

# NEXT GENERATION KNOCK CHARACTERIZATION

V.M. van Essen\*, S. Gersen, G.H.J. van Dijk and H.B. Levinsky  
DNV GL Oil & Gas, P.O. Box 2029, 9704 CA Groningen, the Netherlands

## Abstract

The globalization of the gas market is increasing the diversity of the supply of natural gases. As a rule, "new" gases have different chemical compositions than the gases traditionally distributed. However, different compositions can have different combustion properties, which can lead to unacceptable changes in the safety or fitness-for-purpose of end-use equipment.

Gas-fuelled spark-ignited internal combustion engines are known to be sensitive to variations in fuel composition because of the possible occurrence of engine knock, caused by autoignition of unburned fuel mixture, the so-called end gas, ahead of the propagating flame in the cylinder.

The knock sensitivity of gas engines is a limiting design factor for power output, efficiency and the acceptable variation in fuel gas composition. Empirical methods such as a methane number, which often make use of a standard test engine, have been developed to classify natural gases with respect to their knock resistance. Since the autoignition behavior of fuels and the relative differences in autoignition between fuels depend strongly on the specific regime of temperature and pressure, the generality of the method for engine conditions other than those existing in the test engine is uncertain. Furthermore, empirical methods provide only limited insight in the physical/chemical origins of knock in engines, and are therefore of limited utility for the optimum design for knock-free engine operation when using a wide range of fuels. A correct and accepted method for characterizing knock resistance is not only important for the existing pipeline market but is also an essential enabler for the success of the emerging market for liquefied natural gas (LNG) as a transport fuel. Rather than rely on the empirical methods using gas mixtures and "standard" engines traditionally employed for this purpose, we have derived a method based on the combustion properties of the fuel mixtures, themselves. In this paper we describe the model and compare its predictions with the results of experiments on our fixed-speed, medium-BMEP gas engine using the following gas mixtures: Dutch Natural Gas (DNG), DNG/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>, DNG/H<sub>2</sub>/CO, DNG/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>/H<sub>2</sub>, CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>, CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>, CH<sub>4</sub>/i-C<sub>4</sub>H<sub>10</sub>, CH<sub>4</sub>/n-C<sub>4</sub>H<sub>10</sub>, CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>, CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>/N<sub>2</sub> and CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>/CO<sub>2</sub>.

The core of the knock model described in this paper is the computation of the autoignition delay time of the compressed end-gas during the engine cycle for a given fuel. Autoignition of the end gas is critically sensitive to the pressure and temperature during the burn period, changes in the heat capacity of the fuel-air mixture, variations in initial pressure arising from changes in heating value and changes in the "phasing" of the combustion process with varying fuel composition. All these effects are incorporated into an integrated model for characterizing knock.

Using the integrated model, a propane based scale for knock resistance has been derived. This propane-based scale expressed as a Propane Knock Index (PKI), assigns the knock resistance of a given gas to an equivalent methane/propane mixture. The predicted knock resistance using this method shows excellent agreement with that given by the measured Knock Limited Spark Timing (KLST), and is within the uncertainty of the measurements for all mixtures studied.

## 1. INTRODUCTION

One of the consequences of the increasing diversity of pipeline natural gases, the growing interest in using LNG as a transportation fuel and the introduction of sustainable fuels such as hydrogen into the natural gas infrastructure, is that gases with significantly different composition can be or will be traded and distributed. The introduction of these "new" gaseous fuels may result in the occurrence of engine knock, since most gas engines are developed and adjusted for traditionally distributed (natural) gases,

Knock phenomena are caused by autoignition of unburned fuel mixture, the so-called end gas, in the cylinder before the mixture is completely consumed by the propagating flame. Mild engine knock increases fuel consumption and pollutant emissions, while severe knock can physically damage the engine [11], and should thus be avoided. The traditional methods for characterizing the knock resistance of gaseous fuels such as the methane number developed by AVL [2], in which the knock propensity of a given fuel is compared with an equivalent methane/hydrogen mixture, suffers from a number of

shortcomings [3, 33]. Perhaps most apparent of these is that the number is attached to the behavior of an individual engine under stoichiometric conditions, while the actual diversity of installed designs is great, and modern machines tend to operate substantially fuel lean and at higher pressures. Since the autoignition behavior of fuels and the relative differences in autoignition between fuels depend strongly on the specific regime of temperature, pressure and stoichiometry [e.g. 4-17] the generality of the method for engine conditions other than those existing in the test engine is uncertain. In addition, the suitability of hydrogen as a reference gas has been disputed [3, 18, 33] as well as the treatment of butane and higher hydrocarbons [19]. As such, the necessity of having a correct and unambiguous method to characterize the knock resistance of the variety of fuels for the variety of engine types in the market has become urgent in recent years.

