The Role of High Octane Fuels in Future Mobility - A Technical Review

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Summary

As personal mobility demand is expected to grow globally in the next decades, we will face a greater pressure to reduce total CO_2 emissions from road transport. Most of today's light-duty transport in the world comes from gasoline-powered vehicles. Consequently all efficiency improvement measures, including, but not limited to, the optimization of internal combustion engines - will continue to be key.

It is widely accepted that high octane fuels can help to reduce vehicle CO_2 emissions. The specific CO_2 reduction is heavily dependent on engine technology, detailed fuel properties and finally engine operation. One potential route to increase octane is Ethanol which offers secondary benefits of increased in-cylinder cooling and not negligible significantly lower well-to-tank CO_2 emissions. Research progress in advanced ethanol production might offer ways to introduce high octane fuels based on renewable sources with lowest well-to-tank CO_2 emissions.

To obtain a holistic picture, Shell has conducted a detailed research study to understand the role of High Octane Fuels in conventional and optimized combustion systems. Engine test results based on a de-correlated fuels-matrix to study the impact of various fuel properties such as RON, MON, and ethanol-content on engine efficiency and local emissions will be presented in this paper. Based on these findings, the total well-to-wheel CO_2 emissions in Europe have been modelled in different scenarios for the passenger car segment which provide a differentiated view on the most effective approaches.

1 Introduction

Through the effective use of engine downsizing, significant tank-to-wheel CO_2 reduction has been achieved in gasoline engine development in recent years. The need in society to further decrease CO_2 emissions plays an important role in internal combustion engine research which therefore continues to rely on improving combustion efficiency and reducing losses. It is widely known, that for modern downsized and optimized gasoline engines, a high Research Octane Number (RON) can increase engine efficiency in the operating regions where combustion is limited by engine knock. One of the potential pathways to further improve RON is the addition of Ethanol, not only because of its high anti-knock resistance but also its biomass origin which allows for further improving of the well-to-tank CO_2 footprint. However, the maximum amount of Ethanol in gasoline at present is limited to 10 vol. % in Europe (EN228). Engine modifications will be required to leverage the full potential of higher octane fuel.

Results of a detailed fuels study on the impact of high octane fuels on engine efficiency and engine-out emissions in specifically adapted engines are discussed in the present paper:

- The impact of increased Ethanol splash blend ratios on tank-to-wheel CO_2 emissions and engine performance will be analyzed in the first part (It has to be recognized, that the investigated splash blends do not meet the current EN228 specification. High octane target blended fuels with higher Ethanol content could match to current EN228 limits (except oxygen content)). With that aim tests with specifically designed fuels have been performed to separate individual effects of octane, heat of evaporation and fuel sensitivity (which will be discussed subsequently).
- The focus in the second part is on the assessment of the total well-to-wheel CO_2 emissions of Ethanol fuels in different scenarios for the passenger car segment.

2 The role of high octane fuels in modern engine technology

2.1 Test Engine, Test Matrix, and Fuels Matrix

The engine tests have been performed in a modern downsized boosted gasoline single cylinder engine which was designed to represent future SI engine technology. The engine setup allowed for an easy adjustment of the compression ratio, a critical parameter to leverage the full potential of fuels with increased knock resistance. In this study the compression ratio of the baseline configuration, which has been optimized for E10, was increased by two units from 9.5 to 11.5 for all higher octane fuels. The spark timing was chosen to keep the centre of combustion constant (°crank angle where 50% of the fuel mass is burned) and only retarded where necessary to maintain a constant knock amplitude at higher load, depending on the respective fuel octane level. Detailed specifications of this research tool are displayed below.

The combustion system featured a 4-valve pent roof cylinder head equipped with variable valve timing (VVT) systems for both intake and exhaust camshafts. The cylinder head was equipped with a central-mounted outward opening high pressure piezo direct injector allowing injection pressures of up to 200 bar. Throughout the entire test series, temperatures and pressures of intake air, fuel, coolant and oil were precisely closed-loop controlled by individual conditioning units. The high pressure indication system enabled real time combustion analysis and thereby precise knock control. The engine fuel consumption was measured through a fuel mass flow meter and cross-checked with lambda deviation calculation relevant at lower speeds and loads respectively.

Gasoline Single Cylinder Engine		
Combusiton system		Gasoline DI
Displacement	cm^3	454
Bore	mm	82
Stroke	mm	86
Max mean effective pressure	bar	35 (indicated)
Compression ratio		9.5 (basline conf.)
		11.5 (high octane conf.)
Valves / cylinder		4
Max. injection pressure	bar	200 (piezo actuated)
Max peak pressure	bar	150

Tab. 1: Specification of the single cylinder research engine

To investigate the load and speed impact of different fuel properties, engine tests in a wide range of the engine operating map have been conducted. Injection and valve timing has been optimized for individual load points. Load sweeps at four different engine speeds provided a holistic overview on the benefit of high octane fuels in various combustion regions. The experimental data was subsequently used to model tank-to-wheel CO_2 emissions for different drive cycles. Figure 1 provides an overview of the engine test matrix.

