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Assessment and status of gaseous fuel rating using the methane number

Controls, Automation, Measurement, Monitoring & Predictive Maintenance

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ABSTRACT

The composition of gaseous fuels for spark-ignited (SI) internal combustion engines (ICE) in the marketplace has seen significant change in recent years and is forecasted to change even more. Ethane content in U.S. natural gas has recently increased due to the increased exploitation of shale gas fields, and gaseous fuels with lower carbon content are being actively pursued, e.g., hydrogen blended into natural gas (NG), dimethyl ether (DME) blended into liquefied petroleum gas (LPG). Current engine combustion architectures are expected to operate over this widening range of gaseous fuel quality. Knowing the impact of these new gaseous fuels on critical combustion parameters is critical to the successful operation of SI ICE over the broad range of applications where they are used.

Methane number (MN) is a numerical fuel rating analogous to octane number (ON) and indicates the knock resistance of a gaseous fuel when used in a spark-ignited internal combustion engine. Along with lower heating value (LHV), the MN is a critical parameter for engine manufacturers to know so that the engine may be properly applied to a customer's application. Originating from research work done in Europe over 50 years ago, MN was introduced as an alternative to traditional gasoline rating techniques due to limitations on obtaining experimental values without extrapolative methods. Although the experimental methods and results were published, many specific details remain unpublished. Moreover, a MN test method has never been standardized. Engine manufacturers rely on various analytical methods to predict the MN for a gaseous fuel and may have little experimental data obtained by a standardized method to validate and adjust their predictive models to support these new emerging alternative fuels.

The experimentally determined methane number of gaseous fuel samples is compared with the value predicted by the ASTM D8221 calculated methane number (MNc) method. Differences are noted and analyzed and a new approach to estimating a methane number based on the composition of the gaseous fuel sample is discussed. A new method for determining the MN of a gaseous fuel by using a modified cooperative fuel research (CFR) engine is presented. An essential aspect of the MN test procedure involves identifying and quantifying knock intensity (KI) during engine operation. CFR engines, originally designed for gasoline testing, come equipped with their own knock measurement systems utilizing a capacitive detonation sensor. The original CFR engine system is compared with a Fast Fourier Transform (FFT) approach that uses a piezoelectric pressure transducer. The determination of an MN requires an accurate assessment of the reference methane-hydrogen fuel blend that is used during testing. A comparison is carried out between dynamic fuel blending using mass flow meters and a bracketing method using certified gas sample bottles containing various fuel blends from a gas supplier. Finally, uncertainty of the MN measurement method and the gas composition quantification, required as input for ASTM D8221, are evaluated.

1 INTRODUCTION

The composition of gaseous fuels for spark-ignited (SI) internal combustion engines (ICE) in the marketplace has seen significant change in recent years and is forecasted to change even more. Ethane content in U.S. natural gas has recently increased due to the increased exploitation of shale gas fields, and gaseous fuels with lower carbon content are being actively pursued, e.g., hydrogen (H_2) blended into natural gas (NG), dimethyl ether (DME) blended into liquefied petroleum gas (LPG). Current engine combustion architectures will be required to operate over this widening range of gaseous fuel quality. Knowing the impact of these new gaseous fuels on critical combustion parameters is critical to the successful operation of SI ICE over the broad range of applications where they are used.

End Gas Auto Ignition (EGAI) refers to the spontaneous combustion of unburned fuel in an engine combustion chamber. This phenomenon occurs after the initial spark-induced ignition event, exposing the yet-to-burn mixture to a higher energy environment during the propagation of the flame front throughout the cylinder [1]. EGAI encompasses various classifications that delineate its nature and origin. The term "*knock*" refers to both the audible noise and high-frequency vibrations stemming from EGAI and characterizing the knock intensity of gaseous fuels in terms of a specification is important to the proper matching of SI ICE to the variations in fuel composition.

Methane Number (MN) is an experimentally derived numerical rating indicating the susceptibility of gaseous fuels to EGAI. MN is expressed as the percentage of methane (CH_4) in a methane-hydrogen mixture, that in a test engine under standard conditions has the same knock resistance as the gaseous fuel to be examined. For example, a mixture of 80% CH_4 and 20% hydrogen (H_2) would correspond to a methane number of 80. For MN's greater than 100, the volume fraction of carbon dioxide (CO_2) expressed as a percentage in a carbon dioxide-methane mixture is added to 100. For example, a fuel blend consisting of 75% CH_4 and 25% CO_2 would correspond to a MN of 125.

Originating from pioneering work by Leiker et al. [2] in Graz, Austria, beginning in 1963 and continuing through 1969, MN emerged as a viable alternative to conventional gasoline rating methodologies, primarily due to constraints on maximum attainable values without resorting to extrapolative techniques. Leiker et al. [2] investigated the influence of gas composition on gaseous fuel knock resistance using a Cooperative Fuel Research (CFR) engine, presenting MN test results for 3-gas component mixtures as ternary diagrams as well as MN values for multiple marketplace gaseous fuels. While their method has been emulated by many researchers, many specific details of their experiments including experimental data remain unpublished.

MN is analogous to the octane number (ON) for gasoline, which uses iso-octane and n-heptane as reference fuels. Unlike liquid fuels and octane numbers which have ASTM International (formerly known as American Society for Testing and Materials) standards for determining the Research Octane Number (RON) [3] and the Motor Octane Number (MON) [4], there is currently no standard test method for measuring the methane number of a gaseous fuel (e.g., natural gas) used in SI ICE. With the anticipation of hydrogen blending into natural gas and other new gaseous fuel blends and their subsequent use in automotive applications, it is even more important that the experiments from over fifty years ago [2] be revalidated in a defined and standardized manner. Colorado State University (CSU) has a long history of method development and validation to determine the methane number for alternative gaseous fuels using a CFR engine [5]. Recently the work performed by researchers at CSU [6] was to create a repeatable and reproducible method for determining the MN of gaseous fuels utilizing a modified CFR engine that would support standardization efforts.

In the years following the work by Leiker et al. [2], various engine Original Equipment Manufacturers (OEMs) and technology consulting firms, e.g., AVL, developed their own methods for calculating a numerical rating index, or methane index (MI) that reflected the knock resistance on gaseous fuels, with specific details regarding the experimental MN values used and their calculation methods remaining proprietary. While these methane indexes do not necessarily reflect a true methane number which needs to be determined experimentally, they are extremely useful for comparing the knock resistance of one gaseous fuel to another and are used by engine OEMs for determining the acceptability of a gaseous fuel for their different engine models and applications.

Adoption of the Motoren Werke Mannheim AG (MWM) methane number, by standards organizations (e.g., ASTM [7], ISO, CEN) and regulators (e.g., California Department of Food and Agriculture (CDFA) has taken place within the past ten years.

This paper describes a new method for determining the MN of a gaseous fuel by using a modified CFR engine. An essential aspect of the MN test

procedure involves identifying and quantifying Knock Intensity (KI) via a Knock Integral (K∫) during engine operation. CFR engines, originally designed for gasoline testing, come equipped with their own knock measurement systems utilizing a capacitive detonation sensor. The original CFR engine knock measurement system is compared with a Fast Fourier Transform (FFT) approach that uses a piezoelectric pressure transducer. The determination of a methane number requires an accurate assessment of the reference methane-hydrogen fuel blend that is used during testing. A comparison is carried out between dynamic fuel blending using mass flow meters and a bracketing method using certified gas sample bottles containing several methane-hydrogen fuel blends from a gas supplier. The uncertainty of the MN measurement method and the gas composition quantification, required as input for the ASTM calculated methane number (MNc) is presented.

The experimentally determined MN of gaseous fuel samples is compared to the value calculated by the ASTM D8221 [7] MNc method. Differences were noted and analyzed. Experimentally determined MN values from the literature are compared with ASTM MNc values to examine the impact of certain hydrocarbon species.

