Improvements in vehicle efficiency will be a key factor in ensuring that liquid fuels remain a vital partner in the future of road transport. This article looks at the role of high-octane petrol (HOP) in improving engine efficiency, and summarises the findings of a modelling study designed to assess the impact of HOP on the refining system and the positive effect of HOP on CO_2 emissions.

Authors

Damien Valdenaire damien.valdenaire@concawe.eu

Heather Hamje heather.hamje@concawe.eu

Introduction

Gasoline is a complex mixture of hydrocarbons and other chemical compounds used as fuel for sparkignition internal combustion engines (ICEs), primarily in passenger cars and other light-duty transportation vehicles (LDVs). Gasoline in the European Union (EU) has to meet more than a dozen individual specifications, for which the technical standards and analytical methods are specified under EN 228, the European Standard for unleaded petrol.

The European Commission (EC) also sets limits on other components of finished gasoline. Mandatory environmental regulations for several fuel properties were first introduced in 1998 (Directive 98/70/EC), and were revised in 2003 (Directive 2003/17/EC) and 2009 (Directive 2009/30/EC¹). Other industry specifications limit the tendency and ability of the gasoline blend to foul, damage or corrode gasoline storage facilities as well as the components of vehicle combustion and exhaust systems. These specifications include gum deposition, oxidation stability, colour, NACE corrosion and phosphorous levels.

Petroleum refineries are the main source of finished gasoline and blendstocks for oxygenate blending (BOBs). Ethanol represents approximately 5 volume percent (vol%) of the finished gasoline consumed in the EU.

To burn, liquid gasoline must be vaporised and mixed with oxygen (air). Since gasoline is a blend of hundreds of molecules with different characteristics, gasoline boils (vaporises) over a range of temperatures and must be blended in a way that vaporisation will occur over the entire range of engine operating temperatures. Specifications which measure and control the vaporisation performance of gasoline include:

- Reid vapour pressure (RVP);
- distillation;
- drivability index; and
- vapour-liquid ratio.

Apart from the volatility characteristics mentioned above, the other important fuel quality to be considered is ignition quality. The octane number of a fuel is a measure of its resistance to auto-ignition. Gasoline spark-ignited engines need a high-octane fuel to avoid knocking; this contrasts with diesel engines which rely on auto-ignition and therefore require a low-octane (or high cetane number) fuel. The octane number of a fuel is measured in a special test engine known as a CFR engine, which is a single-cylinder test engine with variable compression ratio dating from 1928. Although the test has been progressively improved over the years, the basic engine configuration and test conditions remain the same. Tests in the early 1930s demonstrated that the knocking behaviour of fuels in vehicles of that era did not correlate with the measured Research Octane Number (RON), therefore a new, more severe Motor Octane Number (MON) was developed. Both methods are still in use today, although in modern passenger cars the relevance of MON is more questionable. A fuel's octane number is determined by comparing and extrapolating its performance in the engine with blends of pure compounds: iso-octane, defined as 100 octane; and n-heptane, defined as having a zero octane number.

¹ See Annex 1: https://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2009:140:0088:0113:EN:PDF



Gasoline octane, particularly the RON, is a critical consideration in the design of today's engines which are optimised for particular octane numbers. A number of studies carried out over the years by the engine manufacturers as well as Concawe members have suggested that engines with higher compression ratios realise improvements in engine performance and efficiency, but they require gasoline with higher octane ratings. A more recent modelling and vehicle study carried out by Concawe has confirmed the results of previous studies and will be the subject of a separate article in the next Concawe *Review*.

Background

The long-term goal of the EU is the decarbonisation of transport.² To achieve this, vehicle efficiency targets for passenger cars and light commercial vehicles have been put in place for 2020/21 and were extended until the 2030 horizon at the end of 2018. Early in 2019, Europe agreed to introduce vehicle CO_2 efficiency targets for the heavy-duty vehicle (HDV) segment for the first time. Additionally, the Renewable Energy Directive II extends the requirement to use sustainable renewable fuels or energies in the transport sector until 2030.