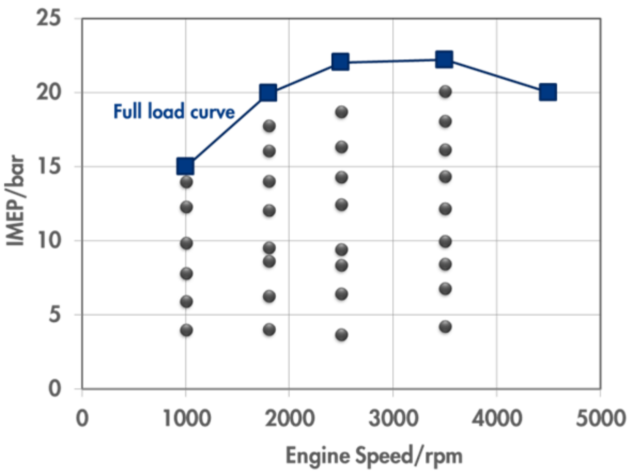


Fig. 1: Engine Test Matrix

A fuel matrix was designed to separate the effects of individual fuel properties such as RON, MON and Ethanol-content on engine efficiency and fuel consumption respectively. Initially, a conventional EN 228 with 10%-vol Ethanol was used to splash blend E20, E30, and E85 (block I). Increasing Ethanol content leads to a higher RON, higher fuel sensitivity and higher heat of evaporation. All of these three properties are expected to have a positive effect on the performance of downsized SI engines. By adjusting the fuel base stock, an E0 fuel has been designed to match the anti-knock properties (RON and MON) of the E30 fuel (block II). This fuel combination was analyzed to separate the effect of octane and Ethanol. Two additional fuels were blended with similar RON values but different MON values, both containing a constant Ethanol volume (E10). The comparison of these fuels enabled the investigation of the impact of fuel sensitivity on engine performance. Detailed properties of all fuels are depicted below.

		Block I				Block II	Block III	
	Unit	**Fuel A**	**Fuel B**	**Fuel C**	**Fuel D**	**Fuel E**	**Fuel F**	**Fuel G**
Ethanol Content	% vol	10	20	30	85	0	10	10
RON		96.5	99	101	107	100	98	98
MON		85	87	88	89	89	92	88
Octane Sensitivity		11	12	13	18	12	6	10
Heat of Vaporisation	kJ/kg	428	490	551	864	366	395	424
Calorific Value	MJ/kg	41,6	40,1	38,4	29,6	42,1	43,0	41,6
	MJ/L	30,8	30,0	28,9	23,3	31,5	30,1	30,3
Density	kg/m3	742	747	753	786	748	699	730

Block 1: Effect of splash blended ethanol fuels, including Fuels A-D
Block 2: Effect of match blended fuels, including Fuel A and Fuel E
Block 3: Effect of octane sensitivity, including Fuel F and Fuel G

Tab. 2: Fuels Matrix

2.2 Impact of Ethanol splash blends on engine performance

Figure 2 presents the engine performance of the Ethanol splash blends at constant speed of 1800 rpm. The results indicate that increased Ethanol splash blends can be used to improve the tank-to-wheel CO_2 footprint in tailored engines. While at lower load, no statistically significant differences can be observed, increased levels of Ethanol provide higher indicated engine efficiencies at higher engine load. This effect can be explained as following:

- The effects of higher octane ratings, in combination with increased in-cylinder cooling effects through the higher heat of evaporation of Ethanol, allow for higher knocking-free engine loads at optimum combustion phasing. In the case of E20, the spark timing had to be retarded as low as 8 bar IMEP to avoid knocking, while with E85, the spark timing was not limited until 15 bar IMEP. At lower engine speed the advantageous fuel properties of Ethanol only played a subordinate role.
- In addition to the spark advance with higher octane blends, the increased knock-resistance allowed for higher compression ratios in tailored engines, resulting in improved thermal efficiency. The impact of the increased compression ratio became obvious through direct comparison of the engine test results with E10 in both engine configurations. Clearly, the engine efficiency was higher with increased compression ratio at low load where knock was not an issue. The opposite trend could be observed at higher load when the increased knock tendency caused by higher end gas temperatures required a later combustion phasing. Consequently this effect forces a fuel depending compromise in engine design.