Finally, the benefit of a new analytical approach for estimating a methane number based on the composition of the gaseous fuel sample which would allow for the use of new and additional experimental data for typical natural gas as well as new gas compositions is discussed.

2 MATERIALS AND METHODS

2.1 Cooperative Fuel Research (CFR) Engine

The engine testing for this research utilized a modified Cooperative Fuel Research (CFR) F-2 Engine, originally manufactured in 1957 by the Waukesha Motor Company. These engines remain commercially available through CFR Engines Inc., Pewaukee, Wisconsin, and are extensively utilized by petroleum refineries and state fuel analysis laboratories. A distinguishing feature of CFR engines is their capability to dynamically adjust the Compression Ratio (CR) without altering other operational parameters.

The CFR engine utilized at the Colorado State University (CSU) Powerhouse Energy Campus has undergone numerous modifications to align with a wide range of research objectives and is pictured in Figure 1. Modifications made directly influencing the testing of the methane number of a gaseous fuel are as follows:

- Knock Measurement System - In-cylinder water-cooled, piezoelectric pressure transducer.
- Engine Control and Monitoring System - LabVIEW™ virtual instrumentation panel.
- Crank Position Measurement - Optical engine encoder.
- Engine Speed Control - Regenerative Variable Frequency Drive (VFD).
- Fuel Delivery System - Dynamic fuel blending system (See Fig. 2).
- Ignition Timing Control - Woodward Large Engine Control Module (LECM).
- Air/Fuel Mixture Monitoring - Motorsports Technology (MoTeC™) lambda meter.
- Intake System - Air conditioning/ dehumidification.
- Intake Manifold Pressurization - industrial air compressor, air flow meter, actuated butterfly valve.
- Intake and Exhaust Manifolds - thermocouples and piezoelectric pressure transducers.

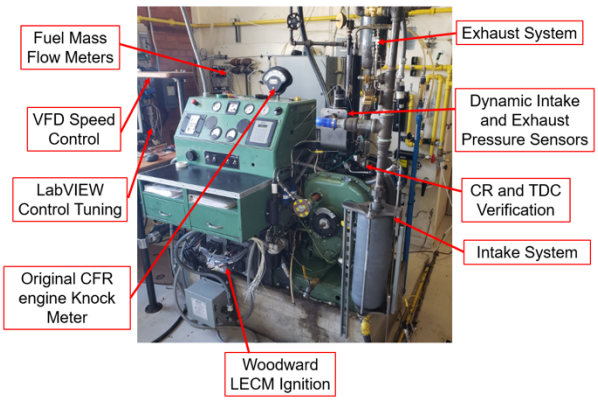

Figure 1. CFR engine at the CSU Powerhouse Energy Campus shown with labeled modifications.

A simplified diagram depicting the dynamic reference fuel blending system, the intake air pressure system, and the exhaust manifold is shown in Figure 2.

2.2 Knock Measurement Systems - CSU FFT vs. CFR

The two methods used for knock quantification within the scope of this project were the CSU-developed Fast Fourier Transform (FFT) of a Bandpass Signal system and the Knock Measurement System that was provided with the original CFR engine. Other viable methods of knock quantification can be found in the literature [10].

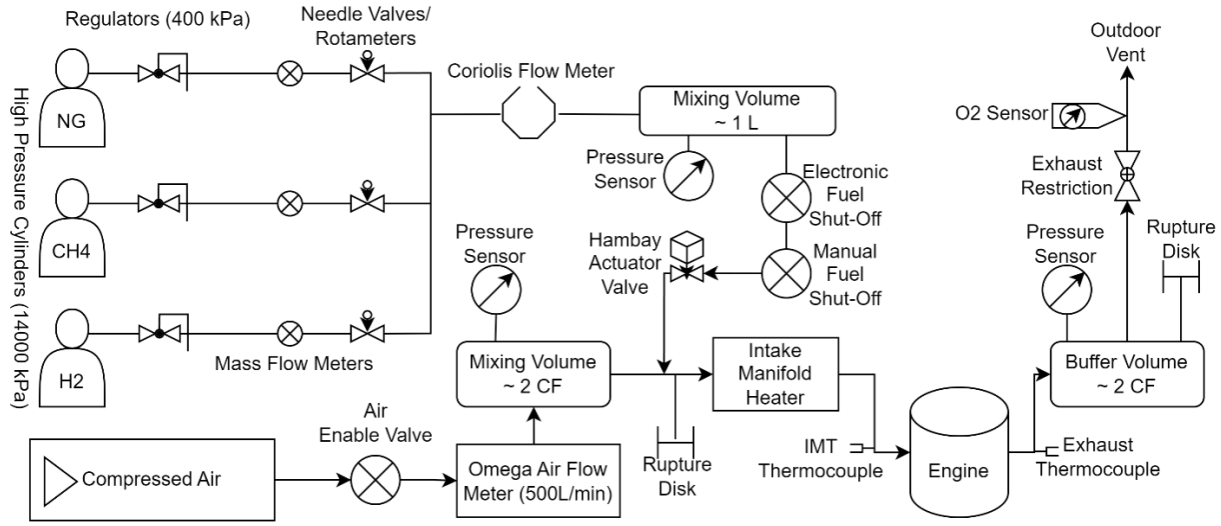

Figure 2. Engine fueling, intake manifold, and exhaust manifold schematic.

2.2.1 CSU FFT

The CSU knock measurement system begins with a water-cooled, piezoelectric transducer (Kistler model 6061A) mounted in the same cylinder detonation port previously housing the CFR detonation pickup. The signal from the transducer is fed to a charge amplifier which converts charge to voltage and relays pressure signal input to the controlling software. A rotary 0.1° incremental optical engine encoder (BEI model L25) provides positive crank angle position indication enabling real-time display of cylinder pressures as a function of crank rotation. Due to high dynamic response and resolution (3600 discreet data points per engine revolution) detailed pressure history is available allowing direct analysis of the combustion event in the cylinder.

The knock measurement method involves a Fast Fourier Transform (FFT) analysis of the cylinder pressure signal to assess pressure trace dynamics in the frequency domain, aligning with methodologies by Brunt et al. [11] and Elmqvist et al. [12]. The method quantifies auto-ignition events by correlating pre-detonation points with cylinder geometry, factoring in the time for a pressure wave to travel twice the cylinder diameter at the local speed of sound.

The frequency associated with the time for a pressure wave to traverse the cylinder, across and back, is used for programming to define an expected knock frequency range. The combustion logger program employs an FFT Power Spectrum function to analyze real-time cylinder pressure signals. A bandpass filter eliminates operating frequency, revealing pressure distortions indicative of knocking. The CFR-F2 engine operates at 900 rpm (15 Hz) which matches the speed used in ASTM's MON method [4] and the past work of Leiker et al. [2]. The CSU FFT system utilizes an in-cylinder water-cooled, piezoelectric pressure transducer from Kistler (Model 6061 A).

Figure 3 depicts light, moderate, and heavy engine knock conditions, with multiple oscillations in pressure occurring after the peak pressure and subsequent peak on the FFT plot with a frequency near 6 kHz corresponding to the anticipated value. The bandpass filter removes low and high-frequency noise tailored to the CFR engine cylinder geometry.