Rather than rely on empirical methods using gas mixtures and “standard” engines traditionally employed for this purpose, we have derived a fundamentally sound method to characterize gases for their knock resistance based on the combustion properties of the fuel mixtures themselves. In this method, engine knock is predicted by modeling autoignition of the compressed end gas during the combustion cycle. Since the autoignition of the end gas is critically dependent upon the pressure and temperature history of the unburned mixture during the combustion cycle, the model takes into account the changes in in-cylinder pressure and temperature experienced by the end gas upon changing gas composition [20]. In this paper we outline the principles underlying the method, and apply it to predict the performance of the DNV GL lean-burn test engine for the following gas mixtures: Dutch Natural Gas (DNG), DNG/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>, DNG/H<sub>2</sub>/CO, DNG/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>/H<sub>2</sub>, CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>, CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>, CH<sub>4</sub>/i-C<sub>4</sub>H<sub>10</sub>, CH<sub>4</sub>/n-C<sub>4</sub>H<sub>10</sub>, CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>/C<sub>3</sub>H<sub>8</sub>, CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>/N<sub>2</sub> and CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>/CO<sub>2</sub>. Further, we demonstrate the veracity of the predictions experimentally.

## 2. EXPERIMENTAL SETUP

The phasing and KLST experiments are performed in DNV GLs combustion laboratory using a 208 kW 1500 rpm lean-burn ( $\lambda=1.5$ ) turbocharged, intercooled 6-cylinder gas engine designed for CHP duty [18, 20, 33-35]. We remark here that this CHP system maintains constant equivalence ratio, engine speed and power output. The engine management system and additional instrumentation provided precise adjustment, monitoring and registration of all relevant engine settings and process conditions. Cylinder pressure indication and post-processing was done using Kistler type 6052 piezoelectric pressure sensors and Kistler type 5011 charge amplifiers connected to a Smetec Combi-Pro indication system. A crankshaft-mounted pulse generator provided 0.1° CA resolution for the cylinder pressure data acquisition. The Combi-Pro system was also used for live detection of borderline knock in the Knock limited Spark Timing (KLST) experiments. Borderline knock was defined here as the occurrence of maximum one (cluster of) knock event(s) within a steady-state test run of roughly 15 minutes. Threshold settings used were 2 bar for the amplitude. A knock event involves exceeding the 2 bar threshold set point for the maximum amplitude of the pressure oscillations in the high-pass-filtered cylinder pressure signal within a window of 30 consecutive combustion cycles.

During the experiments, fuel for the test engine was delivered by a gas mixing unit. This unit allows on-stream variation of the fuel gas composition by independent adjustment of the flow rates of up to six source gas streams, up to a capacity of ~4 MW. The composition of DNG is listed in Table 1. The fuel compositions used in the experiments are shown in Table 2. All mixture compositions were verified by gas chromatography.

**Table 1. Composition of Dutch natural gas used (in mole %).**

CH <sub>4</sub>	81.76	i-C <sub>5</sub> H <sub>12</sub>	0.03
C <sub>2</sub> H <sub>6</sub>	3.01	C <sub>6</sub> H <sub>14</sub> <sup>+</sup>	0.07
C <sub>3</sub> H <sub>8</sub>	0.42	He	0.05
n-C <sub>4</sub> H <sub>10</sub>	0.08	N <sub>2</sub>	13.48
i-C <sub>4</sub> H <sub>10</sub>	0.07	CO <sub>2</sub>	1.02
n-C <sub>5</sub> H <sub>12</sub>	0.02		

Once the composition of the fuel/air mixtures at equivalence ratio  $\lambda=1.5$  and the other relevant cylinder parameters are set, the pressure traces of the gases under non-knocking condition, needed to test the two-zone thermodynamic model discussed below, are measured at a constant spark timing of 14° before top dead center (BTDC). Subsequently, the spark timing was gradually varied up to the point of the onset of borderline knock to determine the KLST.

