

ANALYSIS AND ESTIMATION OF STOICHIOMETRIC AIR-FUEL RATIO AND METHANE NUMBER FOR NATURAL GAS

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ABSTRACT

Stoichiometric air-fuel ratio and methane number are important parameters to optimize natural gas fueled internal combustion engines for power and emissions. The increased production of high energy content natural gas from shale and other sources combined with an increasingly reticulated natural gas transportation system has resulted in widely variable fuel composition for many natural gas fueled engines. In some cases, this requires dynamic adjustments of engine controls to maintain emission compliance, maximize power production, and avoid pre-ignition/detonation conditions.

This paper explores the different methods for calculating stoichiometric air-fuel ratio and methane number for natural gas. Problems and limitations of those methods are identified. In addition, methods are developed to estimate these parameters given only four component information (i.e., nitrogen and carbon dioxide content, specific gravity, and higher heating value). Methods that are suitable for calculation in engine control systems will be highlighted. Those methods have relatively low computational and memory costs yet provide reasonable accuracy.

INTRODUCTION

The introduction of large quantities of shale gas and increased use of natural gas for electrical power generation has resulted in gas compositions varying significantly in some areas of the country. As a general rule, shale gas tends to have a high heating value (due predominantly to increased quantities of ethane and some propane). Often times the shale gas is blended with more traditional gas supplies which historically have a lower heating value. As pipeline end use loads decrease (especially when heating loads or gas fired power plants shut down during low demand periods), the shale gas will displace traditional supplies and result in a higher fraction of the total supply in some localized areas. This will result in an increase in the blended heating value. As the end use loads increase, more traditional gas enters the delivery area resulting in a decrease in the blended heating value.

The day-to-day variation in gas composition can be pronounced (Figure 1). The fuel composition can change by more than a hundred BTU/SCF in a few hours (Figure 2). Many of the engines used in natural gas pipeline transportation were designed assuming a relatively constant fuel gas composition and cannot tolerate these fast changes in fuel gas composition.