Knock Intensity (KI) is the measure of the amplitude of the FFT of an individual pressure trace during a single combustion cycle. The Knock Integral (K∫) used by CSU when operating the CFR engine is simply the sum of the KI values over successive combustion cycles (see Equation 1).

$$K\int = \sum_{i=1}^{n} KI(i) \qquad (1)$$

Where,
n = number of combustion cycles in a data set
KI(i) = knock intensity for a given combustion cycle, i

The FFT amplitude variation over 1000 cycles (73 seconds) at 900 rpm of a typical moderate Knock Intensity measurement is shown in Figure 4. The Knock Integral is used because it quantifies knock severity and persistence and is displayed to the operator as a rolling 200-cycle value is also shown

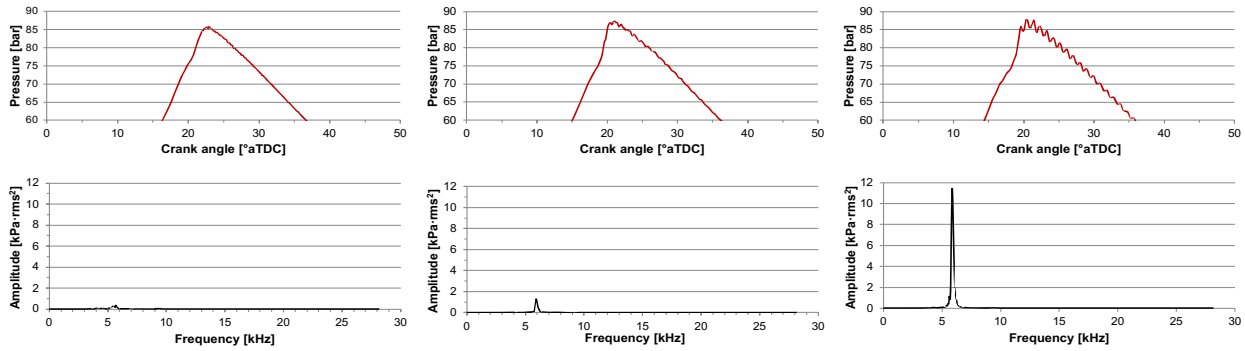

Figure 3. Pressure Trace and FFT plots depicting engine operation with light (left), moderate (center) and heavy (right) knock intensity [5].

in Figure 4. This was performed to allow the operator to better match knock intensities between samples and allow for a greater difference between similar knocking conditions.

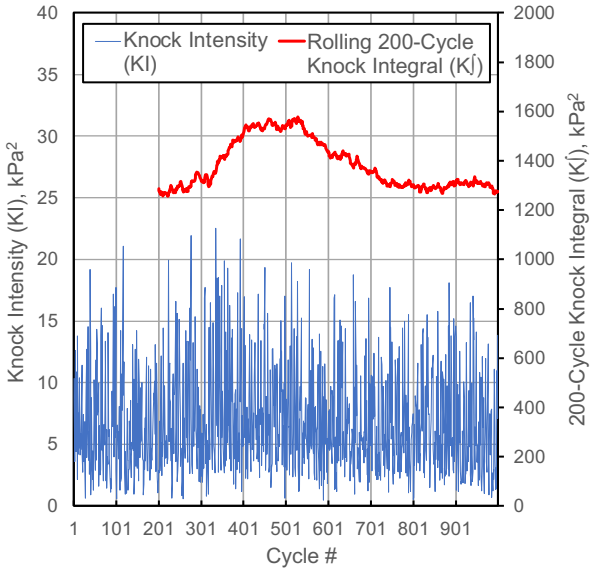

Figure 4. 1000 cycle knock intensity (KI) and knock integral (K∫) plot.

2.2.2 Cooperative Fuel Research (CFR) Engine

The CFR engine and operating system [13] provides a method for gauging the intensity of engine knock during operation and is the standard used for the testing of gasoline knock resistance [3] [4].

For normal operational use, the CFR engine system provides a means to measure the relative changes in knock intensity, requiring operators to determine the onset of knock and change sensitivity impacting the Knock Meter reading in divisions.

The CSU CFR engine was manufactured in 1957 and came equipped with an analog Knock Measurement System which was available until 2009 when the manufacturer switched to a digital system. The knock measurement system consists of a power supply, detonation meter, detonation pickup, and knock meter. The detonation pick-up sensor, mounted through the cylinder head, utilizes a thin flexible diaphragm cover which is exposed to the combustion chamber. The detonation meter (knock meter) is an analog device that can isolate the relative knock amplitude through averaging and filtering the received signal which is then transmitted to the knock meter. The knock meter display reflects the relative intensity of the knock event to establish a comparative scale used as the basis for measuring the intensity of knock experienced in the engine.

One of the focuses of this research was to determine the viability of the CFR Knock Measurement System for the Methane Number test procedure and compare the results to the CSU FFT Bandpass system.

2.3 MN Testing Methods

2.3.1 Knock Intensity of Test Fuel Sample

The following method utilized the CSU FFT Bandpass Knock Measurement system to determine the knock intensity (KI) of the test fuel sample.

1. Start the CFR engine and allow it to reach steady state operating conditions as shown in Tables 1 and 2.
2. Change the gaseous fuel supply to the test fuel sample and allow the engine to reach stable operating conditions.
3. Make gradual increases in compression ratio (+0.5) while maintaining steady-state operating conditions. Continue gradual increases in compression ratio until the onset of audible knock. The compression ratio will remain constant for the rest of the test.
4. If audible knock is not achieved in Step 3 before reaching the maximum CR of the CFR engine, lower the CR, advance the ignition timing and repeat step 3 until audible knock is achieved.

5. Use the knock integral (K∫) to determine operating stability.
6. Record three (3) 1000-cycle intervals of operating conditions including the cylinder-pressure trace data.
7. Terminate the test fuel flow, allowing time for the fuel mixture to leave the CFR engine intake system while the engine continues motoring.
8. The cylinder pressure data is used to determine the Target-K∫ (TK∫) value which is the average K∫ of the three 1000-cycle intervals (2400 K∫ values). The cylinder pressure data is also used to determine the average knock intensity of the fuel sample.

Table 1. Environmental and Testing Parameters established by the ASTM MON method [4] and Leiker et al. [2].

Parameter	Set Point	Allowable Variation (±)
Engine RPM	900 RPM	9 RPM
Humidity	0.00534 kg H_2O per kg Dry Air (37.5 grains of H_2O per lb. Dry Air)	0.0018 kg (12.5 grains)
Coolant Temperature	100 °C (212 °F)	1.5 °C (3 °F)
Coolant Level (HOT)	"*LEVEL HOT*" mark	1 cm (0.4 in.)
Coolant Level (COLD)	Just visible in sight glass	1 cm 0.4 in.)
Oil Temperature	57 °C (135 °F)	8 °C (15 °F)
Oil Level (Running & Hot)	Mid-Level in sight glass	0.5 cm (0.2 in.)
Oil Level (Stopped & Cold)	Top of sight glass	0.5 cm (0.2 in.)
Oil Pressure	190 kPa (27.5 psig)	17 kPa 2.5 psig)
Crankcase Internal Pressure	Atmospheric	−2.5 kPa (−0.36 psig)

Table 2. Research Determined Methane Number Test Parameter Set Points and Variation.

Parameter	Set Point	Allowable Variation (±)
Ignition Timing	12°–21° bTDC	0°
Intake Manifold Temperature	70°C	1.7 °C
Intake Manifold Pressure	Atmospheric	0.62 kPag (0.09 psig)
Exhaust Manifold Pressure	Atmospheric	2.5 kPag (0.36 psig)
Mixture Ratio	Stoich. (λ = 1.000)	0.007 λ

2.3.2 Reference Fuel K∫ Bracketing

Next a series of reference fuel knock integral tests are performed. This approach is based on ASTM's Motor Octane Number (MON) test method [4] where two primary reference fuels (PRF) are selected such that, at the same test conditions of the test sample, "*one knocks harder (higher KI) and the other softer (lower KI) than the sample fuel*."

