

Effects of LPG Fuel Formulations on Knock and Pre-Ignition Behavior of a DI SI Engine

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ABSTRACT

Due to their CO₂ reduction potential and their high knock resistance gaseous fuels present a promising alternative for modern highly boosted spark ignition engines. Especially the direct injection of LPG reveals significant advantages. Previous studies have already shown the highest thermodynamic potential for the LPG direct injection concept and its advantages in comparison to external mixture formation systems. In the performed research study a comparison of different LPG fuels in direct injection mode shows that LPG fuels have better auto-ignition behavior than gasoline. A correlation between auto-ignition behavior and the calculated motor octane number could not be found. However, a significantly higher correlation of $R^2 = 0.88 - 0.99$ for CR13 could be seen when using the methane number. One major challenge in order to implement the LPG direct injection concept is to ensure the liquid state of the fuel under all engine operating conditions. Especially at hot soak conditions, the critical point can be exceeded and the supercritical state can be reached. In this context SI combustion anomalies for LPG depending on the gas mixture components are largely unexplored. Therefore the study also focuses on investigations of the pre-ignition behavior of different LPG fuel formulations in liquid and supercritical state.

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INTRODUCTION

Despite the improvement of hybrid and battery electric vehicles the internal combustion engine remains the dominant source of propulsion in the upcoming decades and offers further development potential. For instance the usage of alternative fuels reveals further CO₂ reduction potential. As a short and midterm action the usage of gaseous fuels seems reasonable, particularly as the adoption to existing engine concepts is less complex compared to other alternative fuels such as advanced biofuels. Besides hydrogen, which is considered as a long term alternative, the two main representatives for gaseous fuels are commonly known as CNG (Compressed natural gas) and LPG (Liquefied petroleum gas). CNG mainly consists of methane whereas propane and n-butane are the main components of LPG. At phase transition from gaseous to liquid state these molecules undergo a significant volume reduction. This results in considerable benefits in terms of transportation and storage aspects. When CNG is liquefied, it is called LNG (Liquefied natural gas) but a higher amount of energy than for liquefying propane and n-butane is required due to a preferable vapor pressure behavior. Furthermore NG liquefaction requires very low temperatures below -160 °C, while LPG can become liquid at ambient temperatures just applying pressure in the magnitude of 10 bar. LPG is currently the most used

alternative fuel for vehicle application in Europe with an already adequate core infrastructure in place *[1]*. Main sources of which the LPG production is based on are the extraction of natural gas and oil, as well as oil refining processes. Due to worldwide increasing natural gas production, a strong supply growth of LPG is expected for the upcoming decades *[2]*. Furthermore, efforts are made in order to produce biogenic LPG either out of glycerin via catalytic hydration or catalytic cracking of waste grease and oil *[3]*. One major benefit of these alternative LPG production routes would be the compatibility with the already existing fuel infrastructure.

Using LPG as a fuel in spark-ignition engines reveals significant advantages. Due to a higher H/C ratio LPG allows a theoretical CO₂ reduction of approximately 10 % depending on the gas mixture compared to gasoline and based on constant engine efficiency. Most of the published studies investigate naturally aspirated, port fuel - liquid or gaseous - injected engine concepts and concede various emission reduction potentials to LPG fuels formulations, which are evaluated in several driving cycles *[4]*, *[5]*, *[6]*, *[7]* and well-to-wheel analyses *[7]*, *[9]*, *[10]*, *[11]*, *[12]*, *[13]*, *[14]*, *[15]*, *[16]*, *[17]*. The existing literature states a tremendous particle emission reduction when using LPG as a fuel, which is especially noteworthy facing

upcoming emission legislations for spark-ignition engines with direct injection /4/, /11/, /15/, /16/, /18/, /19/, /20/, /21/, /22/. Moreover, LPG allows a reduction of non-regulated emissions such as benzene acetaldehyde, formaldehyde and 1,3-butadien /6/, /21/, /23/.