To ensure that liquid fuels can continue to play their vital roles in the future of road transport, FuelsEurope has developed the 'Vision 2050'³ with the objective of demonstrating that the carbon intensity of liquid fuels can be reduced, and therefore, together with vehicle efficiency improvements, contribute to a reduction in GHG emissions from transport. In this context, high-octane petrol (HOP) is one of the many possible improvements that could play a role.

Although vehicle efficiency targets are formulated in a technology-neutral manner, manufacturers do not have many options to ensure compliance, in particular for passenger cars. This is mainly due to the inflexibility in the CO_2 vehicle standards methodology (tank-to-wheels), based on type approval regulations, which do not recognise the fuel contribution. Neither bio-components nor other fuel improvements can count towards the efficiency target.

² European Commission (2018). A Clean Planet for all. A European long-term strategic vision for a prosperous, modern, competitive and climate neutral economy. https://ec.europa.eu/clima/sites/clima/files/docs/pages/com_2018_733_analysis_in_support_en_0.pdf

³ FuelsEurope (2019). *Vision 2050. A pathway for the evolution of the refining industry and liquid fuels.* https://www.fuelseurope.eu/wp-content/uploads/DEF_2018_V2050_Narratives_EN_digital.pdf

Gasoline demand and EU trade balance

EU-28 gasoline demand (consumption) is around 79 Mt/y (2014 data as used for this study) for the fossil content (the ethanol added after the refinery fence being ~5% of the finished grade on average in the EU-28). This demand is expected to decrease significantly towards 2030.

As can be seen from Figure 1, gasoline demand is anticipated to fall from 79 Mt to 52 Mt — a decrease of 34%. This is partly due to the lower efficiency, leading to higher CO_2 emissions, compared to diesel engines. Therefore, every effort to improve gasoline quality needs to be considered from the perspective of an inevitable decline in demand. This decline may be minimised/reduced by quality improvements required to enable an increase in gasoline engine efficiency, which should provide a potential reduction in CO_2 emissions compared to using standard 95 and 98 grade gasoline fuels. Any cost assessment will be a challenge, since it should not be based on a constant demand for fossil fuel, and an accurate assessment of the impact on demand over a long period (to 2030 as for this study⁴) following a product quality change is not rationally possible.



Figure 1: Reconciliated demand for petroleum products in the EU-28, 2014 and 2030 (Mt/year)

⁴ 2030 demand scenario from Wood Mackenzie forecast



The overall net trade in transportation fuels is somewhat unbalanced, with a large amount of the gasoline produced in Europe being exported (nearly 50 Mt) and an equivalent quantity of middle distillates (diesel and jet fuels) being imported. Gasoline and gasoline components are global commodities that are frequently traded between regions and countries. The EU market is particularly integrated with other markets in the US Gulf Coast and in West and North Africa.





Study objective and main assumptions

The objective of this study was to assess the feasibility and impact of a HOP fuel grade in the European (EU-28 + 3) refining system as a contribution to improvements in vehicle efficiency. The work was undertaken using Concawe's modelling tools and capabilities, and attempted to answer the following questions:

- What is the overall feasibility for the refining system, and at which RON?
- What would be the impact on CO₂ emissions from refining and cars (well-to-wheels)?
- What would be the cost impact for refining?

Many different cases were investigated, but for simplicity, only the main case is presented in this article. The simulated HOP is RON 102. For the demand structure, across the EU, the current share is 90% RON 95 grade and 10% RON 98. The results are shown for an estimated 2030 demand structure with 50% HOP (the remaining 50% being RON 95). The biofuel content remains constant at the current level of 3.4% energy (equivalent to an average E5 grade).

As the engine is tuned for a dedicated higher octane, efficiency improves. For this study, and based on previous Concawe research, a 1% efficiency increase per 1 point of RON increase is assumed. The demand for travel being constant decreases the demand for HOP (i.e. for the same passenger-km or weight-km, less energy is required by the transport system, and hence the 'domestic' demand decreases). For the case developed in this article, the decrease in demand is 6.4% (this results in a 40% switch in demand from RON 95 to RON 102 HOP, and a 10% demand switch from RON 98 to RON 102 HOP). Fossil gasoline production remains constant, and domestic volume reduction due to increased engine efficiency can be compensated by additional exports to other markets.