In the proposed method, the primary reference fuel (PRF) is methane (CH4), and the secondary reference fuel (SRF) is hydrogen (H2). Three blends of these two reference fuels, a high, nominal, and a low relative the test sample's Target-K∫ value are used to bracket the knock intensity of the test sample. In general, a bracketing technique eliminates the need to precisely adjust reference fuel flowrates to bracket the TKI or TK∫ value. This reduces test time and uncertainty.

Two types of reference fuel blends may be used. Certified reference fuels (CRF) are blends of CH4 and H2 that are purchased from gas suppliers in various concentrations ranging from 75-95% CH4 corresponding to the expected range of MN for typical natural gas. Dynamically blended reference fuels (DBRFs) are created by blending methane (CH4) with hydrogen (H2) to achieve a reference fuel with a higher, lower, or the same value of the Target K∫ value. The DBRF is provided to the CFR engine using separate supply of CH4 and H2 gases using precise fuel flow control and flow rate measurements.

2.3.2.1 Bracketing Target-K∫ Value (CRF)

1. Select two (2) CRF blends that bracket the test fuel and one (1) CRF blend that is close to the anticipated MN.
   a. If GC data is unavailable, begin with CRF-1 = 85-15 (85% CH4-15% H2, 85 MN) and select CRF-2 and CRF-3 based on CRF-1's K∫ value.
2. Activate the CRF-1 flow and let the engine stabilize before recording a 1000-cycle interval.
3. Terminate the CRF-1 fuel flow, allowing time for the fuel mixture to leave the CFR engine intake system while the engine continues motoring.
   NOTE: If CRF-2 and CRF-3 have not been selected, determine the closer two blends that will bracket the fuel. Examples are provided below:
   a. Target-K∫ = 500, CRF-1(85-15) = 700, CRF-2 (80-20), and CRF 3 (90-10)
   b. Target-K∫ = 500, CRF-1(85-15) = 100, CRF-2 (80-20), CRF-3 (75-25)
4. Activate CRF-2 and let the engine stabilize before recording a 1000-cycle interval.
5. Terminate the CRF-2 fuel flow, allowing time for the fuel mixture to leave the CFR engine intake system while the engine continues motoring.
6. Activate the CRF-3 flow and let the engine stabilize before recording a 1000-cycle interval.

7. The Bracketing Target-K∫ MN test is now complete. Turn off the CRF-3 fuel flow and stop the engine.

2.3.2.2 Bracketing Target-K∫ Value (DBRF)

1. Activate the CH_4 flow for the primary reference fuel (PRF) and let the engine stabilize to measure the Current K∫.
2. Select the secondary reference fuel (SRF) based on the relation between the Current-K∫ and the Target-K∫.
   a. If Current K∫ < Target K∫: SRF = H_2
   b. If Current K∫ > Target K∫: SRF = Carbon Dioxide (CO_2)
3. Make gradual adjustments in the SRF until
   a. Current-K∫ = ~1.2 x Target-K∫ (DBRF-High) and record 1000-cycle intervals while keeping both PRF and SRF flows constant.
   b. Current-K∫ = ~1.0 x Target-K∫ (DBRF-Med) and record 1000-cycle intervals while keeping both PRF and SRF flows constant.
   c. Current-K∫ = ~ 0.8 x Target-K∫ (DBRF-Low) and record 1000-cycle interval while keeping both PRF and SRF flows constant.

   Note - A 20-30% difference between DBRF values is recommended.
4. The Bracketing Target-K∫ MN test is now complete. Turn off the SRF fuel flow and stop the engine.
5. Calculating the MN value for a DBRF requires converting the PRF and SRF mass flow rates to standard volumetric flow rates (Q). When the SRF is hydrogen, the MN is given by Equation (2).

$$MN = \left(\frac{Q_{CH4}}{Q_{CH4} + Q_{H2}}\right) \cdot 100 \qquad (2)$$

When the SRF is carbon dioxide, the methane number is given by Equation 3.

$$MN = \left(\frac{Q_{CO2}}{Q_{CH4} + Q_{CO2}} + 1\right) \cdot 100 \qquad (3)$$

2.3.3 Post-Processing Procedure

Utilizing the Methane Number (MN) of the three reference fuel blends enables the establishment of a relationship between MN and Average-Knock Integral (K∫), facilitating direct calculation of the MN based on the sample fuel knock integral. Alternatively, the average knock intensity (KI) values can be used. Although the relationship between MN and knock integral is non-linear, linear regression offers a viable approximation when the total range of RF's is less than 5 MN. The coefficient of determination (R^2) can be used to determine the best regression method to be used with R^2 greater than 0.99 desired.

1. The Knock Integral (K∫) or Knock Intensity (KI) values for all tests are averaged over each 1000-cycle data collection period generating four datapoints for evaluation.
   a. Average of the three (3) 1000-cycle intervals for the test sample
   b. DBRF-High, or CRF-1
   c. DBRF-Med, or CRF-2
   d. DBRF-Low, or CRF-3
2. Plot MN vs. Avg. K∫ (or KI) for the three reference fuel blends (DBRF or CRF).
3. Generate a linear or exponential regression equation using the three (3) reference fuel blend MN-Avg. K∫ (or KI) datapoints, evaluating the validity of the three reference blend tests based on the R^2 value achieved.
4. Using the average K∫ (or KI) from the three test fuel sample tests which is also the TK∫ of the test fuel sample, calculate the MN of the test fuel sample.

2.3.4 Comparison of CRF and DBRF Bracketing K∫ Methods

A comparison of the CRF and DBRF Bracketing K∫ methods is illustrated in Figure 5 and tabulated data shown in Tables 3 and 4. In the example case, the TK∫-target value based on the three tests of the sample fuel was 719 kPa^2, which was also an average knock intensity value 3.61 kPa^2. The K∫ Bracketing tests for both the CRF and DBRF blends were run as described above. Using the average-K∫ values from the three CRF and three DBRF tests, exponential and linear regression curve fits were calculated based on their respective average K∫ values. The MNs for the CRF and DBRF K∫ Bracketing methods were 86.12 and 86.44, respectively.

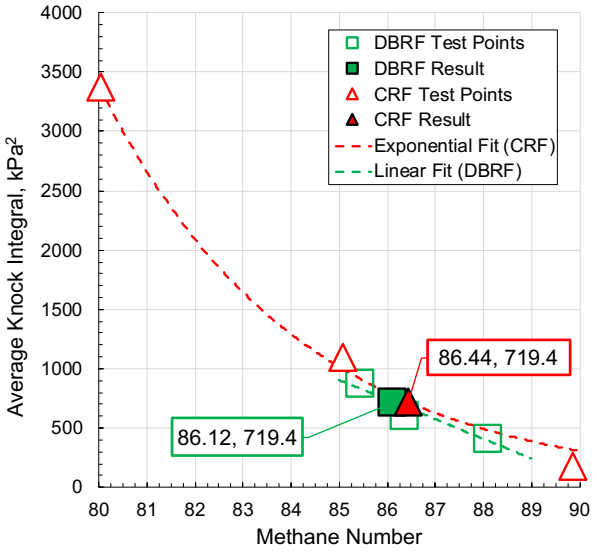

Figure 5. Bracketing Target-K∫ Value, CRF vs DBRF Methods.

Table 3. CRF Data.

Parameter	Avg-K∫, kPa2	Avg-KI, kPa2	MN
CRF-1	3364 ± 42.0	16.85 ± 0.387	80.01
CRF-2	1091 ± 45.6	5.45 ± 0.403	85.06
CRF-3	172 ± 25.8	0.85 ± 0.228	89.86
Exponential Curve Fit	$K\int = 7.709 \cdot 10^{11}\, e^{-0.24055MN}$ $R^2 = 0.9947$		
Target-K∫	719.4	3.61	86.44

Table 4. DBRF Data.