### 3. KNOCK MODEL

#### 3.1 Thermodynamic model

To predict the influence of fuel composition on the changes in the phasing of the combustion in our gas engine, we developed a conventional two-zone thermodynamic model [1]. A detailed description of this thermodynamic model can be found elsewhere [18, 20, 34]. Briefly, in this one-dimensional model the combustion chamber is divided into a zone consisting of unburned gases and a zone with the burned gases separated by an infinitely sharp flame front. In the model we assume that no heat exchange occurs between the two zones during the entire engine cycle, and that the pressure is uniform throughout the cylinder. All gases are considered as ideal gases and the components in the zones are homogeneously mixed. The enthalpy changes of the gases flowing in and out of the cylinder are neglected in the model. The input data needed for the model are the engine geometry, in-cylinder conditions (P, T) at closure of the inlet valve, operating conditions such as spark timing, air factor, humidity and the fuel composition.

The simulation is based on solving the time dependent state of the two zones in the combustion chamber using the conservation equations for mass and energy, and the ideal gas equation of state. Until the time of ignition and after the mixture is completely burned the mixture is simulated as a single zone. Immediately after spark ignition the burned zone is created. The combustion process is simulated using the approach proposed by Chmela [26] where the mass burning rate is related to the laminar burning velocity and a fit parameter ( $C_{model}$ ) which was used to account for the turbulence effects in the burning rate model. In previous work it was found that a single model parameter, independent of the gas composition, is sufficient to predict the effect influence of the fuel composition on the pressure profiles accurately.

**Table 2. Overview of fuel compositions used during phasing and KLST experiments**

Mixture	Fuel composition in mole-%	Mixture	Fuel composition in mole-%
CH <sub>4</sub>	100%	CH <sub>4</sub> /i-C <sub>4</sub> H <sub>10</sub>	99.3% / 0.7% 98.5% / 1.5% 97.7% / 2.3% 96.6% / 3.4% 94.1% / 5.9% 93.1% / 6.9%
CH <sub>4</sub> /C <sub>2</sub> H <sub>6</sub>	96.6% / 3.4% 93.3% / 6.7% 88.6% / 11.4% 87.2% / 12.8% 82.4% / 17.6%	CH <sub>4</sub> /n-C <sub>4</sub> H <sub>10</sub>	98.8% / 1.2% 97.9% / 2.1% 96.6% / 3.4% 94.9% / 5.1%
CH <sub>4</sub> /C <sub>2</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub>	91.1% / 6.6% / 2.3% 81.1% / 13.7% / 5.1%	DNG/C <sub>2</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub>	100% / 0% / 0% 97.3% / 0% / 2.7% 95.5% / 0% / 4.5% 90.9% / 0% / 9.1% 97.3% / 2.7% / 0% 91.9% / 8.1% / 0% 82.1% / 17.9% / 0% 91.9% / 8.1% / 0% 88.3% / 4.7% / 7.1% 79.9% / 10.2% / 9.9%
CH <sub>4</sub> /C <sub>3</sub> H <sub>8</sub>	99.1% / 0.9% 98.8% / 1.2% 98.2% / 1.8% 97.0% / 3.0% 96.1% / 3.9% 94.4% / 5.6% 94.3% / 5.7% 92.6% / 7.4% 92.5% / 7.5% 90.0% / 10.0%	DNG/H <sub>2</sub>	100% / 0% 97% / 3% 94% / 6% 89% / 11% 85% / 15% 80% / 20%
CH <sub>4</sub> /C <sub>3</sub> H <sub>8</sub> /N <sub>2</sub>	96.1% / 3.9% / 0.0% 90.1% / 3.7% / 6.2% 85.0% / 3.4% / 11.6% 77.5% / 3.2% / 19.3%	DNG/H <sub>2</sub> /CO	100% / 0% / 0% 90% / 10% / 0% 85% / 10% / 5% 80% / 10% / 10% 70% / 10% / 20%
CH <sub>4</sub> /C <sub>3</sub> H <sub>8</sub> /CO <sub>2</sub>	95.6% / 4.4% / 0.0% 90.6% / 4.4% / 5.0% 80.0% / 5.0% / 15.0% 75.0% / 5.0% / 20.0%	DNG/ C <sub>2</sub> H <sub>6</sub> /C <sub>3</sub> H <sub>8</sub> /H <sub>2</sub>	100% / 0% / 0% / 0% 93.8% / 3.8% / 2.4% / 0% 87.2% / 3.4% / 1.9% / 7.5% 81.2% / 3.2% / 2.0% / 13.6%