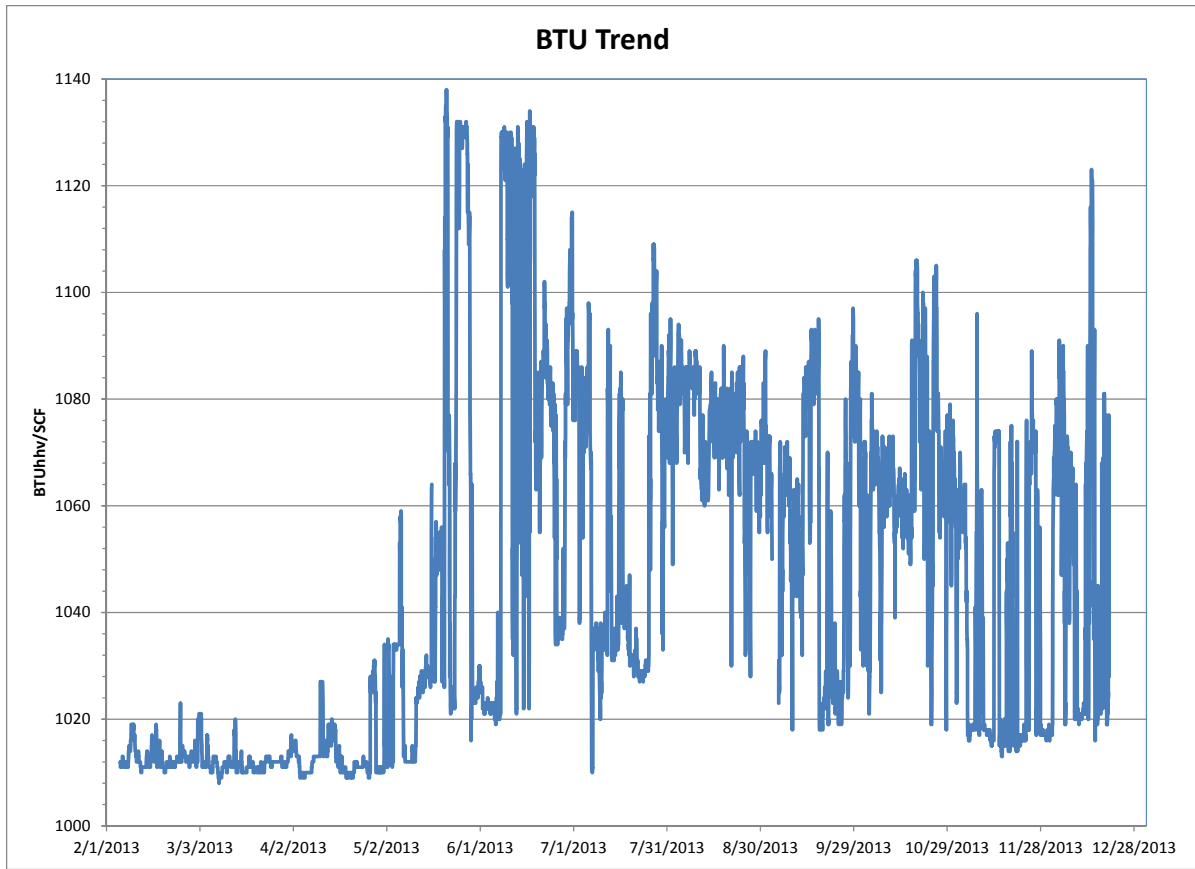


Figure 1 - BTU Trend

To achieve specific air emission limits at maximum power, many engines need to be tuned and configured to the fuel gas they are operating on. When the composition frequently and significantly changes, significant engine damage and/or air emission excursions are possible. [1] [2] If the engine is tuned and configured to operate under the worst case gas compositions, it is likely the maximum power capability and/or the efficiency will have to be reduced. [3] [4] Ideally engines subjected to wide variations in fuel gas composition will use adaptive control methods to automatically adjust the engine to the fuel composition.