Parameter	Avg-K∫, kPa2	Avg-KI, kPa2	MN
DBRF-High	878 ± 59.1	4.42 ± 6.15	85.45
DBRF-Med	606 ± 140.0	3.07 ± 5.09	86.37
DBRF-Low	420 ± 95.8	2.10 ± 3.80	88.08
Linear Curve Fit	$K\int = -165.32MN + 14957.1$ $R^2 = 0.9225$		
Target-K∫	719.4	3.61	86.12

2.4 Recommended Test Conditions - Parameter and Sensitivity Studies

The testing environment is an important consideration when measuring the knock resistance of a fuel. There are multiple parameters that have varying levels of impact on the knock tendencies and repeatability of an MN test. The impact of certain operating conditions and test parameters was investigated in prior research and subsequently reported on in detail [6]. There are two main considerations for test parameters held constant during a methane number measurement, which are (1) the specific values chosen, and (2) the allowable variation, or control boundaries. Significant test parameters identified included ignition timing (IT), intake mixture temperature (IMT), intake manifold pressure (IMP), and lambda. A summary of those parameter and sensitivity studies is provided in Table 5.

Table 5. Parameter Variability and Sensitivity Results.

	dKI / d(Variable)	Allowable Variation (±)	d(MN) / d(Variable
Ignition Timing	Non-linear	Not Applicable*	0.029
Intake Manifold Temp.	0.209	1.66 °C	−0.004
Intake Manifold Pressure	0.562	0.615 kPag	−0.049
Mixture Ratio (λ)	52.2	0.007 λ Units	20.9

* Ignition timing is a parameter set using a digital encoder and is based on precise engine crank angle position. Thus, this parameter does not vary.

2.4.1 IT, IMT and IMP

Ignition timing, IMT, and IMP have weak correlations to the MN value and thus will allow operators some flexibility in selecting their respective values for stability and ease of operation while minimizing variation.

While the ignition timing has a substantial impact on the KI for a given compression ratio, the CSU ignition timing system uses a digital encoder and is based on precise engine crank angle position. Thus, this parameter does not vary between the sample test fuel and reference fuels during testing.

While the intake mixture temperature does influence the knock intensity of a sample test fuel, it has minimal influence on MN results. It was maintained at 70 °C (158 °F) ± 1.7 °C (3.1 °F) to facilitate knock intensity measurements while mitigating the risk of backfire.

The CFR engine is naturally aspirated and is operated with minimum intake and exhaust restrictions. Since CSU's elevation is 1,525 m with a barometric pressure of 85 kPa, the impact of intake manifold pressure was studied. The IMP was regulated using the test facility's compressed air system while the exhaust manifold pressure (EMP was altered using a manual restriction valve. However, lowering the EMP beyond ambient conditions was not feasible. The lab systems can simulate elevated pressure conditions in the CFR engine but introduce fluctuations in the intake pressure system of ±5 kPa. These variations occur every few seconds but still allow the average K∫ value, which encompasses 1000 cycles, to be used as the IMP remains constant during that time.

IMP variations within the expected ambient pressure range of 85–105 kPa were smaller than the registered variation between test days at identical operating conditions, and so higher pressures (115–200 kPa) were tested. Overall, there is a negative, but negligible relationship between MN and IMP over the expected range of IMP. It was concluded that MN tests should occur at ambient atmospheric pressure, with fluctuations restricted to ±0.62 kPa. Based on tests taken on four separate days, it was concluded that a 10 kPa increase in IMP yields a 0.5 MN variation, which is within the anticipated parameter fluctuation.

2.4.2 Lambda (λ)

Lambda (λ), the ratio of the actual air fuel ratio (AFR) to the stoichiometric AFR for a given fuel is a crucial parameter and influences many engine performance characteristics. Historically [2] [4] CFR engines have been operated at "*the stoichiometric combustion air ratio, λ=1*", or ideally balanced combustion. While rich operation (λ<1) offers the highest knock intensity for a gaseous fuel [2], controlling a rich-mixture and reproducing knock intensities between a sample fuel with unknown chemical composition and several reference fuels is challenging and time consuming. Instead, an exhaust O_2 sensor was used to control λ and the variable compression ratio feature of the CFR engine was used to maximize the knock intensity. For the CSU system, a MoTeC™

Professional Lambda Meter (PLM) was used in conjunction with a Bosch O_2 sensor.

Comparative testing between CR and KI with different λ values involved incrementally increasing CR and recording the knock intensity as shown in Figure 6. Among the λ values tested, there was a notably stronger correlation for λ = 1 compared to the others. KI values were less consistent outside the 0.95–1.05 range, and misfires occurred outside the 0.8–1.2 range, making an average KI value impractical. The results from this study indicated a significant benefit of running at λ = 1 to achieve reproducible knock characteristics.

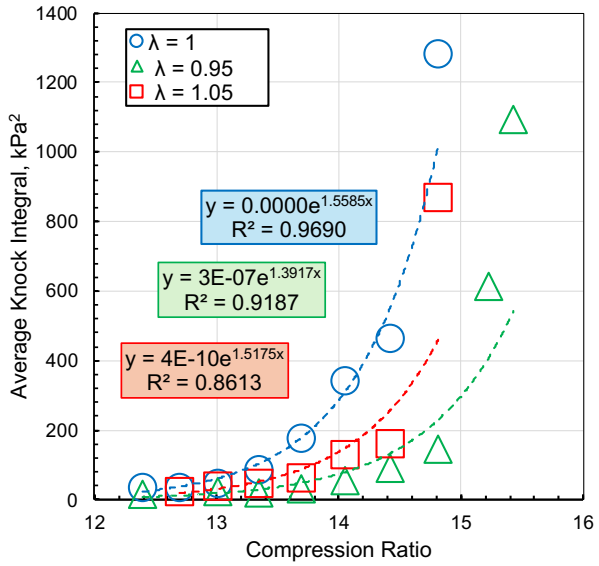

Figure 6. λ and KI Variability Study.

A set of tests were conducted with a constant CR of 14:1, ignition timing of 15° bTDC, IMP and EMP at ambient conditions, and an IMT of 70° ± 0.25 °C. Other testing parameters, such as coolant and oil temperature, were maintained at nominal values. Figure 7 shows a piecewise linear relationship between λ and average KI. The absolute value of the trendline slopes on either side of the peak value occurring at λ = 1.00 are about the same allowing for a symmetric tolerance band to be applied to λ. Multiple tests were run to determine an average fluctuation of KI, and it was determined that a 0.0065 change in λ on the rich side resulted in a change in KI of 0.363 kPa² and that a change in λ of 0.0074 on the lean side resulted in a change in KI of 0.363 kPa². Considering the air–fuel ratio system only registers 0.001 λ, the maximum allowable variation in λ was determined to be ± 0.007.

The MN measurement requires bracketing the knock intensity of a test fuel with several reference fuels. Multiple MN tests were performed with several values of λ within a 0.9–1.2 range because the KI was found to be highly unstable outside this range. The results of two separate series of tests shown in Figure 8 reveal the significant relationship between λ and MN. Maintaining control of λ within ±0.007 equates to a 0.15 MN variation.

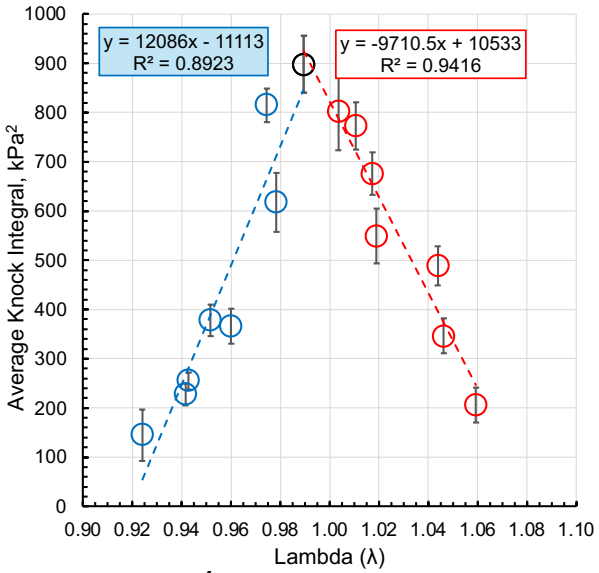

Figure 7. λ and K∫ Sensitivity Study.