### 3.2 Autoignition model

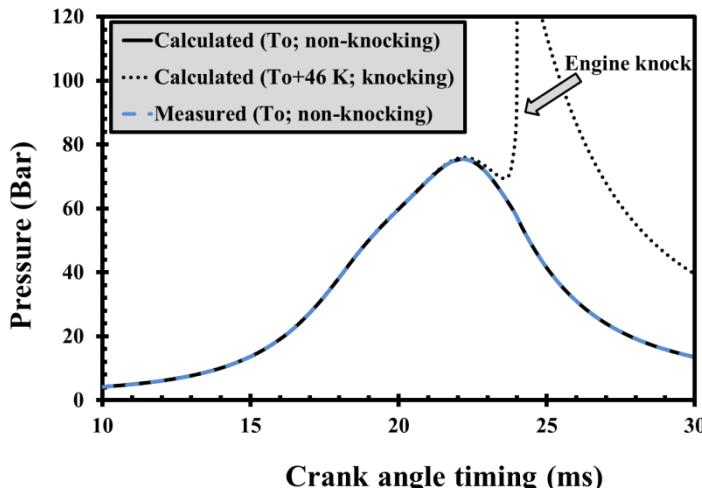
Knock in spark-ignited gas engines occurs when the compressed unburned end gas ignites spontaneously before being consumed by the propagating flame front. To understand the autoignition behaviour of gaseous fuels under conditions relevant to the DNV GL engine, we performed autoignition delay time experiments in the DNV GL Rapid Compression Machine (RCM), see for more details Refs.

[7,8,13,18,20,33-35]. The measurements have been performed for CH<sub>4</sub>, CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub>, CH<sub>4</sub>/C<sub>3</sub>H<sub>8</sub>, CH<sub>4</sub>/i-C<sub>4</sub>H<sub>10</sub>, CH<sub>4</sub>/n-C<sub>4</sub>H<sub>10</sub> and CH<sub>4</sub>/H<sub>2</sub> mixtures. Both stoichiometric ( $\lambda=1$ ) and fuel-lean ( $\lambda=2$ ) conditions were examined at in-cylinder conditions relevant to the DNV GL gas engine, with temperatures at the end of compression ranging from roughly 850 to 1120 K and pressures at the end of compression up to nearly 80 bar.

The measurements have been compared with numerical simulations using the SENKIN code [31] in the CHEMKIN II library [23] and the chemical mechanism developed in [9-12]. Based on sensitivity analyses the chemical mechanism used in this study is optimized by altering the rate coefficients using a least square fit in order to get the best correspondence between simulated and measured autoignition delay times. This optimization of the chemical mechanism substantially improved the predictive power of the knock resistance; agreement between RCM data and simulations using the improved mechanism changed from 40% to better than 15% at pressures relevant to the DNV GL engine [34, 35, 36].

### 3.3 Knock model

To account for the changes in pressure and temperature of the unburned end-gas during the engine cycle, we derive the specific volume of the assumed adiabatic core [24] of the unburned end gas from the pressure history computed by the two-zone thermodynamic phasing model. Together with the gas composition of the fresh cylinder charge, the input manifold temperature and pressure the specific volume is used as input into the autoignition model. Clearly, when using non-knocking input data, the simulation model should not (and does not) predict autoignition of the end gas, as seen Figure 1. To induce autoignition, however, we increase the initial temperature of the end gas in the simulation. Here, increasing the initial temperature by 46 K results in spontaneous ignition of the end gas at roughly 90% burn; the sudden spike observed in the simulated pressure history shown in Figure 1 is used here to indicate knock in the end gas. This temperature offset is chosen such that the model predicts autoignition of the end gas near the end of the burn period for an arbitrarily chosen fuel.