However, important factors for high efficiency and further CO₂ reduction are the quality of the fuel being used and the engine concept. So far most of the LPG fuelled vehicles are bivalent concepts. Monovalent engine concepts offer the advantage to optimize the engine especially to the changed fuel properties and thus exploit the full potential of LPG engine technology. Compared to gasoline engines, dedicated LPG engines can then be operated at higher compression ratios with high thermal efficiencies due to high octane ratings of the hydrocarbons which LPG contains. Even if a RON is not officially standardized for LPG, for pure propane for example a research octane number (RON) of 112 has already been found in very early studies /24/, /25/. In Europe the current fuel quality standard EN 589 for LPG fuels does not consider any RON /26/. Only a minimum motor octane number (MON) of 89 is specified. According to a calculation procedure, the mass fractions of the contained molecules are divided into groups with respect to their number of carbon atoms and determine the MON of the fuel. For an increased usage of LPG fuels in the future, the accuracy of this method needs to be reviewed with regard to modern engine

technology. There is still little knowledge about the suitability of different LPG fuel formulations for the application to modern spark-ignition TC-DI engines, their potential to increase engine efficiency for stoichiometric combustion systems and combustion anomalies depending on the gas mixture components and the state of the fuel.

This paper is believed to be the first study on experimental investigations of the auto-ignition behavior of LPG fuel formulations in liquid and supercritical state burned in spark-ignition engines with direct-injection. On the one hand, the investigations focus on the knock tendency, the combustion characteristics and the regulated emissions of different LPG mixtures burned in a modern spark-ignition turbocharged series production engine with liquid direct injection. On the other hand, the pre-ignition behavior of LPG mixtures in liquid and supercritical state is studied on a direct-injection spark-ignition single cylinder research engine. Comparisons for both auto-ignition phenomena are made to results obtained with RON 95 E5 on the corresponding engine. In the following sections, the experimental setup and procedures for tests conducted on both engines are briefly discussed, followed by the results of the performed tests. Finally, major conclusions from this work are drawn in the last section.

Table 1. Fuel properties

	RON 95 E5	LPG 1	LPG 2	LPG 3	LPG 4	LPG 5	LPG 6	LPG 7	LPG 8
Motor octane number (EN ISO 5163, EN 589)	86.3	95.9	86.7	93.2	94.6	94.6	89.4	93.3	91.5
Methane number (DIN 51624 / AVL method)	-	32.3	18.4	21.4	17.6	28.5	26	30.7	15.2
Density (15 °C) / kg/m ³	749	508	566	548	553	526	515	520	560
Carbon mass fraction / %	84.43	81.73	83.45	82.30	82.45	81.99	83.68	82.25	82.75
Hydrogen mass fraction / %	13.22	18.28	16.56	17.70	17.59	18.01	16.32	17.75	17.25
Ethane mass fraction / %	-	0.14	0.13	0.16	0.13	0.28	0.4	0.8	0.1
Propane mass fraction / %	-	98.98	28.61	38.22	25.83	67.39	48.3	82.1	16.1
Propene mass fraction / %	-	0.17	0.05	0.24	0.16	0.18	50.2	0.2	8.2
n-Butane mass fraction / %	-	0.16	30.46	41.57	25.82	21.21	0.4	2.3	50.7
iso-Butane mass fraction / %	-	0.55	3.61	19.49	47.68	10.80	0.7	1.6	24.6
C4 olefins mass fraction / %	-	-	36.84	0.13	0.08	0.03	-	13.0	0.2
n-Butene mass fraction / %	-	-	19.92	0.02	0.02	-	-	7.9	
iso-Butene mass fraction / %	-	-	0.27	0.06	0.04	0.03	-	0.3	
cis-2-Butene mass fraction / %	-	-	4.41	0.02	-	-	-	1.3	
trans-2-Butene mass fraction / %	-	-	12.24	0.03	0.02	-	-	3.4	
C5 mass fraction / %	-	-	0.31	0.19	0.44	0.10	-	0.1	0.1
Spec. enthalpy of vaporization at $\lambda = 1$ / kJ/kg _{air}	~29.5	27.0	24.8	24.1	23.9	25.2	28.2	26.1	23.9
Stoichiometric air requirement / 1	14.17	15.64	15.21	15.49	15.45	15.56	15.19	15.52	15.40
Lower heating value / MJ/kg	41.99	46.35	45.75	45.96	45.86	46.17	46.08	46.20	45.82
Mixture heating value (DI, $\lambda = 1$) / kJ/m ³	3509	3510	3561	3513	3515	3512	3591	3525	3522