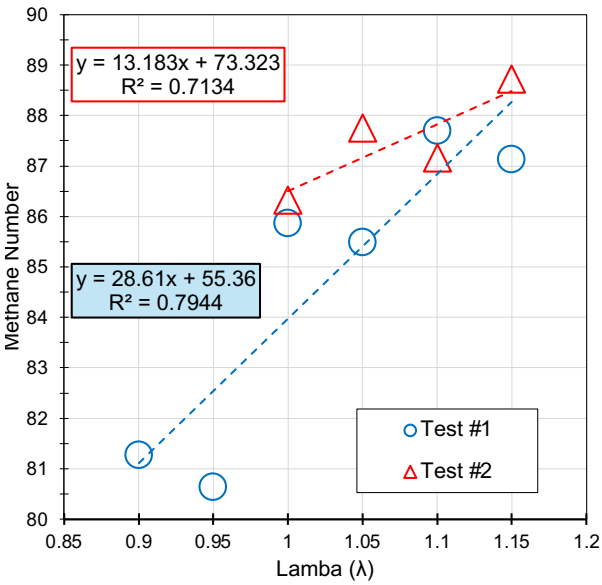

Figure 8. Effect of λ on Methane Number.

2.5 Comparison between CSU FFT Bandpass and CFR Knock Measurement Systems

The CSU FFT and CFR knock measurement systems each provide a benefit and yet have inherit drawbacks depending on the application. The FFT Bandpass system provides consistent KI (or K∫) values without intervention from the operator and operational parameters. The system also provides insight into cylinder pressures and a detailed analysis of the engine operation. In a research environment, such insight is beneficial, but in a regulatory environment, such information would not be necessary. The drawback to the FFT Bandpass method is its real benefit, with the sensitivity of the method not being able to be adjusted to gain finer resolution between knocking conditions. The CFR

knock meter system provides such adjustment in resolution and allows a definitive KI metric without the use of post-processing. Even with these differences between methods, both produce a KI (or K∫) parameter that can be used to accurately determine MN.

Direct comparisons between the CSU FFT Bandpass system and the CFR engine knock meter system are limited by the subjective nature of the CFR system. However, a method was developed for adjusting the settings of the CFR Detonation Meter to provide readings similar to the CSU FFT Bandpass method.

The CFR engine design is such that there is one port in the cylinder head for a pressure transducer or the CFR detonation meter. This means only one knock measurement system can be tested at a time, and hence, differences in knock intensity must be recreated at two different times. There are many adjustments available on the original CFR knock measurement system for precise tuning of knock measurement. Through trial and error, the CFR "*METER READING*" and "*SPREAD*" values were adjusted to match the CSU FFT Bandpass system so direct comparisons could be made.

Figure 9 shows the results from tests investigating the relationship between each method with similar operating conditions using the 90-10 CRF. The results for the comparison between the two methods were not scaled in any way, but rather, the initial CRF KI value was set to a low value using the SPREAD dial. When referencing the CFR system, the unit used is the Knock Meter Reading (KMR), and the CSU system used the average-K∫. The data show that the two methods have similar trends with ignition timing. Consequently, both methods are expected to produce accurate MN measurements.

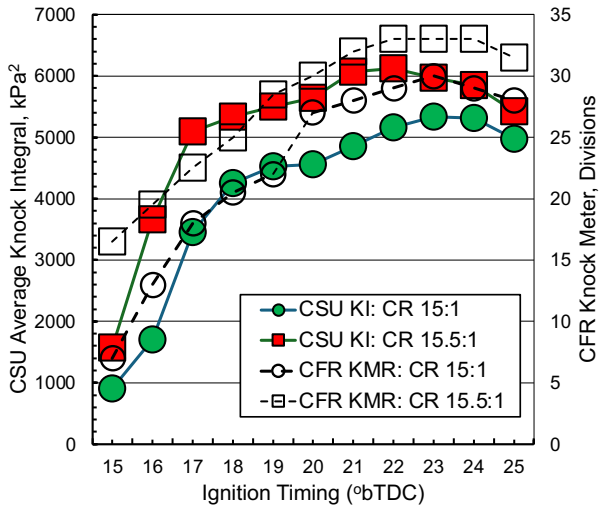

Figure 9. Knock Metric Comparison between CFR FFT Bandpass and CFR Knock Meter.

2.6 MN Measurement Uncertainty

Direct calculation of the total uncertainty associated with the MN test procedure is a challenging ordeal, with many different variables adding variation to the measurement. To estimate the total uncertainty associated with the measured MN, multiple tests using three different samples (see Table 6) of the natural gas supplied to the facility over a 6-month period were conducted and are shown in Figure 10. All tests used the DBRF Bracketing K∫ method, and the following testing parameters were used: ambient intake/exhaust pressures, stoichiometric mixture, 70 °C intake mixture temperature, and 15° bTDC ignition timing. All six tests had an average MN value of 85.6 with a standard error of 0.65. However, the second sample with four separate tests had a MN standard error of 0.86. While more repeatability tests using only one specific gas sample would be useful, the estimate is that the MN using this method may have an uncertainty of ± 1.5 MN-units. Note - Leiker et al. [2] indicated the same uncertainty with their method using a similar approach.

Table 6. Typical CSU Natural Gas (mol%).

Compound	Gas Sample #1	Gas Sample #2	Gas Sample #3	Average
Methane	89.35	89.16	87.80	88.77
Ethane	8.70	8.36	9.01	8.69
Propane	0.52	1.05	1.50	1.02
iso-Butane	0.024	0.050	0.038	0.037
n-Butane	0.040	0.098	0.072	0.070
iso-Pentane	0.005	0.018	0.012	0.012
n-Pentane	0.005	0.018	0.012	0.012
Hexane	0.004	0.003	0.002	0.003
Nitrogen	0.013	0.013	0.016	0.014
Carbon Dioxide	1.33	1.23	1.55	1.37
MN (measured)	85.4	85.4	86.0	85.6
MNc	77.9	76.3	75.0	76.4

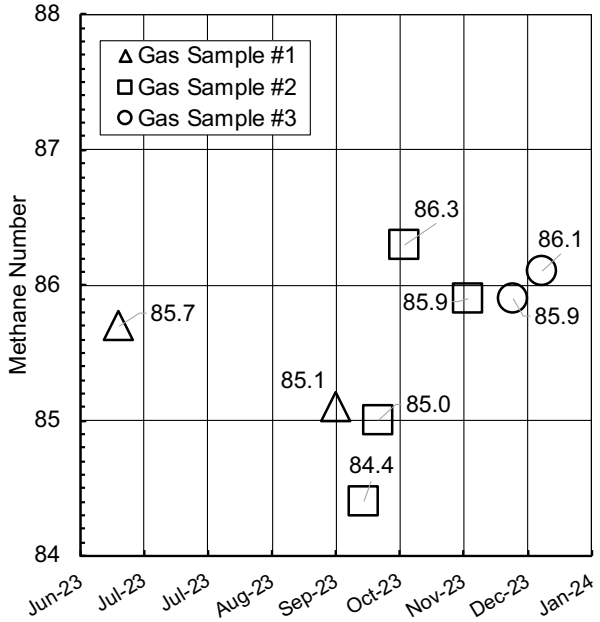

Figure 10. Methane Number Uncertainty Test Results.