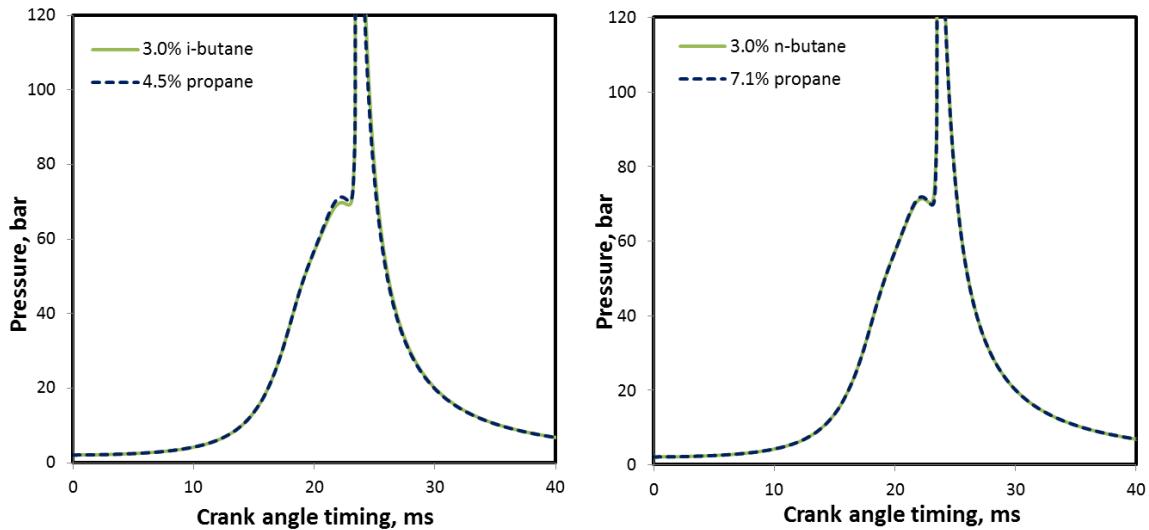


**Figure 1. Measured pressure history and calculated autoignition of DNG, constrained to the complete measured pressure and temperature history, at both the actual intake temperature  $T_0$  (non-knocking) and at  $T_0+46$  K (knocking).**

## CONSTRUCTION OF THE RANKING TOOL

To compare the knock resistance of different gases with each other, following a suggestion in Ref. [3], we use a propane-based scale that we have developed [34]. In this scale, which we refer to as Propane Knock Index (PKI), the knock resistance for a given gaseous fuel mixture is expressed as an equivalent fraction of propane in methane under the identical engine conditions. In this procedure, which is illustrated in Figure 2, the occurrence of engine knock at the point at which 90% of the fuel is burned is calculated for a given fuel composition, in this example 3.0% butane in methane (Figure 2). To find the “propane equivalent”, propane is added to methane and engine knock is calculated by the integrated knock model (simulation of both phasing and autoignition). The model automatically changes the propane fraction in methane iteratively up to the moment that knock occurs at the same position in the cycle as the gas under comparison.

The calculations shown as an illustration in Figure 2 (left) indicate that 3.0% i-butane is equivalent to 4.5% propane, while 3.0 % n-butane is equivalent to 7.1% propane (Figure 2, right). The observed difference in knock propensity of the butanes is mainly caused by the differences in the burning velocity: n-butane burns faster than i-butane [32] which results in a higher end-gas temperature for the n-butane/methane mixtures. The increase in end-gas temperature reduces the autoignition delay time and thus lowers the knock resistance. Here we note that the observed difference between the isomers of butane is also confirmed by our KLST experiments in the DNG GL engine; differences in knock behavior between butane isomers has also been observed in the literature [19].