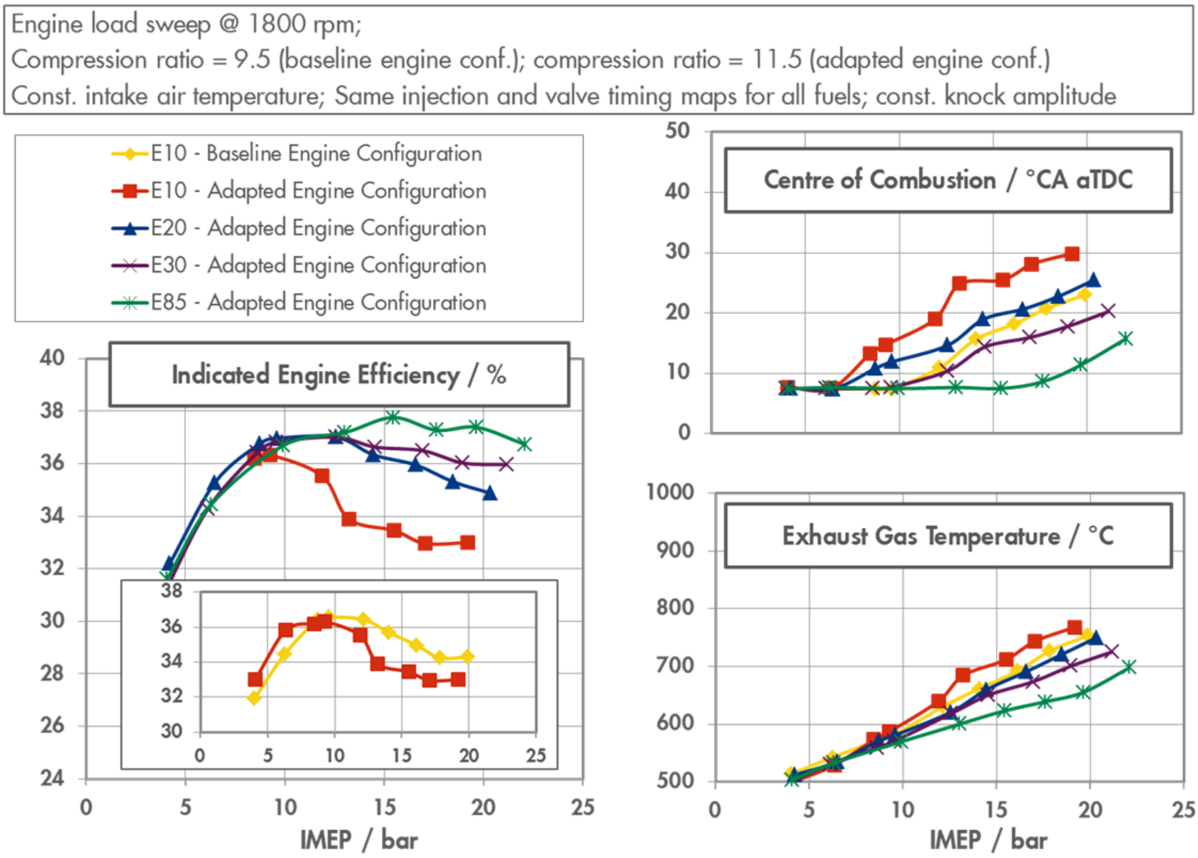


Fig. 2: Impact of Ethanol splash blends on engine efficiency at 1800 rpm

The engine test results at full load operation confirmed the findings of the load sweep operation. Increased Ethanol blending using the same base stock will help to significantly increase the engine efficiency if the engine design is adapted to the benefit of the fuel properties. In addition to the effects described above, higher Octane fuels offer additional benefit potential at full load as shown in Figure 3. In consequence of the earlier combustion phasing, reduced fuel enrichment requirements can be observed with higher octane fuel grades. This effect becomes much more apparent at higher engine speeds as fuel enrichment is often needed to protect engine components such as the turbocharger being exposed to too high temperatures. Fuel enrichment with E85 is obsolete under the chosen boundary conditions allowing for an efficiency improvement of more than 30 % compared to the baseline case with E10. Overall, the adaptation of the engine design to specific high octane fuel properties offers a considerable potential to further reduce TtW CO_2 emissions.

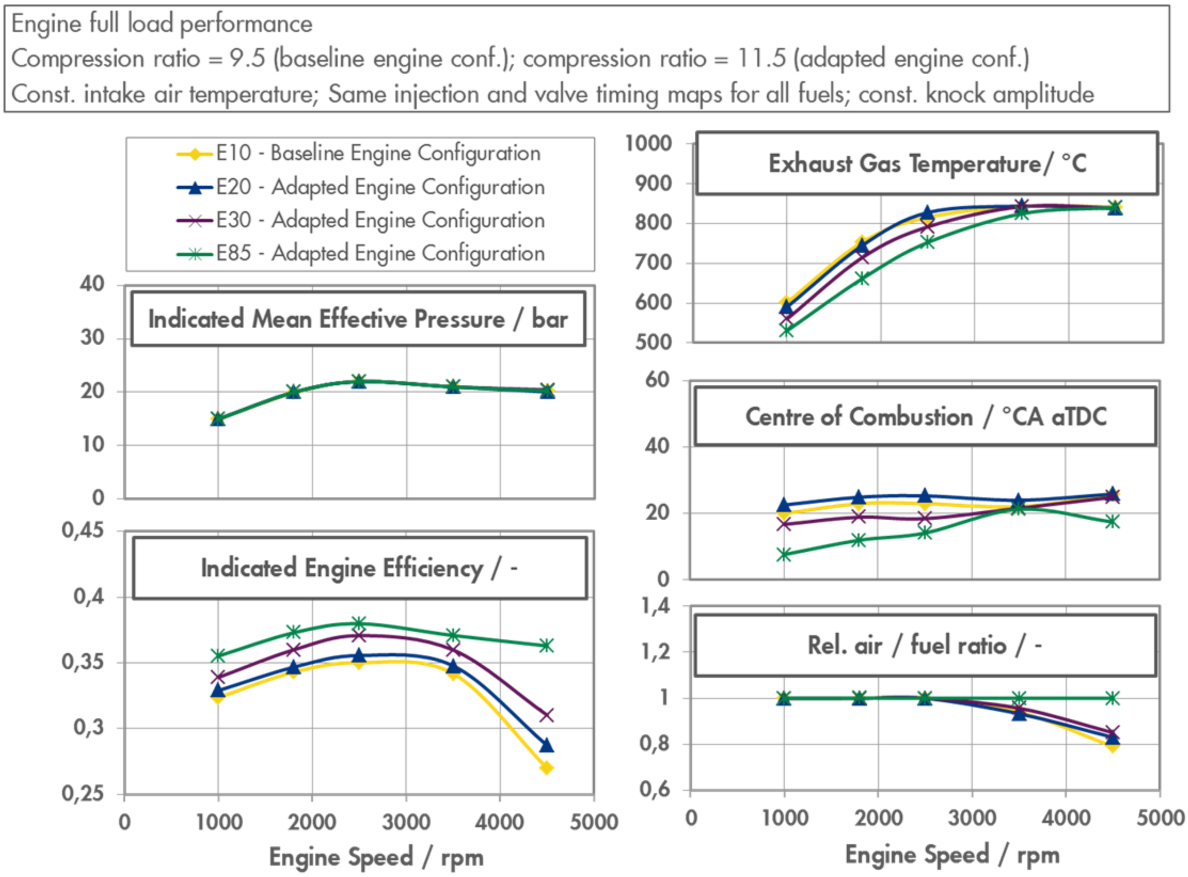


Fig. 3: Impact of Ethanol splash blends on engine full load performance

The introduction of Euro 6c in combination with urban air quality challenges in mega cities has brought increased attention to particulate emissions in DI gasoline engines. The obtained data provide an indication that particulate number (PN), as well as particulate mass (PM) emissions, can be significantly reduced in Ethanol splash blends. The effect might be attributed to the increased oxygen content of the fuel which hinders the formation of soot particles. This effect outweighs the increased heat of evaporation of Ethanol which leads to slightly reduced temperatures during compression and potentially cooler droplets. However, the later effect might become more critical under cold start conditions. As the single cylinder engine can only be operated in steady-state conditions further work is needed to confirm the particulate reduction potential in transient and cold start operation. One additional effect on the PN/PM formation with Ethanol splash has to be considered: the splash blend approach results in a dilution of the original base fuel. The aromatic content of the fuel decreases with higher Ethanol splash blends. As C6+ aromatic components lead to a higher boiling range and are less prone to evaporate in contact with the cylinder wall, the reduced aromatic content with higher Ethanol splash blends contributes to reduced PN/PM emissions. Further investigations based on a de-correlated fuels matrix will be necessary to separate the individual effects of a changed fuel composition [1].