3 COMPARISON OF EXPERIMENTAL METHANE NUMBER (MN) TO CALCULATED METHANE NUMBER (MNc)

3.1 ASTM MNc Method

In 1972, Leiker et al. [2] published a technical paper [2] based on an FVV/AVL (Forschungsvereinigung Verbrennungskraftmaschinen e.V./Anstalt fur Verbrennungskraftmaschinen List) research program [14] and included a method for "*for calculating the methane numbers of gas mixtures from their chemical compositions*" based on the experimental methane number results from that FVV/AVL research program.

Following this publication, various engine Original Equipment Manufacturers (OEMs) and technology consulting firms, e.g., AVL [15], developed their own methods for calculating a numerical rating index, or methane index (MI) that reflected the knock resistance of gaseous fuels. In most all cases, specific details regarding the experimental MN values used in calibrating their calculation methods, as well as the calculation method itself, remain proprietary. While these indexes do not necessarily reflect a true methane number which needs to be determined experimentally, they are extremely useful for comparing the knock resistance of one gaseous fuel to another and are used by engine OEMs for determining the acceptability of a gaseous fuel for their different engine models and applications.

MWM (Motoren Werke Mannheim AG) leveraged Leiker et al. [2], experimental data shown as ternary mixture diagrams by creating algorithms for these diagrams and developed an automated method (Fortran computer code) for estimating a methane number based on the hand calculation method first proposed by Leiker et al. [2]. Over time, MWM made some amendments to the original method. Unlike the CFR engine operating at stoichiometric conditions, their method was intended for modern lean-burn combustion engines where the nitrogen in the fuel is insignificant, so MWM excluded it. They also developed factors to be used when considering iso-butane, pentanes, hexanes and higher hydrocarbon gases, based on tests they ran on their large, lean-burn engines.

Adoption of the MWM methane number method by standards organizations (e.g., ASTM, ISO, CEN) and regulators (e.g., California Department of Food and Agriculture (CDFA)) has taken place within the past ten years. MWM's methodology was published by CEN [16] in EN 16726 Annex A, and the computer code was published by Euromot [17] in 2018. Based on these two publications, ASTM created a Microsoft Excel® program, augmented by a VBA macro. that allows users to determine the Calculated Methane Number (MNc) based on volumetric gaseous fuel composition and standardized it [7]. ASTM also cites MNc limits in two gaseous fuel motor vehicle specification standards [8] [9].

3.2 Comparison of Measured and Calculated MN Values

Over the course of testing in 2023, it was observed that the ASTM MNc method under-predicted the knock resistance of the CSU natural gas by at least 7.5 MN-units (see Table 6). Several available MN calculation tools from engine OEMs and technology consulting firms also under-predicted the knock resistance.

The precision of the MNc method is dependent on the precision of the original gaseous fuel components that are entered into the calculation. Specific checks of gas chromatograph (GC) readings including using multiple GCs was performed and the uncertainty of the GC readings was estimated in accordance with the general principles of metrology, as summarized in the ISO Guide to the Expression of Uncertainty Measurement (GUM) [18] using a Monte Carlo analysis. It was found that the MNc uncertainty with a 95% confidence level was typically less than ± 0.5 MN-units.

A blind test using a CRF sample was performed using the CRF K‚ Bracketing method and confirmed the MN of the sample. The test method resulted in a MN of 86.5 ± 1.30. The CRF contained 85.06 % by volume of CH_4 and 14.94 % by volume of H_2 so the theoretical MN value would be 85.1. The test method over-predicted the knock resistance by 1.4 MN-units (1.6%).

Using the nominal CRF component values and their 2% uncertainties in a Monte Carlo analysis, the MNc value was 84.1 ± 0.33. The MNc method under-predicted the knock resistance by 1 MN-unit (1.2%). Hence, while the nominal calculated MN is an exact value, the uncertainty due to typical gas chromatograph uncertainties is very small and generally can be ignored when reporting the MNc as an integer value.

Leiker et al. [2] tested sixteen types of gas found in the marketplace and published both the experimental MN values and their prediction of the MN using their new calculation method. While both the Leiker et al. [2] hand calculation method and the ASTM MNc method under- and over-predicted the measured MNs, the MNc method has a higher error with an RMS value of 3.7 MN-units. There were two samples representing Austrian and USSR natural

gas shown in Table 7, that had high methane concentrations (95-96 % by volume) with the total of butanes, pentanes and hexanes at less than 0.7 % by volume. In those two cases, the ASTM MNc method significantly under-predicts the knock resistance. CSU natural gas (Table 6) also had low amounts of these higher hydrocarbons.

Table 7. Two Test Samples reported by Leiker et al. [2] (vol%).

Compound	Gas Sample #14	Gas Sample #15	Average CSU Sample[2]
Methane	96.85	95.01	88.77
Ethane	1.43	2.62	8.69
Propane	0.40	0.73	1.02
iso-Butane	0.09	0.15	0.037
n-Butane	0.09	0.20	0.070
iso-Pentane	0.05	0.09	0.012
n-Pentane	0.04	0.06	0.012
Hexane	0.30	0.22	0.003
Nitrogen	0.55	0.54	0.014
Carbon Dioxide	0.18	0.38	1.37
MN	90.0[1]	82.5[1]	85.6
MNc	80.3	77.6	76.4

[1] Measured by Leiker et al. [2]
[2] See Table 6.

The experimental work by Leiker et al. [2] utilized n-butane but did not perform any tests on higher hydrocarbons. Leiker et al. [2] indicated that iso-butane could be considered as equivalent to n-butane. Based on tests MWM ran on one of their lean-burn engines, MWM updated their algorithm to treat iso- and normal-pentane the same and with an equivalency to n-butane by a factor of 2.3. Hexane and higher hydrocarbon gases were given an equivalency to n-butane by a factor of 5.3. The algorithm has an extreme sensitivity to very small levels of butanes as 0.1% by mole of butane lowers the MNc value by approximately 3.5.

Callahan et al. [19] reported that while "*the addition of heavier hydrocarbons to methane lowered the knock resistance of the fuel, the effect of methyl groups in the molecule tended to enhance the knock resistance of the gas resulting in higher MNs for the isomers compared to the normal alkanes.*" This confirmed previously published data on this phenomenon [20]. Figure 11 shows Callahan's findings and overlays the respective MNc values. It is interesting to note that iso-butane had slightly comparable knock resistance to propane at a 3% blend with methane. Their findings reveal significant differences between their measured and ASTM's calculated methane numbers for higher hydrocarbons even at low amounts.

The treatment of iso-butane and higher hydrocarbons by the MNc method which uses a unity equivalency factor is a possible contributing factor for the MNc method under-predicting the knock resistance of the CSU sample fuels by such a significant amount.

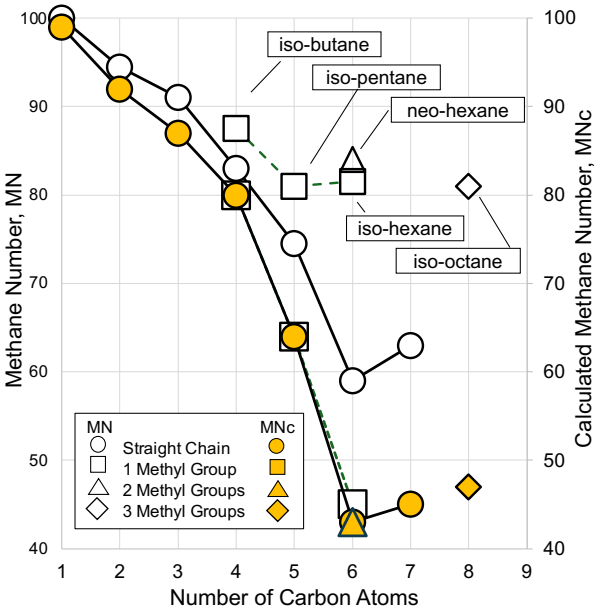

Figure 11. Methane number as a function of carbon chain length for normal paraffins and isomers at a 3 % concentration in methane [19].