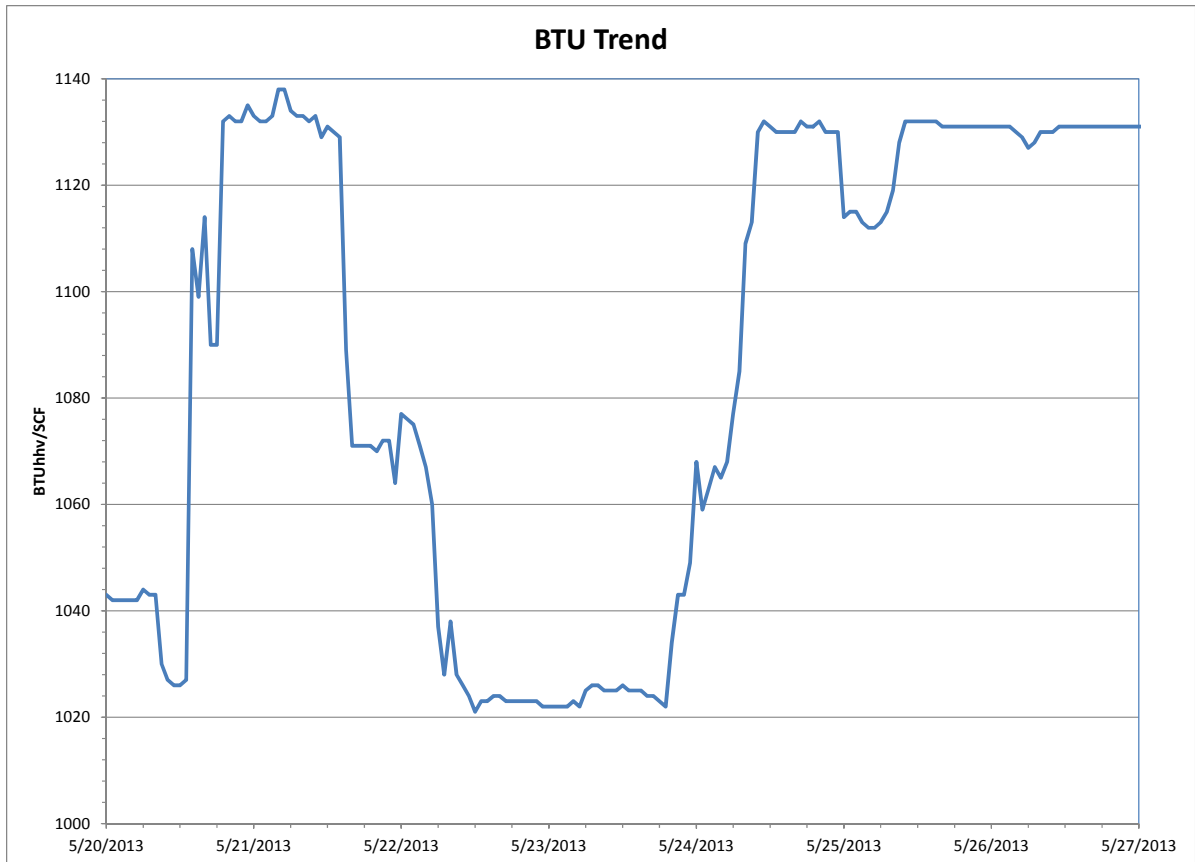


Figure 2 - BTU Trend Detail

DISCUSSION

Two key parameters associated with engine operation are dependent on the fuel gas composition. The first is the stoichiometric air/fuel ratio (SAFR) which is defined as the ratio of the air to the fuel (by mass) such that there is just enough oxygen to burn all of the fuel. While many engines (such as lean burn engines) do not operate at stoichiometric conditions, the SAFR is still important parameter in the control of nitrogen oxide emission levels. Adjusting an engine to the proper air/fuel ratio based on the fuel composition is the single most important control to avoid knock and maintain air emissions.

The second parameter discussed in this paper is the methane number (MN). The MN is one measure of a gaseous fuels propensity to cause knock¹ in an engine. It is determined by measuring the onset of

¹ Knock is used here to describe either the effect of pre-ignition (ignition of the air/fuel mixture prior to the initiation of controlled ignition) or detonation (when the fuel/air mixture in the end gas region ignites ahead of the flame front that originated from the ignition source). Detonation is also sometimes referred to as autoignition. While pre-ignition and detonation are distinctly different mechanisms, they both produce higher stress levels on the engine when compared to normal combustion. Both pre-ignition and detonation can be damaging to the engine because the abnormal combustion produces higher pressures and temperatures in the power cylinder and therefore increased stresses on the head, liner, piston, bearings, connecting rod, and crankshaft. The fuel characteristics that produce either pre-ignition or detonation are much the same.

The usage of knock is not defined or used consistently in the industry. The usage in this paper is consistent with Haywood. (41) For most large bore engines, knock by detonation is more prevalent.

knock in a CFR engine.² The MN scale was defined by setting the knock rating of a fuel having a high knock resistance (in this case pure methane) to a value of 100 and a fuel having a low knock resistance (pure hydrogen) to a value of 0 when operating at stoichiometric conditions. Based on that scale, various gas compositions were measured and their MN determined. It should be noted that the MN is not limited to the range of 0-100, high quantities of heavy hydrocarbons can produce a negative MN and high levels of carbon dioxide in a largely methane mixture can produce a MN greater than 100.

The chemical kinetics of combustion are very complex; the methane number is not a perfect model for predicting knock for a specific engine. Rather, it is a general parameter that can be used to provide guidance on how likely a given fuel composition is to cause knock. There are several fuel combustion properties that correlate to the likelihood of knock:

- Low ignition delay time
- High flame speed
- Low autoignition temperature
- High heat release rate

The heat release rate is a combination of the heating value of the gas and the flame speed. Hydrogen has relatively low chemical energy but has a very high flame velocity and a relatively low autoignition temperature which is why it has a low knock resistance. Similar combustion characteristics exist for hydrogen sulfide. [5] Laminar flame speeds, heating values, and autoignition temperatures for common natural gas components can be found in Appendix A.