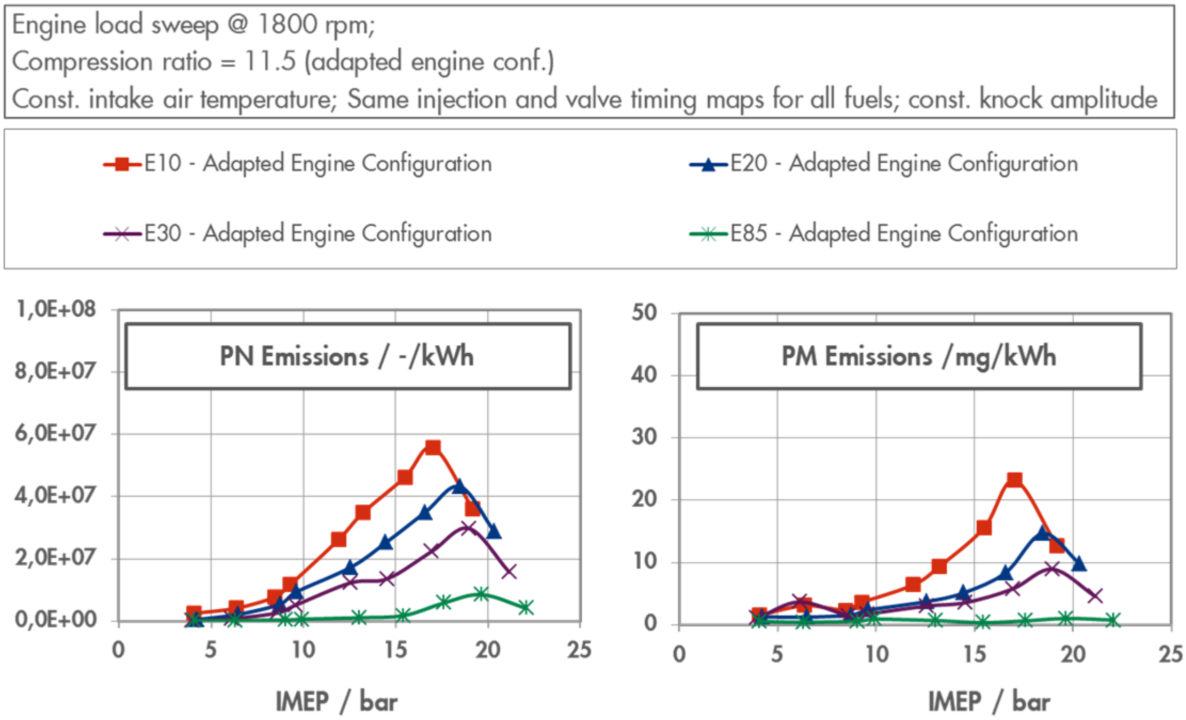


Fig. 4: Impact of Ethanol splash blends on particulate emissions

2.3 Impact of heat of evaporation on engine performance

As outlined above, the fuel octane rating significantly contributes to increased engine efficiency in adapted engines. However, as shown in table 2, the increase of Ethanol also led to higher heat of evaporation. As more energy is required to evaporate Ethanol, lower compression end gas temperatures can be expected. Fuel E was specifically designed to match the octane (RON and MON) of E30. Due to the absence of any Ethanol, Fuel E provided lower levels of heat of evaporation. The cooling effect of the heat of evaporation together with a higher flame speed provided an additional benefit of the higher Ethanol blend, as shown in Figure 5. At higher engine load, E30 allowed for an earlier combustion phasing at constant knock amplitudes. As a consequence, the indicated efficiency was measured to be 4 % higher at full load with the E30 splash blend compared to the E0 with similar RON and MON. The Ethanol route to increase octane hence provides secondary benefits over fossil high octane fuels which lead to a further reduction in tank-to-wheel CO_2 emissions. This effect has been observed in earlier studies as well [9]. However, different data suggest that the octane measurement covers the cooling effect of Ethanol up to 40 vol.-% and therefore fully describes the overall knock resistance of the fuel [4]. Further work is needed to fully understand how the cooling effect impacts the RON measurement at lower Ethanol contents.