2030 scenario modelling results

Linear programming (LP) is a mathematical tool that helps the decision-making process. LP consists of an optimization driven by an economic objective function (profit maximization or cost minimization), where variables involved are constrained by means of linear equations. Concawe has a unique LP model which includes all the individual process unit capacities of the EU refining system. With more than 25 years' experience in modelling, this is the most relevant tool for assessing refinery operations.

Overall gasoline pool results

To meet the new quality demand, the model increases the octane rating of the gasoline pool. This is done by a combination of factors, including increasing oxygenate imports (MTBE), decreasing naphtha blending to gasoline (low octane component, more exports of petrochemicals), and increasing the use of alkylate (unit optimisation). For the reformer, the model increases severity, resulting in lower reformate yield but with a higher octane. To avoid a result based on the economic incentive to incorporate oxygenate (which is an unknown factor for 2030) in the gasoline pool, the data are shown for a 'high oxygenate case' (imported component) and a 'low oxygenate case' (more octane coming from the refinery).

Table 1: Overall gasoline pool results

	HOP RATIO	POOL RON ⁵	МТВЕ	ALKYLATE	NAPHTHA
Base case	10% (98)	94.6	1.1%	9.3%	5.4%
HOP RON 102 High oxygenate case	50%	95.8	5.9%	13.5%	1.3%
Low oxygenate case	50%	95.8	4.4%	14.9%	1.0%

⁵ The gasoline pool produced by the model consists of RON 95, RON 98 (base case) and low-octane export grade (RON 91).



Regional balances

To understand the behaviour of different refinery configurations, the results were extracted for the nine regions embedded in the LP model. The purpose was not to forecast or predict actual future local trade flows, but to provide a view on how different refinery configurations may react to a higher octane demand for EU gasoline. Figure 3 shows the evolution for each region, for the 2030 HOP RON 102 case for the light oxygenate pathway compared with the 2030 base. The regions have a different behaviour, some of them importing and others exporting HOP. However, in comparison to the total demand, these interregional trade flows remain limited. Each of the simulated refineries manage to adapt and produce some of the HOP demand.



Figure 3: Regional balances for the 2030 HOP RON 102 case (light oxygenate pathway) vs 2030 base case

The Central and Southern EU model refinery configurations show the highest imbalance between demand and production. However, if the constraints on intermediate trade flows and blending of oxygenates were to be relaxed, this would lead to a more closely balanced situation for these sections of the model.

Sensitivity case

In the standard cases, increasing unit capacities through investment was not allowed as the choice was to push the refining system based on existing capacities. However, in a clear and foreseeable environment, investing to adapt refinery yields to local demand is a strategic opportunity that some refiners may chose. In this case, giving the freedom to the model to invest and increase process units capacities results in a significant evolution, including an increase in alkylation units, and reformer and isomerisation recycling. The direct impact is on MTBE imports, which go back down to the level in the base case (1.1%).

Direct CO₂ emission balance

Table 2 shows the CO_2 balance taking into account the refinery, the vehicle emissions from cars and the oxygenate well-to-tank (WTT) impact. The key hypothesis for the impact on 'cars' is a 1% efficiency increase per 1 point of RON increase. Different engine testings are currently ongoing. In the case of a lower value, the impact on 'cars' is proportional. For example, at 0.50% efficiency/point of RON, the CO_2 balance goes from -5.1 Mt/y to -2.55 Mt/y.