FUELS

Table 1 summarizes the most relevant properties of the fuels investigated in this study. A conventional RON 95 E5 according EN 228 /28/ with octane numbers determined on a CFR engine in accordance to EN ISO 5163/64 /29/, /30/ serves as reference fuel for all investigations. All LPG fuels are market relevant fuels according EN 589. Their motor octane number is calculated using this applicable standard while the methane number is calculated in accordance to DIN 51624 /31/ established in /32/, /33/, /34/ in 1968.

The gaseous test fuels are selected in order to cover a wide range of characteristic numbers describing the knocking resistance. LPG 1, with a purity grade of 99 % propane, shows the highest knock characteristic numbers (methane number and motor octane number). LPG 2, a gas mixture with high olefin content, holds a motor octane number slightly below the minimum acceptance level of DIN EN 589 and close to the MON of the reference fuel RON 95 E5. In order to increase the octane rating, the two components with the highest MON impact (LPG 3: propane; LPG 4: iso-butane) are blended into a similar base composition as LPG 2 instead of olefins. Despite their different formulation, LPG 4 and LPG 5 have the same motor octane number. LPG 5 represents a typical winter fuel, LPG 6 consists of propane and propene, whereas LPG 7 and LPG 8 are homologation fuels according /27/ with high propane and high butane content. Comparing the properties, the lower density of all LPG fuels can be noted. While the heating value is higher for the LPG fuels, the lower densities lead to lower volumetric heating value in comparison to conventional gasoline. Due to high vapor pressures high propane and especially high propene content is reflected in high enthalpies of vaporization approximated via Clausius-Clayperon equation. The stoichiometric air requirement of all LPG fuels is similar to conventional fuel compared to other gaseous fuels. The mixture heating values indicate that similar cylinder charges will be required to achieve the same power output.

In order to investigate which characteristic number describes the knocking behavior best, LPG 1 to LPG 5 are being used as fuels for measurements on the series production engine. LPG 5 to LPG 8 is burned in the single cylinder engine to investigate the pre-ignition behavior.

EXPERIMENTAL SET-UP

Series Production Engine

Hardware

As a modern downsizing concept with a state of the art level of specific power, the 1.6 l inline turbocharged gasoline direct injection engine of the Ford Motor Company was chosen. A summary of the technical data of the engine is given in **Table 2**.

The engine is quantity controlled with stoichiometric combustion system and conventional valve train. Variable cam phasing on intake and exhaust side is applied to enable scavenging operation under low speed full load conditions and improved part load efficiency by means of internal exhaust gas recirculation strategies. The four valve combustion chamber roof with central arranged injector and spark

plug position engine lengthwise reveals a compression ratio of CR = 10 for the base version. For a more comprehensive analysis of the octane requirement and knock behavior of the LPG fuels, the compression ratio is increased up to CR = 13, utilizing three different piston designs. The piston crown design for each compression ratio is depicted in the following figure.

