied. A first blend of 60 vol% B0 and 40 vol% RF_{A30P70} is selected, owing to its CN and density meeting the EN590 norm. Furthermore, a second blend, having a higher share of RF_{A30P70} (i.e. 80 vol%) with B0, is simulated to derive trends at increasing renewable substitution share in the fuel mixture.

Figure 7 presents the comparison of the air utilization for different blends of RF_{A30P70} and diesel at cruise point operation. It can be seen that with an increasing blending proportion of RF_{A30P70} in diesel, the share of lean mixture (i.e. AU between $1 < \lambda < 2$) is larger. Hence, a higher degree of air/fuel mixing and a high potential to soot oxidization during combustion is expected. The bottom of Figure 7 shows the cut-sections of the piston bowl modelled in CONVERGE that corroborate the trends of the air utilization curves. At the selected crank angle of 22 °CA a larger share of lean equivalence ratios can be seen and a smaller share of rich zones ($\lambda < 1$). This indicates that the soot is expected to be better oxidized in case of the blends with RF_{A30P70}. Further, it can be seen from Table 6 that at the cruise point operation, the RF_{A30P70} blends resulted in higher OPN as compared to diesel.

Impact of the most promising blends are also studied at the rated power point, as shown in Figure 8. Similarly to cruise point operation, increasing RF_{A30P70} blending proportion with diesel yields larger lean mixture shares (i.e. AU between $1 < \lambda < 2$), indicating a higher degree of air/fuel mixing and a high potential to oxidize soot during combustion.



Table 6 Comparison of OPN for different blends of B0 and RF_{A30P70} at cruise point and rated power point operation

Fuel	OPN @ cruise point	OPN @ rate power point
100 % B0 diesel	22.2	9.3
60 % B0 + 40 % RF _{A30P70}	25.2	12.8
20 % B0 + 80 % RF _{A30P70}	28.62	17.7

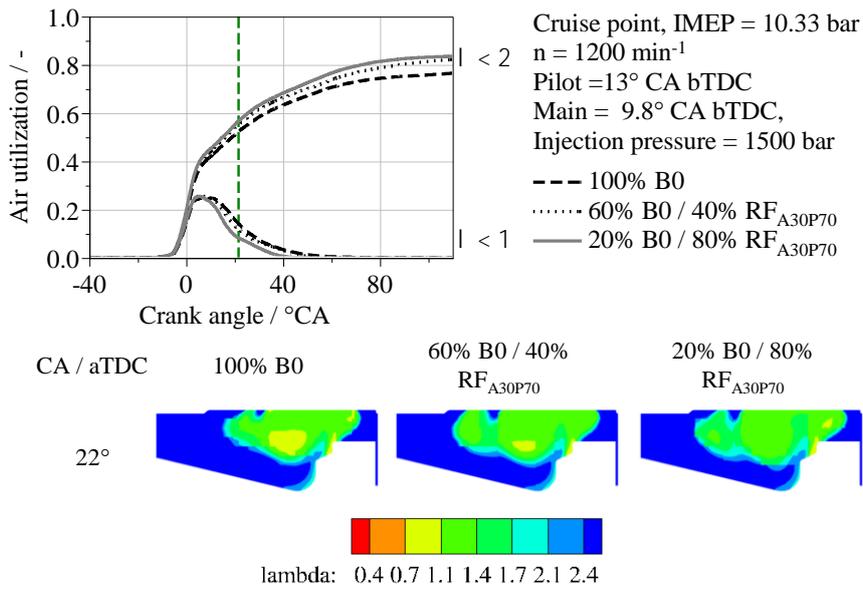


Figure 7 Comparison of air utilization (top), and lambda plots for RFA30P70 and diesel (bottom), at cruise point