The MN requirement of each engine (the fuel with the lowest MN that the engine can accommodate without knock) is specific to the design of that engine. The MN requirement is dependent on the engine geometry (i.e. the bore, stroke, compression ratio, piston/cylinder head shape, scavenging efficiency, location of the ignition source, air/fuel mixing, turbulence, etc.) and the operating conditions (temperatures, pressures, torque, trapped air/fuel ratio, ignition timing, and speed). In general, knock in a lean combustion spark ignition engine has the following sensitivities to operating conditions: [6] [7] [8] [9] [10]

Operating Parameter	Change	Impact
Trapped air temperature	Higher temperatures are more likely to knock	Very high
Torque	Decreasing torque reduces knock	Very High
Ignition timing	Retarding timing generally reduces knock ³	High
Air/fuel ratio	Increasing combustion air generally reduces knock ⁴	Moderate

² [Cooperative Fuel Research engine.](#)

³ If the mode of knock is autoignition, adjusting the ignition timing may have limited effect on reducing knock.

⁴ This statement is generally true for lean burn units, but air adjustment is dependent on the fuel composition. For example, in fuels with high hydrogen content, increasing air will increase the flame speed until the equivalence ratio approaches 1.6; faster flame speeds are more prone to lead to knock conditions. As the air is increased, the heat release rate is generally decreased, scavenging increased, and cooling increased all of which reduce the potential for knock. Moreover, additional airflow is typically achieved by increasing the air manifold pressure, which can result in higher trapped temperatures increasing the potential for knock.

Operating Parameter	Change	Impact
Coolant temperature	Reducing the coolant temperature decreases the potential for knock	Low
Peak compression pressure	Higher pressures can increase or decrease knock ⁵	Low
Speed	Decreasing speed generally increases knock ⁶	Low
Exhaust backpressure	Excessive exhaust backpressure can increase knock ⁷	Very low

As some of these operating conditions can, to some degree, be controlled, the MN requirement of an engine has some variability. For example, lowering the trapped air temperature will lower the MN requirement of the engine. By knowing the MN of the fuel, the some engine operating conditions can be adjusted to maximize power, control air emissions, and avoid knock.

In researching this paper, several additional options were identified that could be reasonably applied to engines to reduce the potential for knock. For example, the addition of water vapor reduces the propensity of knock. Water has a high specific heat which decreases the heat release rate and, therefore, should improve the MN requirement. Recirculating cooled exhaust gas will also reduce knock. Water or water/alcohol injection has also been used as knock control which achieves knock reduction through inlet cooling caused by the vaporization of the water/alcohol and by adding water vapor to the combustion air. [10] [11]

GAS COMPOSITION ANALYSIS

For this review, over 25,000 gas compositions were downloaded from informational postings of interstate natural gas transportation pipelines. The compositions were reviewed for integrity. In addition, publically available compositions from reference documents were added to the dataset including the source data used to calculate methane numbers. These compositions include single component gases such as propane. Several sample compositions were created to parametrically assess the sensitivity of the models to changes in gas compositions. A detailed analysis was performed from a subset of these compositions (6,330 compositions). Statistics on these compositions are:

	HHV (BTU/SCF)	LHV (BTU/SCF)	Specific Gravity	CO2%	N2%	C2%	C4+%	H2
Max	2567	2362	1.522	50.00	16.81	100.00	17.97	30.00

⁵ With all other conditions constant, the flame speed generally decreases with increasing pressure (which reduces the likelihood of knock) but the ignition delay decreases with increasing pressure (which increases the likelihood of knock). The impact on knock is dependent on which effect has the higher impact for a given pressure/temperature condition. It should be noted that increasing the compression pressure (which is achieved through turbocharging or supercharging on an engine with fixed compression geometry) also increases the temperature. Of the two mechanisms, temperature has the higher impact. Therefore, increasing the compression pressure without additional air intake cooling will generally increase the incidence of knock.