Table 2. Series production engine hardware specification

Bore / mm	79
Stroke / mm	81.4
Number of cylinders	4
Cylinder displacement / cm ³	399
Stroke/bore ratio / 1	1.03
Valves per cylinder	4
Maximum Torque / Nm	240
Compression ratio / 1	10; 11.5; 13
Injection system	Bosch Multihole
Maximum fuel pressure / bar	150



Figure 1. Piston designs

The intake ports are designed as high tumble ports with an increased charge motion level and optimized flow coefficients in order to enable best mixture preparation conditions even under difficult boundary conditions /35/. The engine is boosted by a monoscroll turbocharger with wastegate control. The intake air temperature is controlled by an intercooler.

For LPG direct injection the conventional components of the gasoline high pressure injection system are used (high pressure pump, fuel rail, fuel injectors). No modifications of the fuel-carrying components have been made. An additional middle pressure pump has been applied upstream the high pressure pump in order to precompress the LPG to a pressure level of 15 to 35 bar and keep it in liquid phase.

Test Bench Instrumentation

For the thermodynamic measurements the cylinder pressure is measured with Kistler 6041 pressure transducers mounted flush in the combustion chamber roof of each cylinder. Sampling is performed via Kistler 5011 charge amplifiers and a FEV combustion analysis system (CAS) in a resolution of 0.1° CA between 30° CA BTDC and 70° CA ATDC and 1° CA in the rest of the cycle. The higher resolution around TDC is used to enable knock detection. Dynamic intake and exhaust gas pressures are measured with Kistler 4045 A5 pressure transducers and sampled in 1° CA resolution. In total, 200 consecutive cycles are measured. Measurements of static pressures and temperatures are performed with conventional pressure transducers and thermocouples during an averaging interval of 30 s. Oil and water conditioning systems allow steady-state operation. The pressure upstream the air filter and downstream the air filter is measured.

controlled to 1013 mbar. The engine was coupled to an electric dynamometer to maintain the desired engine speed with an accuracy of $\pm 1 \text{ min}^{-1}$.

The gaseous exhaust gas composition is determined from a partial mass flow of exhaust gases which is sampled downstream the turbocharger and upstream the three way catalyst. The exhaust gas sample is fed to the following emission analyzers via a transfer line heated to 193 °C. Regulated and unregulated emissions, i.e. CO, CO₂, HC and NO_x are measured at engine exhaust via these sampling systems:

- HC: Flame ionization detector (Rosemount NGA 2000)
- O₂: Paramagnetic oxygen analyzer (Rosemount NGA 2000)
- CO: Infrared gas analyzer (Rosemount NGA 2000)
- CO₂: Infrared gas analyzer (Rosemount NGA 2000)
- NO_x: Chemiluminescence analyzer (Eco Physics 700 EL ht)

The flame ionization detector is calibrated with C₃H₈. Particle emissions are measured close to the exhaust gas sample extraction point using a smoke meter (AVL 415s).

Experimental Procedure

An engine speed variation from 800 to 6000 1/min in warm conditions, with linearly increased intake air temperature from 30 °C at 1000 1/min to 55 °C 6000 1/min, is used to study the fuel influence on engine efficiency and to determine knock sensitivity. Tests are performed in homogenous operation mode with single injection into the intake stroke and typical valve timings for a turbocharged engine using scavenging at full load. Engine calibration settings such as fuel rail pressure as well as cam and injection timing correspond to the production calibration, vary versus engine speed and are kept constant for all fuels. Spark timing is adjusted for each fuel to keep the center of combustion (MFB50) constant at 7.5° CA ATDC $\pm 1^\circ$ CA. It is set at the knock limit for operation points where the optimal combustion phasing cannot be realized. The knock limit is defined via the cylinder pressure indication system by the occurrence of combustion cycles with peak-to-peak knock amplitudes of engine speed divided by 1000 1/(min·bar). The exhaust gas temperature upstream turbine is limited to 1000 °C for these investigations.