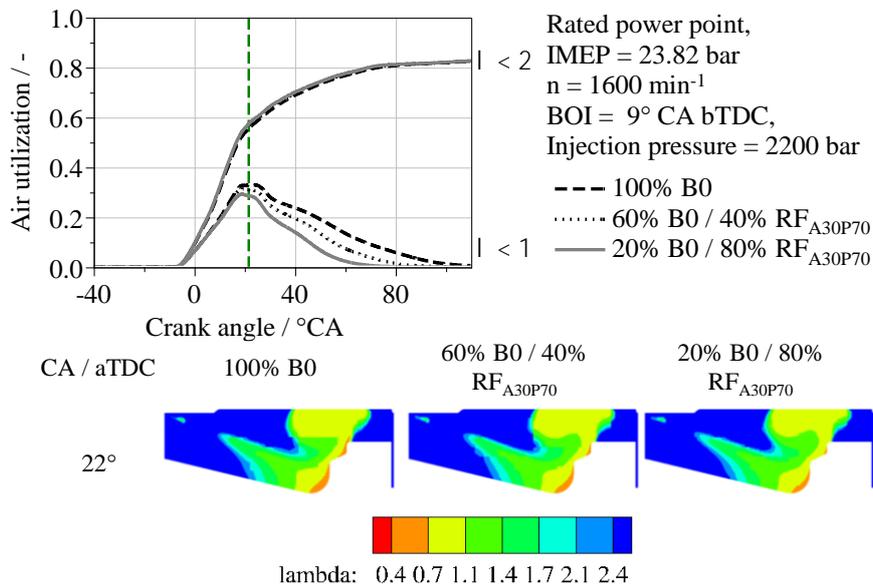


Figure 8 Comparison of air utilization (top), and lambda plots for RFA30P70 and diesel (bottom), at rated power operation

4 Discussion and Conclusions

4.1 4.1 DISCUSSION

No decisions are made based on the described results, that have provided a deviation from the grand agreement.

4.2 4.2 CONCLUSIONS

The potential of the novel drop-in biofuels containing high-Cetane (C₁₁-C₂₁) bio-hydrocarbons and (C₆-C₁₁) bio-alcohols was examined with regard to mixture formation, engine performance and emission reduction.

- The thermo-physical and physicochemical properties of fuel surrogates are estimated using models over a wide range of temperatures, featuring very good agreement with measured data.
- The fuel blend with 40 vol% REDIFUEL (i.e. RF_{A30P70} - alcohol of 30 vol% and a paraffinic content of 70 vol%) in diesel satisfies both the minimum requirement for Cetane Number and density stated by the EN590 norm.
- All the blends of REDIFUEL with diesel exhibit a marginal rise in efficiency and reduced engine out CO₂ emissions. Generally, the particulate matter, carbon monoxide and hydrocarbon emissions are reduced with an increase in the renewable drop-in fuel.
- The fuel blend with 40 vol% REDIFUEL in diesel exhibits a relative reduction in indicated specific particulate matter, indicated specific carbon monoxide, indicated specific hydrocarbon and CO₂ emissions by 12 %, 6 %, 18 %, and 2.7 % respectively with reference to diesel. A marginal rise in thermal efficiency by 0.6 %-points is noticed for this blend.
- In the numerical modelling, the blends of REDIFUEL with diesel show enhanced mixture formation, as indicated also by a higher level of oxygen entrainment in the spray plume as compared to diesel. This indicates a better soot oxidation potential of the REDIFUEL blends, as confirmed by the engine tests.

Overall, the REDIFUEL blends show similar performance as diesel with reduced particulate matter, hydrocarbon and CO₂ emissions. This suggests that REDIFUEL will help in a reduction in TtW CO₂ emissions and, thanks to its renewable nature to an overall reduction in WtT CO₂ emissions. Further, the blend with 40 vol% REDIFUEL in diesel satisfies the EN590 norm and can be on the immediate term used in current heavy duty fleets, without necessity for hardware adaptation or engine calibration.



5 Deviations from Annex 1

There are no deviations with respect to the description of work.



6 References

Please include references when necessary.