Table 2:	CO ₂ balance v	s 2030 base case	(Mt/year)
----------	---------------------------	------------------	-----------

	REFINING	CARS	OXYGENATE IMPACT (WTT)	TOTAL CO ₂
Base case	Base	Base	Base	-
HOP RON 102 High oxygenate case	-0.9	-5.1	+1.6	-4.4
Low oxygenate case	-0.5	-5.4	+1.0	-4.9

Looking at Table 2 in more detail, the evolution of 'Refining' + 'Oxygenate impact (WTT)' is +0.7 and +0.5 MtCO₂/year for the 'high' and 'low' oxygenate cases, respectively. It could be deduced that the octane from the refinery system is less CO_2 -intensive than oxygenate production; however, the change vs base case is quite small (~1 Mt versus a total ~140 Mt for the refining system), hence it is more reasonable to consider that both pathways (refinery and oxygenate) are equivalent in terms of their CO_2 intensities.

The refining system is under higher constraints with regard to the gasoline units, but importing oxygenates allows a slight decrease in crude processing and hence lower CO_2 emissions. This decrease is compensated for by the carbon content of the oxygenate on a WTT basis.

Economics

To run HOP cost sensitivity cases, step changes in the HOP price differential versus the current RON 95 price are modelled. Two historical price sets were considered, one at a high Brent value (100 \$/bbl, 2014) and the second at low Brent (43 \$/bbl, 2016). This assessment was undertaken without process investment (this was only allowed in a sensitivity case as mentioned on page 45). For a better understanding and to provide confidence in the behaviour of the model, Figures 4 and 5 on page 47 show the curves for HOP RON 98 and RON 100. However, in this discussion, comment is only made on the RON 102 curve and results as this is the main case for the study.

HOP cost sensitivity - 2014 price set, Brent @ 100 \$/bbl

To reach 50% of the market demand (2030 hypothesis), the model needs an incentive of 17 \$/t and 53 \$/t for a RON of 98 and 102, respectively (see Figure 4). As expected, with the study being undertaken without process investment, the model reaches a plateau at different levels of domestic demand depending on the RON increase. Investments or innovative solutions/technologies would allow the model to reach 100% of domestic demand even for RON 102. Our estimation shows that the HOP RON 95 price differential is driven by the MTBE value for one third, and the remaining two thirds by other components.



Figure 4: HOP domestic demand % vs HOP-RON 95 price differential (2014 price set, Brent at 100 \$/bbl)

HOP cost sensitivity - 2016 price set, Brent @ 43 \$/bbl

At a lower Brent value, the incentives are quite different, being only 24 \$/t for HOP RON 102 (see Figure 5). In this case, the MTBE contribution to this price differential increased to about 50%.

For RON 102, at 50% of domestic demand, the break-even point (above RON 95) is worth between 7.5 and 3.5 \$/t/point of RON (2014 and 2016 price scenarios, respectively—see Figures 4 and 5, HOP RON 102 curve at 50% of domestic demand). Being a cost for refiners, this has to be compared to the octane value on the market, as the cost could potentially be recovered via market price differentials.





To appreciate the order of magnitude, it can be noted that the average historical octane value in the US Gulf Coast is estimated at around 12 \$/t/point of RON (2010–2017). Since gasoline is a commodity traded in a free and open market with multiple competing companies, the market price and product differential are the result of a supply/demand equilibrium. In this context, refiners cannot always pass their costs on to their clients, as there is no direct correlation between refinery costs and market value. Therefore, historical figures may be considered as an indication but in no way as a forecast.

Conclusion

This study recommends the endorsement of RON 102 as a pragmatic way forward for high-octane petrol in discussions with industry stakeholders.

The main takeaways from the HOP study are as follows:

- The set of assumptions in the LP modelling study demonstrate the feasibility of producing a HOP in the EU refining system, requiring either more oxygenates or investments in gasoline units.
- The evolution of the LP economical function is in the same order of magnitude as the historical octane value (USGC quotation).
- A significant reduction in CO₂ emissions is expected (refining process + combustion in ICEs at high compression ratio + oxygenate WTT).

Refiners have been improving fuel quality for decades and will continue to do so into the long-term future. The demand for cleaner and more efficient fuels is increasing, and the successful implementation of HOP would represent a significant contribution to climate change mitigation.