Research Engine

Hardware

For the pre-ignition investigations, a homogeneously operated direct injection spark ignition single cylinder research engine was used. Injector and spark plug are placed in central cross position in the combustion chamber roof, which means that the spark plug is

installed between the exhaust valves, while the injector is installed between the intake valves, as depicted in the sectional view of the cylinder head in [Figure 2](#).

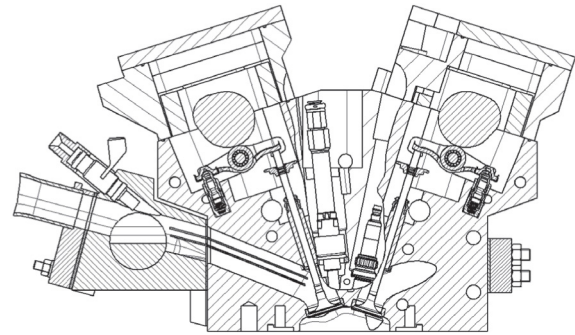


Figure 2. Sectional view of cylinder head

The intake ports are designed as symmetrical filling ports to minimize the charge motion and thus, raising the likeliness of the occurrence of pre-ignitions. If needed the tumble ratio can be varied in two steps by an additional tumble flap. The following [Table 3](#) summarizes the most important engine parameters.

Table 3. Research engine hardware specification

Bore / mm	75
Stroke / mm	82.5
Displacement / cm ³	364
Number of valves	4
Max. charging level / bar (abs.)	3.5
Compression ratio / 1	10.93
Cylinder peak pressure / bar	170
Injection system	Bosch HDEV 5.2
Maximum fuel pressure / bar	200

The direct-injection gasoline injector is a six-hole solenoid actuated injector, which was found to be optimal for the engine in terms of oil dilution behavior, mixture homogenization and thus creating an important pre-condition in order to provoke gas phase pre-ignitions. Since pre-ignitions can be induced by oil droplets, the blow-by gas is not returned to the intake manifold, but it is discharged alternatively. The used lubricant oil is denoted Mobil Super™ 2000 X1 10W-40. In order to avoid glow-ignitions caused for example by the ground electrode a relatively cold prototype spark plug with a short-nosed insulator is used. Concerning the fuel system the utilized high pressure fuel pump is volume flow controlled. To reach the supercritical state, the fuel is heated up by an electrical heater mounted to the complete fuel line downstream the high pressure pump including the fuel rail and pipes upstream the injector. For fuel changes, the system was completely drained, purged with air, and flushed with the new fuel to minimize possible contamination by other fuels.

Test Bench Instrumentation

The single cylinder engine instrumentation is similar to the one used for the series production engine and includes only minor differences, such as the used cylinder pressure transducer Kistler A6043 A100.

Identical pressures upstream of the throttle flap and in the exhaust manifold are applied to simulate turbocharging. In total, 500 consecutive cycles are measured ten times to reach a high level of statistical confidence of pre-ignition events. The engine was coupled to an eddy-current brake and an electric dynamometer to maintain the desired engine speed with an accuracy of $\pm 1 \text{ min}^{-1}$, regardless of the engine load. The intake air mass flow is measured with an ultrasonic air mass meter.

Experimental Procedure

The investigation of the pre-ignition behavior focuses on gas phase pre-ignitions triggered by the thermal in-cylinder conditions, together with chemical reactivity of any ignitable substances. In this case, the in-cylinder pressure and temperature history determine the auto-ignition behavior significantly. Therefore boost pressure sweeps at high intake air temperature were investigated for LPG 5 to LPG 8 and compared to the reference fuel. The methodology was already established in previous work where numerous tests were made to find a special operating point with pre-ignitions, but with limited intensities [36]. The selected settings are summarized in Table 4.