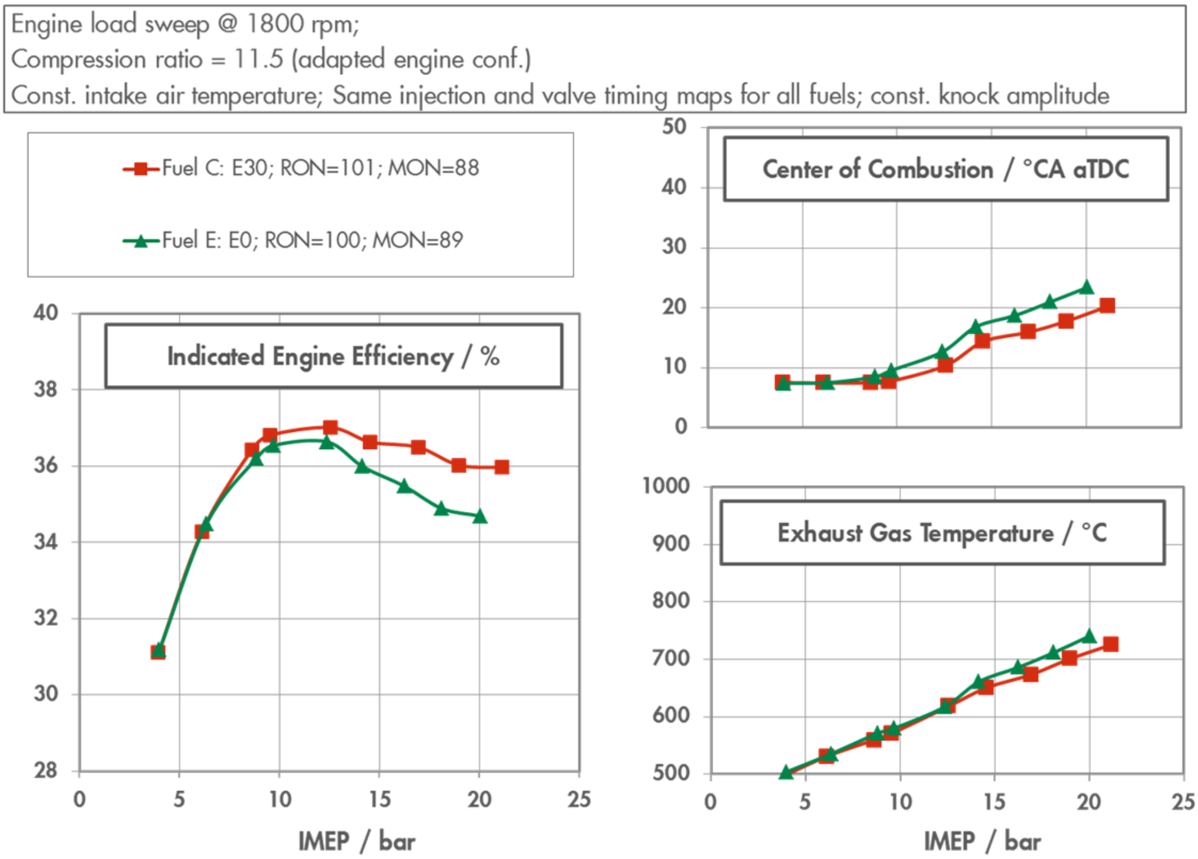


Fig. 5: Impact of Ethanol content on engine efficiency in similar octane fuel grades

2.4 Impact of fuel sensitivity on engine performance

A fuel's knock resistance is historically characterized by the research octane number (RON) and motor octane number (MON). The MON test uses a higher temperature, lower manifold pressure and higher engine speed condition than the RON test. The difference of these numbers is referred to as fuel sensitivity (RON-MON). Several fuel studies in different engines suggested that octane requirements of modern downsized boosted gasoline engines might be different from requirements derived in the past, as we see lower temperatures for given pressures in real engines today [2].

The addition of Ethanol into EN228 also increases the sensitivity of the fuel. Two high octane fuels with similar RON and Ethanol content but different MON have been designed to separate the effect of sensitivity in high octane fuels and to analyze the impact on engine performance. The above described behavior can also be observed in Figure 6. Fuel G provided a higher sensitivity and also slightly higher engine efficiency at high load as it allowed for an earlier combustion phasing. This means for a given level of RON, a high MON value can actually be disadvantageous in modern boosted downsized gasoline engines. However, potential backwards compatibility issues for specially designed high MON vehicles have to be taken into account.