⁶ Reducing the speed generally increases the scavenging efficiency, which reduces free radicals that can help initiate combustion and, more importantly, lower the residual temperatures in the power cylinder. However, increasing speed lowers the pressure in the cylinder faster resulting in the associated temperature of the end gases to more likely be below the autoignition temperature and, therefore, reduce the likelihood of knock.

⁷ Backpressure has little impact on knock according to Taylor. (10) To the extent that high backpressure inhibits power cylinder scavenging efficiency, it can increase the likelihood of knock.

	HHV (BTU/SCF)	LHV (BTU/SCF)	Specific Gravity	CO2%	N2%	C2%	C4+%	H2
Min	749	675	0.409	0.00	0.00	0.00	0.00	0.00
Average	1041	939	0.598	0.56	1.73	5.07	0.14	0.01

STOICHIOMETRIC AIR/FUEL RATIO

Three different methods to calculate stoichiometric air/fuel ratio were evaluated.⁸

Composition Method

The standard method to calculate stoichiometric air/fuel ratio performs a mole balance of the individual gas components in the fuel to air ratio. Inerts (carbon dioxide, nitrogen, and helium) are ignored in the oxygen requirement calculations but are used in the mass balance calculations.

The basic principle of this method is to multiply each gas component fraction (not percent) by the number of carbon and hydrogen atoms for each component to calculate the amount of air required. One oxygen molecule is required for each carbon atom and one oxygen molecule is required for each four hydrogen atoms. This then needs to be multiplied by 4.7738 to account for the nitrogen in the air. Dividing this by the specific gravity of the fuel gas will yield the stoichiometric air to fuel ratio on a mass basis. Specifically:

$$SAFR = \left(C_{Mol} + \frac{H_{Mol}}{4} \right) * \frac{4.7738}{SG} \quad (1)$$

Where

C_{Mol} is the composition weighted carbon content

H_{Mol} is the composition weighted hydrogen content

SG is the specific gravity of the gas relative to air

As a worked example, consider a gas composition that has 5% carbon dioxide, 94% methane (CH₄), and 1% ethane (C₂H₆) by volume. This sample composition has a specific gravity of 0.607 (including inerts). The SAFR would be calculated as:⁹

$$SAFR = \left((0.94 * 1 + 0.01 * 2) + \frac{(0.94 * 4 + 0.01 * 6)}{4} \right) * \frac{4.7738}{0.607} = 15.06 \quad (2)$$

Urban/Sharpe Method

The Urban and Sharpe method [12] is similar in nature to the composition method but was created to estimate the air/fuel ratio based on measuring exhaust gases. The principal also works using the gas

⁸ For these calculations, it is assumed that the amount of free oxygen in the fuel gas is negligible. If there are significant quantities of oxygen in the fuel gas, the amount of air decreases accordingly.

⁹ Methane has one carbon atom and four hydrogen atoms; ethane has two carbon atoms and six hydrogen atoms. Complete combustion of methane will result in one carbon dioxide molecule (requiring two oxygen atoms, one oxygen molecule) and two water molecules (requiring two oxygen atoms or one oxygen molecule). The number of carbon and hydrogen atoms for typical natural gas components can be found in Appendix A. Air is approximately 78% nitrogen and 21% oxygen (with the balance being argon and other gases) and has a mole weight of 28.964.

composition. The method first determines the weighted sum of carbon, hydrogen, oxygen, and nitrogen in the fuel gas components. This method differs from the composition method by including carbon dioxide in the fuel in the mole sums. The specific gravity of the gas is not required for this method.

$$SAFR = \frac{(1 + \frac{H_{Mol}}{4 C_{Mol}} - \frac{O_{Mol}}{2 C_{Mol}}) * (31.999 + 3.7738 * 28.159)}{(12.011 + 1.008 * \frac{H_{Mol}}{C_{Mol}} + 15.999 * \frac{O_{Mol}}{C_{Mol}} + 14.007 * \frac{N_{Mol}}{C_{Mol}})} \quad (3)$$

Where

N_{Mol} is the composition weighted nitrogen content

O_{Mol} is the composition weighted oxygen content

This method will give the exact same answer as the composition method.