Table 4. Single cylinder engine calibration settings

Engine speed / (1/min)	1500
IMEP / bar	11 - 20
MFB50 / ° CA ATDC	44 - 45
Fuel pressure / bar	150
Start of injection / ° CA BTDC	variable
End of injection / ° CA BTDC	240
IVO (1mm) / ° CA ATDC	10
EVC (1mm) / ° CA BTDC	10
Relative air/fuel-ratio / 1	1
Air temperature in runner / °C	102
Coolant and oil temperature / °C	110

The engine speed of 1500 1/min is characteristic for the low end torque and particularly critical with regard to pre-ignition and combustion stability. In order to have equal combustion phasing and residual gas temperatures, a constant negative valve overlap and a constant center of combustion was chosen. The late combustion phasing results in an increased period of homogenization and more available time for the mixture to reach its auto-ignition delay due to pre-reactions taking place. Pre-investigations had shown that the additional tumble flap in the intake manifold had to be deactivated in order to provoke pre-ignition events at boost pressure below 3 bar also for LPG fuels with high auto-ignition resistance.

Thermodynamic Analysis

Combustion delay, combustion duration and the center of combustion are determined for every operation point via the FEV Combustion Analysis System following the Rassweiler and Withrow approach [37]. In order to evaluate the in-cylinder temperature, a more detailed

thermodynamic analysis is performed for some operation points, using the Three-pressure-analysis (TPA) function of the commercial software GT Power, version 7.4.0, from Gamma Technologies. This model is able to account for the effects on the in-cylinder charge caused by direct injection. Fuel properties are considered according to the fuel analysis. The evaporation heat of the LPG fuels is described by NASA polynomial functions. Moreover, it features a two-zone temperature model to determine the temperature in the burned as well as in the unburned gas.

RESULTS

Knock Behavior

At first the differences regarding knock behavior and the potential of LPG fuel formulations regarding efficiency increase will be discussed for an engine speed variation under full load conditions for the base compression ratio of the series production engine. Thus, effects of combustion chamber design changes on combustion and emission behavior are excluded. In a second step the efficiency potential of an increased compression ratio will be investigated.

As depicted in Figure 3, all LPG fuel formulations achieve the same engine torque as the reference fuel RON 95 E5. The auto-ignition characteristics are significantly enhanced by all LPG fuels compared to the reference gasoline fuel. This leads to considerably advanced combustion phasing in terms of MFB50, along with positive effects on specific fuel consumption, combustion stability and enrichment demand for component protection. As a result, a maximum fuel consumption reduction at $n = 6000 \text{ 1/min}$ of approximately 17 % and a maximum brake specific efficiency of 36.3 % at $n = 3000 \text{ 1/min}$ are achieved. Thereby an improvement of 6.7 % in efficiency compared to the reference fuel RON 95 E5 is gained. The highest efficiency increase arises for LPG 1 and LPG 5 at $n = 5000 \text{ 1/min}$ with 26 % compared to gasoline. Due to the low knock tendency of LPG 1 (99 % propane) and LPG 5 (70 % propane), those fuels achieve the limitation for the mean peak cylinder pressure of 110 bar already at $n = 1750 \text{ 1/min}$. Heat delay and heat duration are decreased compared to the reference fuel. Both characteristics are slightly shorter in comparison to RON 95 E5. On the one hand this can be possibly explained with the high volatility of the LPG fuels and therefore excellent mixture preparation properties. Consequently different thermal in-cylinder conditions during and after injection due to the different evaporation behaviors of the fuels also affect the heat delay and heat duration. On the other hand a potential impact of burn velocity can be taken into consideration. In a stoichiometric mixture the laminar burning velocity for example of pure propane is higher than for conventional gasoline fuel at standard ambient temperature and pressure [38]. Due to the fact that the investigated LPG fuels contain several hydrocarbons, the burn velocities vary from fuel to fuel. Nevertheless, LPG 1 and LPG 5 both fuels with high propane content show the lowest heat duration in Figure 3. However, the most advanced combustion phasing of these fuels is evident throughout the entire engine speed range at full load conditions.