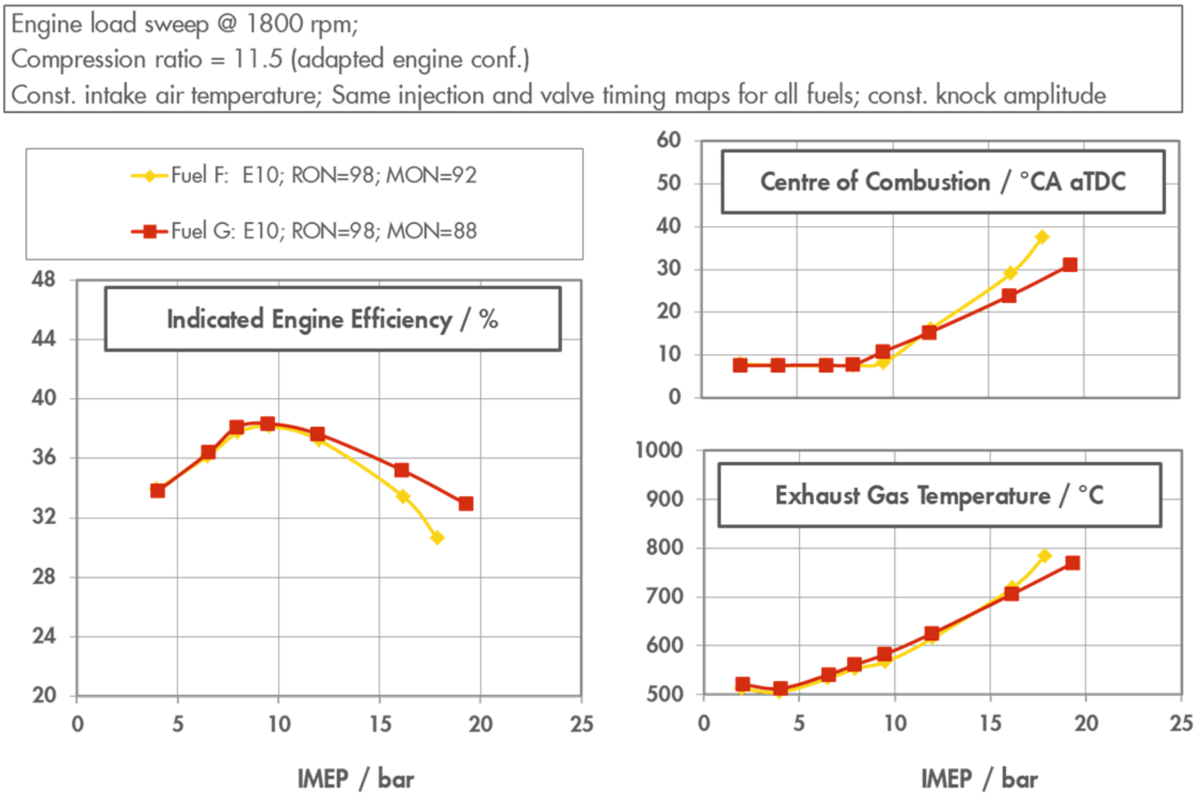


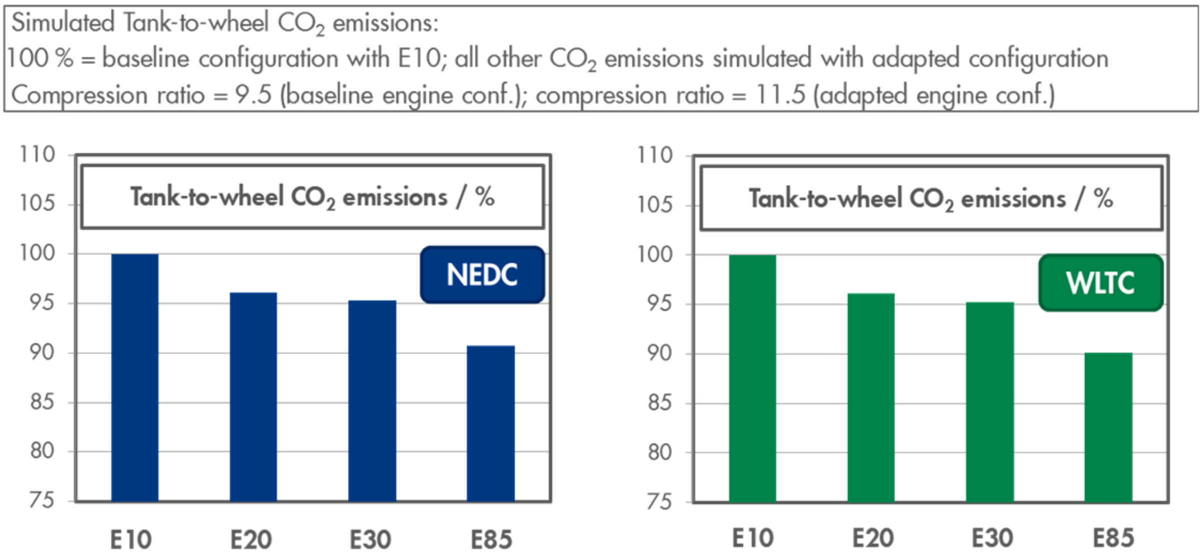
Fig. 6: Impact of fuel sensitivity on engine efficiency

Overall, the results confirm previous studies which concluded that increased Ethanol splash blends improve the tank-to-wheel CO_2 footprint in adapted engines [3,4]. Furthermore, the data suggest that the increase in engine efficiency cannot be exclusively attributed to the increase in octane, but is likely a combination of the simultaneous increase of RON, heat of evaporation, flame speed and sensitivity. Hence, the ethanol route provides additional TtW CO_2 savings over fossil high octane fuels. To realize the full potential further work is needed to understand impact of sensitivity on optimized engines as well as potential limitations to increased compressions ratios such as pre-ignition [5].

2.5 Comparison of TtW CO_2 emissions for different Ethanol splash blends

Using the single cylinder test results, tank-to-wheel CO_2 emissions for different Ethanol splash blends were calculated by simulating the new European driving cycle (NEDC) and the worldwide harmonized light vehicles test cycle (WLTC) for a typical C-class passenger vehicle. Figure 7 indicates that higher ethanol blends showed a benefit of reduced tank-to-wheel CO_2 emissions in both test cycles. The TtW CO_2 reduction potential of E20 was modelled to around 4% compared to E10 with the baseline engine configuration. This improvement was related to higher engine efficiencies but also the fuel properties itself. Due to the improved H/C ratio, Ethanol released less carbon atoms per unit of energy during combustion, which contributed to decreased CO_2 emissions for higher ethanol blends. Further Ethanol increase from E20 to E30 should only have a very minor effect on the CO_2 emissions in the two test cycles. However, this will be subject to change if the compression ratio is further increased for E30. As outlined by the results, it can be expected that the shift from

NEDC to WLTC will have no major impact on the CO_2 emission reduction potential because the engine is primarily not operated in the knock limited area of the engine map.



Simulated Tank-to-wheel CO_2 emissions:
100 % = baseline configuration with E10; all other CO_2 emissions simulated with adapted configuration
Compression ratio = 9.5 (baseline engine conf.); compression ratio = 11.5 (adapted engine conf.)

Fig. 7: Simulated tank-to-wheel CO_2 emissions in NEDC and WLTC

3 Well-to-Wheel CO_2 impact of E20

The key driver for a potential increase in octane of future fuels is clearly the potential for CO_2 reduction in gasoline combustion engines. However, in order to understand the full impact on CO_2 emissions along the value chain a WtW approach is needed to identify which fuel options could deliver the biggest CO_2 saving. Primarily there are two routes to increased octane:

1. Via increasing the use of higher octane fossil hydrocarbon derived components such as platformate, alkylates, isomerates, MTBE etc. (or a reduction of the use of lower octane components such as light naphthas)
2. Via renewable fuel components such as ethanol or derivatives such as ETBE

Directionally increasing the octane level of fuels with crude derived components requires increasing amount of processing and energy resulting in increased CO_2 WtT intensity of gasoline. Bearing in mind that CO_2 is the key driver for increased octane it therefore seems sensible to focus on ethanol as a source of increased octane.