Four Component Estimation

In some cases, full gas composition analysis is not available but the four components of higher heating value, specific gravity, carbon dioxide content, and nitrogen content are available. In those cases, the SAFR can be estimated by:

$$SAFR = \frac{0.0094098 HHV}{SG} \quad (4)$$

Where

HHV is the higher heating value of the gas in BTU/SCF at 14.73 psia and 60 °F

In most cases this method, although greatly simplified, does a very good job modeling the actual SAFR as shown in Figure 3. This method will not be accurate if the fuel gas contains significant quantities of oxygen without applying an adjustment factor. Likewise, this method should not be used if the hydrogen content exceeds 30% by volume. Because this is an estimation method, it is strongly recommended that either of the other two options presented here be used when the full gas composition is available.

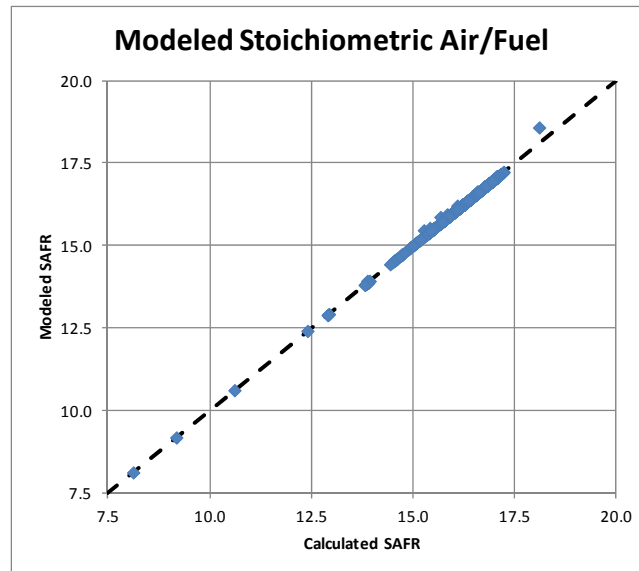


Figure 3 - Modeled vs. Calculated SAFR

METHANE NUMBER

Several different methods of calculating MN were evaluated. Some of these methods are related to each other while other methods are completely different. In many cases, the methods are limited in their applicability based on gas compositions. While there are other methods to calculate MN available as well, this analysis is limited to methods that are either generally available or commonly used by the natural gas industry.

All of the methods discussed here ignore the presence of water in the fuel gas (or combustion air for that matter). The presence of water should act as a diluent and improve the effective MN of the fuel. [13 p. 2] [10 p. 70] The presence of carbon dioxide and nitrogen in the fuel increase the MN because they act as diluent to the air/fuel mixture. This lowers the gas temperature during combustion which increases the actual MN. [14]

There is a wide variability in the calculated MN by calculation type. This is attributed to variability in the calculation methods and in the actual measurement MN. Figure 4 shows the MN measured vs calculated MN for several different calculation methods. Measured MN values were taken from several sources including [15], [14], [16], [17], and [18].