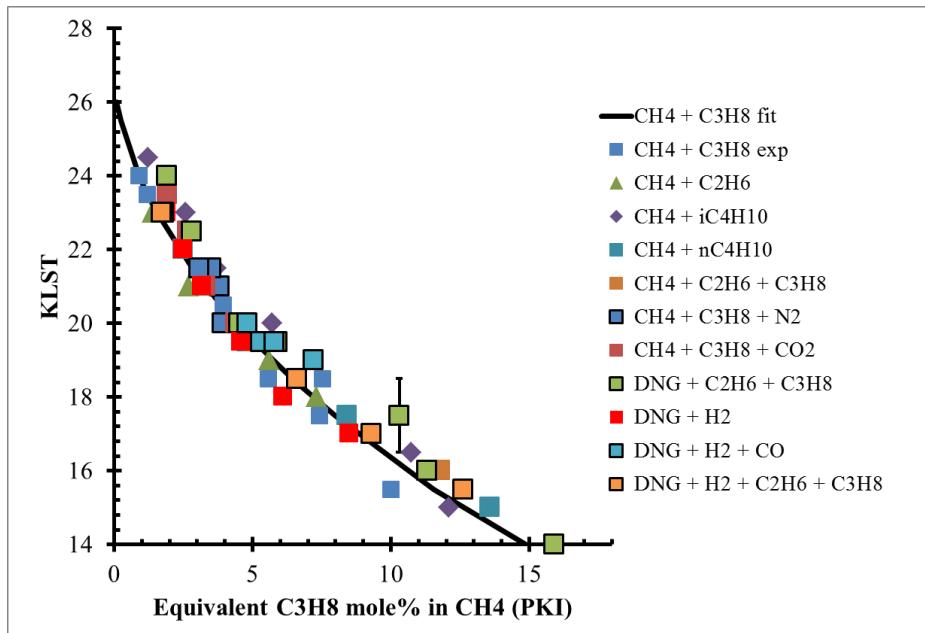


**Figure 2.** Knock simulations for 3.0% i-butane (left) and 3.0% n-butane (right) both shown with their “propane equivalent”, performed using the integrated model.

## COMPARISON WITH EXPERIMENTS

As illustrated above, the PKI is a measure for the *calculated* knock resistance of a given fuel; mixtures with the same *calculated* PKI have identical knock resistance. To test the veracity of the predictions we calculated the PKI's for the measured gas mixtures from Table 2, according the procedure described above, and also presented in Ref. [34]. The *calculated* PKI's are plotted in Figure 3 as function of the

*measured* KLST; mixtures with the same KLST also have identical knock resistance. Also shown in the figure are the measured KLST for the methane/propane mixtures used as the basis of the method (blue diamonds), and the best fit to these data (grey line). As can be seen in the figure, the deviations of the computed PKI from the fit of the methane/propane data are well within the uncertainty of the KLST measurements for all gases studied, demonstrating the excellent predictive power of the method.

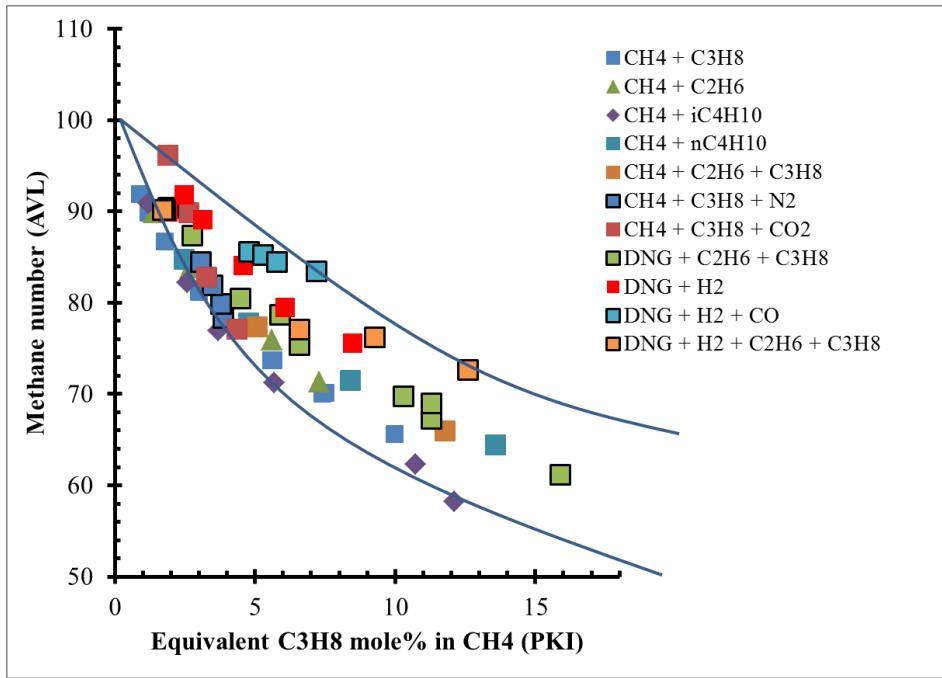


**Figure 3. Measured KLST vs. computed equivalent fraction of propane in a methane/propane mixture (Propane Knock Index, PKI)**