3.3 Proposed New Method for Calculated MN

The FVV/AVL work [14] reported by Leiker et al. [2] developed a calculation method using a modified linear mixing rule where individual gaseous components are first separated into two- or three-component mixing groups for which experimental data exists, and then volumetric proportions of these mixing groups along with their local methane numbers are used to determine the methane number of the total mixture. This resulted in an estimate of MN that was fairly accurate, when compared to the experimental work they had undertaken. Subsequent modifications to their method included arbitrary criteria for the selection of the mixing groups, equivalency factors for gas components that did not have CFR engine mixture data, and a minimization routine to solve the inherent set of underdetermined linear equations. The method resulted in a numerical rating, or analytical estimate, indicating the knock resistance of the gaseous fuel sample. The method is extremely useful in comparing the knock resistance of one gaseous fuel to another.

However, in addition to being difficult to program and deploy into commercial/process applications, e.g., gas chromatographs, the method does not easily support changes to its estimates of the knock resistance of current or future gaseous fuels of interest, e.g., hydrogen/natural gas blends, dimethyl ether (DME) blended with liquefied petroleum gases (LPG), and ammonia (NH_3).

The viability of using a regression equation to predict the methane number as a function of the

composition of the gaseous fuel using experimental data has been previously demonstrated [21]. It is practical for CFR engine experimentation to utilize single-, two-, or three-component gaseous fuel mixtures.

A new predictive methane number method has been developed, featuring a second-order regression equation involving linear, binary, and ternary interactions of gaseous fuel components. So far, the new method employs regression equations with coefficients tuned using the experimental data based on the method described in Section 2.3. If made public, the large data set from the FVV/AVL work [14] could be used to develop the initial model. Moreover, inert and diluent gas components could be treated in the same regression equation which would support gaseous fuels containing high amounts of diluents. Otherwise, first determining the methane number of an inert-free mixture using the regression equations and then correcting for the inerts per the MWM method [16] could be the methodology. Furthermore, as experimental data for new gaseous fuel components of interest becomes available, these components could be added to the new method and new coefficients determined. While the regression equation would be lengthy, it could be easily programmed for a variety of commercial applications.

A simple example for a five-gas component mixture is shown.

n	Component, x_n
1	CH_4
2	C_2H_6
3	C_3H_8
4	n-C_4H_{10}
5	CO_2

x_n, mole %
L_i, linear coefficients
$B_{i,j,1\text{-}3}$ binary coefficients
$T_{i,j,k,1\text{-}6}$ ternary coefficients

Linear interactions:

$$MN_{linear} = \sum_{i=1}^{n} L_i \cdot x_i$$

Binary interactions:

$$MN_{binary} = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} x_i \cdot x_j \cdot \left[B_{i,j,1} + B_{i,j,2} \cdot \frac{x_i}{(x_i+x_j)} + B_{i,j,3} \cdot \left(\frac{x_i}{(x_i+x_j)} \right)^2 \right]$$

Ternary interactions:

$$MN_{ternary} = \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=j+1}^{n} x_i \cdot x_j \cdot x_k \cdot \left[\begin{array}{c} T_{i,j,k,1} + T_{i,j,k,2} \cdot \frac{x_i}{(x_i+x_j+x_k)} + T_{i,j,k,3} \cdot \left(\frac{x_i}{(x_i+x_j+x_k)} \right)^2 \\ + T_{i,j,k,4} \cdot \frac{x_j}{(x_k+x_j+x_i)} + T_{i,j,k,5} \cdot \left(\frac{x_j}{(x_i+x_j+x_k)} \right)^2 \\ + T_{i,j,k,6} \cdot \left(\frac{x_i}{(x_i+x_j+x_k)} \times \frac{x_j}{(x_i+x_j+x_k)} \right) \end{array} \right]$$

$$MN_{calculated} = MN_{linear} + MN_{binary} + MN_{ternary}$$

Binary interaction terms correct for the deviations shown by the experimental binary data from the assumption of a linear combination of pure component data. Similarly, ternary interaction terms correct for the deviations shown by the experimental ternary data from the assumption of a linear combination of pure component data and the binary interactions.

Note - Where there are no experimental data for linear, binary or ternary combinations of components, those coefficients are set to zero.

4 CONCLUSIONS AND FUTURE WORK

4.1 Conclusions

The purpose of this work was to develop a method for determining the MN of gaseous fuels and evaluate the effect of environmental factors and test parameters on end gas auto-ignition on a spark-ignited gaseous fuel engine. This evaluation was completed using a Cooperative Fuel Research engine with modifications implemented to operate using gaseous fuels and control environment parameters.

It was shown that ignition timing, IMT, and IMP have weak correlations to the MN value and thus will allow operators some flexibility in selecting their respective values for stability and ease of operation while minimizing variation.

The Air/Fuel ratio can vary significantly over the course of a test and has a significant impact on the knock intensity (KI). It was determined that a λ of 1.000 corresponded to the peak KI value and provided the most stable operating condition. KI values were less consistent outside the 0.95–1.05 range, and misfires occurred outside the 0.8–1.2 range, making an average KI value impractical. The results from this study indicated a significant benefit of running at λ = 1 to achieve reproducible knock characteristics.

This study compared the CSU FFT Bandpass and CFR Knock Detection methods, each offering advantages and disadvantages. Both systems are considered viable for determining the MN. Using a knock integral (K∫) when analyzing the cylinder pressure signal from a water-cooled, piezoelectric transducer provides a reasonable parameter for stabilizing the knock intensity during testing using a CFR engine.

This work produced a viable test method for determining the methane number (MN) of a gaseous fuel using a CFR engine. Two reference fuel methods to determine the MN were developed and validated. While these two methods are fundamentally the same, a certified blend of methane with hydrogen would be the most pragmatic.

MN test uncertainty was approximated by testing a consistent fuel sample multiple times over a 6-month period with consistent test parameters and different environmental conditions. Analysis of the MN test results from these data result in an uncertainty of 1.5 MN units.

This work observed that the ASTM MNc method as well as several available MN calculation tools from engine OEMs and technology consulting firms under-predicted the knock resistance for typical natural gas fuels. However, these MN calculation tools are extremely useful for comparing the knock resistance of one gaseous fuel to another.

Prior research shows that iso-butane has more knock resistance than n-butane. Methane number calculation methods should consider this when using equivalency factors for n- and iso-butane as well as higher hydrocarbons.

A new method to calculate a methane number utilizing a second-order regression equation involving linear, binary, and ternary interactions of gaseous fuel components has been presented. It could be developed and the adjustable coefficients tuned using experimental data based on the test method described in Section 2.3.

4.2 Future Work

A consistent test method for measuring the methane number of gaseous fuels is needed. Similar to ASTM RON and MON methods, it should be developed by a standards organization. This will establish a method for quantifying the MN of new gaseous fuels and confirming MN predictions by existing models.

It is recommended that detailed testing of the impact of n-butane, iso-butane and higher hydrocarbons on the methane number be performed. This effort could be published and would provide experimental data to support new regression equation methods as well as to offer possible adjustments to existing equivalency factors used by current methane number calculation methods.

The proposed new method for calculating a methane number using a regression equation has been developed from the FVV data set [14] and the intent is to publish the details of the model, including coefficients, when appropriate permissions have been obtained, or the data set has been made public.

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