Advanced ethanol from waste and residual feedstock material (wheat straw, waste wood) shows more WtW GHG reduction than produced from farmed crops (wheat, sugar beet). The following values are considered for an assessment of the WtW impact of higher octane fuels, here different ethanol pathways compared to neat gasoline shown as Well-to-Combustion (WtC), the efficiency of the engine in MJ/km not included yet:

	Wt-Combustion CO_2 Footprint	
1st Generation Ethanol (sugar beet, wheat)	gCO_2 / MJ fuel*	33 - 57
2nd Generation Ethanol (wheat straw, waste wood)	gCO_2 / MJ fuel*	11-17
Normal crude derived gasoline (E0)	gCO_2 / MJ fuel**	93.2

* Typical greenhouse gas emissions as in [6]

** Typical greenhouse gas emissions as in [7]

Tab. 3: Assessment of the WtW impact of higher octane fuels

Based on above engines results it is predicted that raising the octane level of gasoline from E10 RON95 to E20 RON 99 can improve engine efficiency by 3.2% in the WLTC. Clearly this number depends on the starting octane level as well as other parameters such as sensitivity.

As seen in Figure 8, an E20 splash blend shows significant potential for reducing GHG emissions on a WtW basis from up to 11% compared to E10 (EN228). This result highlights the potential for further optimization of the internal combustion engine both through improved hardware and more efficient combustion as well as improved fuels to deliver an integrated CO_2 reduction.

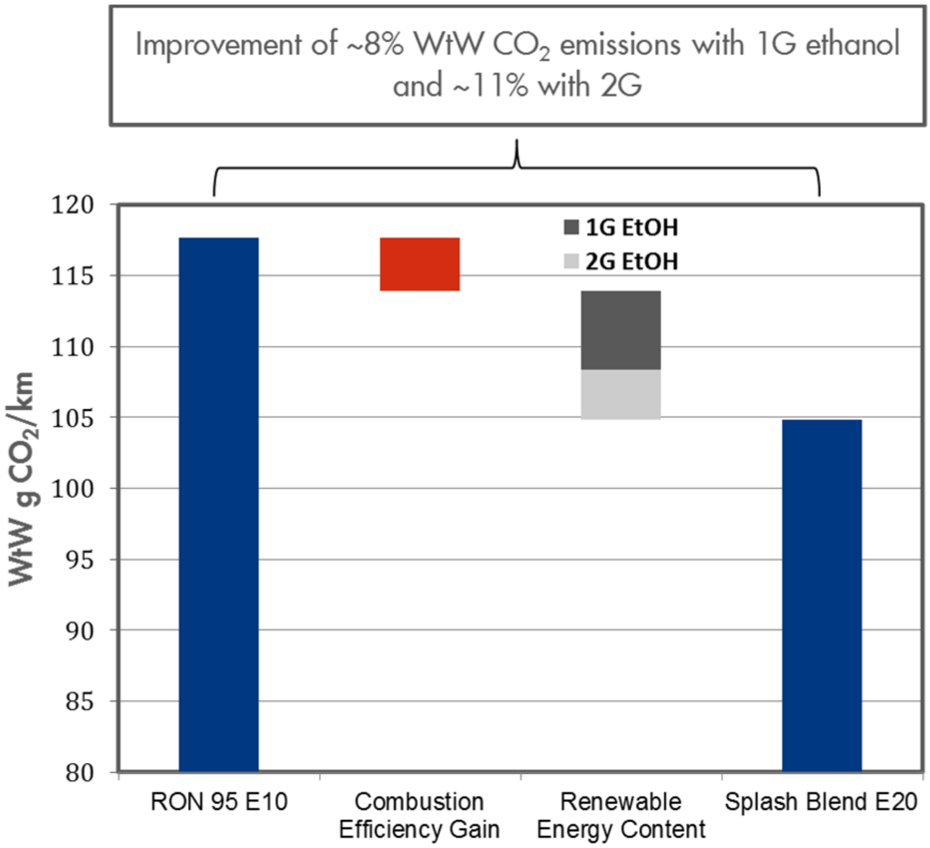


Fig. 8: 2020 WtW CO_2 improvement potential of combining higher ethanol levels with increased octane levels

Following assumptions have been made to calculate the WtW CO_2 improvement potential:

- Fuel consumption of 132MJ/100 km for RON 95 E10
- Engine efficiency improvement of 3.2% from E10 to E20
- 1G Ethanol WtC CO_2 emissions of 33.5 CO_2e /MJ (Assumption in 2020+ all 1G biofuel in the market complies with requirements as in [6] 60% WtC reduction from 2018 for ethanol from new installations compared to the fossil comparator of 83,8 gCO_2e/MJ).
- 2G Ethanol WtC CO_2 emissions of 14 CO_2e /MJ

Comparing the GHG intensity of fuel pathways provides a guidance on which fuel could deliver the lowest GHG emissions in a gasoline car. More important is to understand the potential of GHG reduction that can be achieved within a fleet with high octane ethanol blends. Based on the data of the recently published Auto-Oil II study [8] and the above results, a scenario has been developed to predict the European CO_2 reduction potential for 1G and 2G Ethanol in an E20 splash blend. These results can be compared to the CO_2 reduction potential of other fuel/drivetrain combinations.

Scenario boundary conditions were chosen as following:

- Whereas vehicles brought into the market are assumed to be E20 capable from 2015 onwards, gasoline powertrains are not optimized to high octane before 2025.
- It is assumed that high octane E20 is available from 2025 onwards.
- The cumulated effect of a high octane E20 on total WtW CO_2 reduction vs. an E10 is calculated in two steps: for the gasoline vehicles entering the market between 2015 and 2024 the calculated WtW CO_2 reduction is due to the higher bio ethanol content in the fuel only. For the gasoline cars entering the market between 2025 and 2030 in addition a better engine efficiency of 3.2% is included as well in the CO_2 reduction calculation.
- Average fuel consumptions for the gasoline cars are estimated to be 1.50, 1.32, 1.30, 1.28 MJ/km for 2015, 2020, 2025 and 2030 respectively [8].
- New gasoline sales scenario as in [8]
- Average mileage assumed to be 10.000 km/year [8]
- An average energy consumption of 15 kWh/ 100 km and an average electricity grid intensity for Europe of 78 gCO_2/MJ in 2025 and 12 kWh/100 km and 67 gCO_2/MJ in 2030 are assumed to calculate the CO_2 reduction potential of electric vehicles [8].