## COMPARISON WITH OTHER METHODS

With an eye towards possible standards, it is illustrative to compare the possible differences between the method described here and the existing methods. Here, we compare the PKI for the gases shown in Fig. 5 with the methane number (MN) computed using the AVL method [2] (version 3.2). The plot of MN versus PKI is shown in Fig. 4. We see that for the same knock resistance in our engine, expressed as the same PKI, a substantial difference in the AVL MN is observed. The difference becomes significant even at the relatively low PKI, growing to more than 13 MN ‘points’ at PKI=10 and above for the gases examined here.

As shown in Fig. 3 the largest differences are observed for the i-butane- and hydrogen-containing mixtures. The underestimation of the knock-enhancing effect of hydrogen seen in our engine is also observed in Ref. [32]. In contrast to our methodology the AVL method does not discriminate between isomers of butane as a result AVL substantially overestimates the knock-enhancing effect of iso-butane is substantially overestimated by treating it as n-butane. Here we note that the difference in knock resistance between i-butane and n-butane is also observed by others [19].



**Figure 4.** Methane number (AVL 3.2) plotted versus PKI for the gases shown in Figure 5.

## ALGORITHM

While the integrated knock model predicts the knock resistance very well for the DNV GL engine, it is very time consuming in use. To convert the method into an easy-to-use tool, a first-generation, gas-input-only algorithm has been formulated for binary and ternary mixtures of methane with ethane, propane, and i-butane and n-butane; typing in the gas composition readily gives the PKI for the gas [34]. The current version of the algorithm gives PKIs with a standard error of  $\pm 0.2$  when compared to the PKI derived from the full knock model. While the interpretation of the PKI in terms of an equivalent methane/propane mixture is relatively transparent, it can also be converted to a 0-100 scale, similar to other knock methods. The merits of one scale or the other is a subject of further discussion. Currently we are extending the gas-input-only algorithm to pipeline gases and sustainable gases.

## DRIVE TOWARDS STANDARDIZATION

For both pipeline gases and LNG as a transportation fuel, the way to guarantee the widest range of fuels and maintaining optimum engine performance in an open market is to agree on standards. A standard based on a correct characterization of knock resistance is essential in this process. Fuel suppliers and OEMs must now be sure that the way in which the fuel is specified indeed guarantees the desired performance of the engines in the market. A “correct” standard safeguards the end user by ensuring that engine performance is not unnecessarily compromised (unnecessary derating) or is unnecessarily at risk. It also ensures that gases are not excluded from the market, or “overtreated” to remove knock-enhancing components without cause.

Since the methodology presented in this paper is based on the physical and chemical processes that govern knock, and thus quantifies the differences in the behavior of engine types, the proposed method is well suited to serve as the basis for a standard. Since the method can be readily adapted to new engines and

fuels, a standard can also be adjusted to account for the changes in the market in a straightforward manner, without losing relevance.

## SUMMARY AND CONCLUSIONS

In this paper we have presented a method to characterize the effects of changes in fuel composition on engine knock in the DNV GL test engine. The method represents the physical and chemical phenomena responsible for these effects in sufficient detail to be able to accurately characterize pipeline gases, LNG gases and hydrogen containing natural gases for their knock resistance, as demonstrated by comparison with measurements. The method uses a propane-based scale, which can be converted to an algorithm for ease of use in practice. Comparison with the AVL method points to shortcomings in this yardstick for knock resistance for our engine, and potential consequences for their use in standards for fuel quality.

Since the DNV GL method is based on the physical and chemical processes that govern knock, it can be adapted in a straightforward manner to new engines and fuels. This fundamentally correct approach, together with the predictive power of the DNV GL method makes this methodology well suited to serve as the basis for a standard.

## Acknowledgement

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