- [1] Graziano, B.; Perez, J. M.; Kremer, F.; Pischinger, S.; Reddemann, M. A.; Kneer, R.; Heufer, K. A.; Rohs, H.: Virtual Fuel Approach: a new simulative methodology to analyse effects of fuel properties on mixture formation in compression ignition combustion. In Proceedings of THIESEL Conference on Thermo- and Fluid Dynamic Processes in Diesel Engines, Valencia, (2014).
- [2] Graziano, B., Heuser, H., Kremer, F., Pischinger, S. and Rohs, H.: The oxidation potential number: an index to evaluate inherent soot reduction in DI die-sel spray plumes. SAE International Journal of Engines,9(1), 222-236 (2016).
- [3] Kitano, Koji, Ichiro Sakata, and Richard Clark. "Effects of GTL fuel properties on DI diesel combustion." SAE transactions (2005): 1415-1425.
- [4] Wu, Tao, et al. "Physical and chemical properties of GTL– diesel fuel blends and their effects on performance and emissions of a multicylinder DI compression ignition engine." Energy & Fuels 21.4 (2007): 1908-1914.
- [5] Farrell, J. T., Cernansky, N. P., Dryer, F. L., Law, C. K., Friend, D. G., Hergart, C. A., McDavid, R. M., Patel, A. K., Mueller, C. J., Pitsch, H.: Development of an experimental database and kinetic models for surrogate diesel fuels. SAE Technical Paper, No. 2007-01-0201 (2007).
- [6] Yadav, Jaykumar, Vikram Betgeri, Barbara Graziano, Avnish Dhongde, Benedikt Heuser, Markus Schönen, and Nina Sittinger. "Renewable drop-in fuels as an immediate measure to reduce CO 2 emissions of heavy-duty applications." In Internationaler Motorenkongress 2020, pp. 353-372. Springer Vieweg, Wiesbaden, 2020.
- [7] Choudhury, H. A., Intikhab, S., Kalakul, S., Khan, M., Tafreshi, R., Gani, R., Elbashir, N. O.: Designing a surrogate fuel for gas-to-liquid derived diesel. Energy & Fuels, 31(10), 11266-11279 (2017).
- [8] Pischinger, Stefan , et. al, " Fuel Design for Future Combustion Engines – A View from the Cluster Tailor-Made Fuels from Biomass" 37th Internationales Wiener Motorensymposium 28-29 (2016):224-252.
- [9] Graziano, B., Ottenwälder, T., Manderfeld, D., Pischinger, S., Grünefeld, G., "Advanced methodology for the detection of smoke point heights in hydrocarbon flames." Energy and Fuels (2018): 3908-3919.
- [10] Alkidas, A.C., "Combustion-chamber crevices: the major source of engine-out hydrocarbon emissions under fully warmed condition. " Progress in Energy and Combustion Science, (1999): 253-273.

7 Acknowledgement

H2020-LC-SC3-RES-21-2018-DEVELOPMENT OF NEXT GENERATION BIOFUELS AND ALTERNATIVE RENEWABLE FUEL TECHNOLOGIES FOR ROAD TRANSPORT

Acknowledgement:

The author(s) would like to thank the partners in the project for their valuable comments on previous drafts and for performing the review.

Project partners:

- 1 - FEV – FEV EUROPE GMBH - DE
- 2 - MPI – MAX-PLANCK-GESELLSCHAFT ZUR FORDERUNG DER WISSENSCHAFTENEV - DE
- 3 - CSIC – AGENCIA ESTATAL CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS - ES
- 4 - VTT – Teknologian tutkimuskeskus VTT Oy - FI
- 5 - RWTH – RHEINISCH-WESTFAELISCHE TECHNISCHE HOCHSCHULE AACHEN - DE
- 6 - OWI – OWI Oel-Waerme Institut GmbH - DE
- 7 - VUB – VRIJE UNIVERSITEIT BRUSSEL- BE
- 8 - NESTE – NESTE OYJ – FI
- 9 – MOL - MOL HUNGARIAN OIL AND GAS PLC - HU
- 10 – INER - INERATEC GMBH - DE
- 11 – T4F - TEC4FUELS - DE
- 12 – UNR - UNIRESEARCH BV – NL

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under Grant Agreement no. 817612



Disclaimer:

This document reflects the views of the author(s) and does not necessarily reflect the views or policy of the European Commission. Whilst efforts have been made to ensure the accuracy and completeness of this document, the REDIFUEL consortium shall not be liable for any errors or omissions, however caused.

8 Risk register

Risk No.	WP	What is the risk?	Probability of risk occurrence ¹	Effect of risk ²	Solutions to overcome the risk
1	3.4	Possible engine damage (rebuild / repair not possible in time)	2	1	Procurement of spare parts, spare cylinder head; definition of engine shut-down limitations
2	3.4	Lead time of ordered components too long	2	2	Regular (monthly) alignment of delivery time plan with suppliers

¹ Probability risk will occur: 1 = high, 2 = medium, 3 = Low

² Effect when risk occurs: 1 = high, 2 = medium, 3 = Low