The potential WtW CO_2 savings compared to E10 are shown in figure 9, up to 3.9 Mt CO_2/year and 7.6 Mt CO_2/year for an E20 based on 1G ethanol and up to 6.6 Mt CO_2/year and 9.9 Mt CO_2/year for a 2G ethanol in 2025 and 2030, respectively.

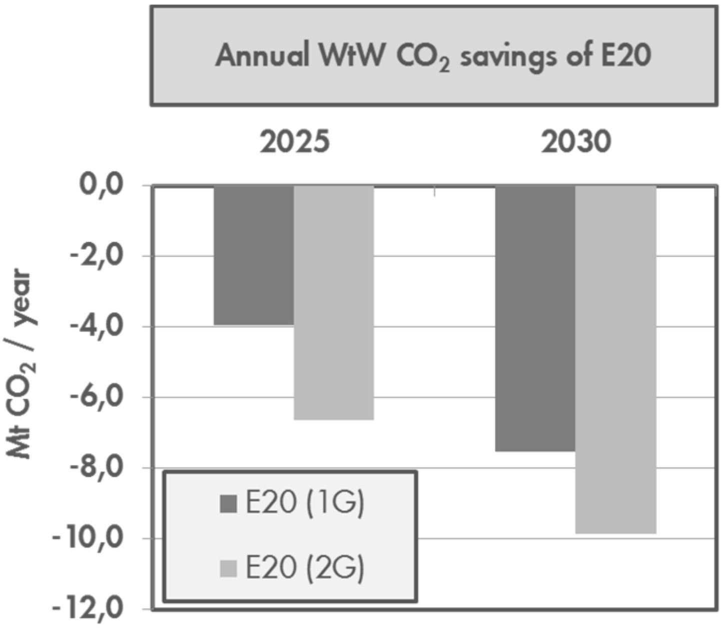


Fig. 9: Annual WtW CO_2 savings of E20 high octane in new gasoline sales that entered the markets from 2015 up to the shown year in Europe

To set these numbers into context with other potential CO_2 reduction pathways, it will be required to have

- ~ 9 million BEV on the road in 2025
- ~ 12 million BEV on the road in 2030

to achieve the same CO_2 saving as with the E20 (2G) pathway in Europe.

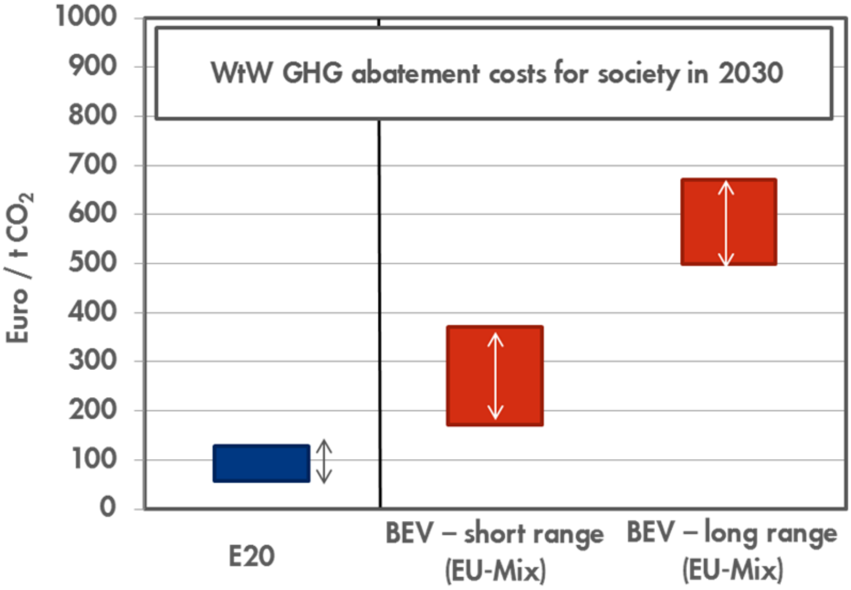


Fig. 10: Comparison of WtW CO_2 abatement costs for society highlighting the potential of biofuels as cost-efficient carbon abatement options [8]

The Auto-Oil coalition study [8] also highlighted this potential, particularly taking into account the cost to society recommending biofuels as cost-efficient and high effective option for decarbonisation of transport as shown in Figure 10. The WtW CO_2 abatement cost to society are quite moderate for an E20 fuel-powertrain combination around 100 Euro/ton CO_2 (mid of span) abated. Compared to 280 Euro/ton CO_2 (mid of span) for a short range or 613 Euro/ton CO_2 (mid of span) for a long range battery electric vehicle (BEV). Consequently, the Ethanol route is a potential pathway to achieve highest CO_2 savings at moderate costs.

4 Conclusions

Overall, the results of the investigations highlight the potential for further optimization of the internal combustion engine both through improved hardware and more efficient combustion as well as improved fuels to deliver an integrated CO_2 reduction at moderate costs to society:

- Increased Ethanol splash blends improve the vehicle tailpipe CO_2 emissions in adapted engines. Using an E20 splash blend, the TtW CO_2 footprint could be reduced by around 4% in the WLTC.
- The data suggest that the increase in engine efficiency cannot be exclusively attributed to the increase in octane, but is likely a combination of the simultaneous increase of RON, higher heat of evaporation of ethanol compared to standard gasoline and sensitivity. Consequently, the ethanol route provides additional tank-to-wheel CO_2 savings over fossil high octane fuels.
- On a WtW basis E20 shows significant potential for reducing GHG emissions by up to 11% compared to E10 (EN228).

5 Acknowledgement

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