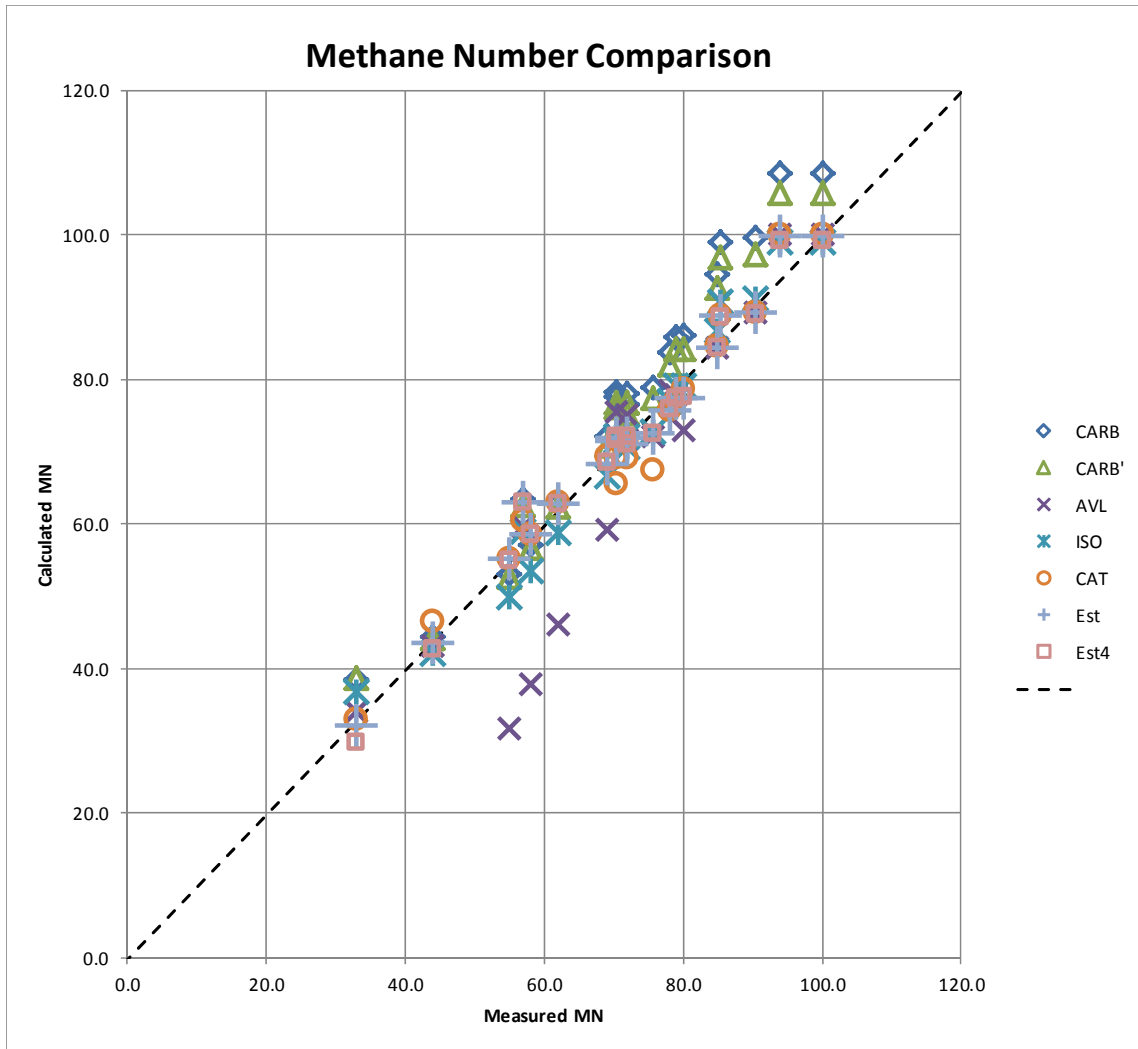


Figure 4 - Measured vs. Calculated MN

GRI/SwRI Methods

Kubesh et al. [14] of the Southwest Research Institute generated several different correlations to estimate motor octane number (MON). The MON is then curve fitted to determine a MN. The first MON method is based on a data regression of six gas compositions.

$$MON = 137.78 C1 + 29.948 C2 - 18.193 C3 - 167.062 C4 + 181.233 C02 + 26.994 N2 \quad (5)$$

Where the fuel gas compositions are in fraction by volume and

C1 represents methane content as a fraction of the total mixture

C2 represents ethane content as a fraction of the total mixture

C3 represents propane content as a fraction of the total mixture

C4 represents the sum of iso and normal butane and all heavier hydrocarbons content as a fraction of the total mixture

CO₂ represents carbon dioxide content as a fraction of the total mixture

N₂ represents nitrogen content as a fraction of the total mixture

As stated by Kubesh, this regression is limited to gases with methane content between 82-100%. The information from the Kubesh paper was used to perform my own least square fit based on the nine samples that had reliably measured MONs:

$$MON = 125.53 C_1 + 82.571 C_2 + 42.694 C_3 + 94.426 C_4 + 480.805 CO_2 + 41.274 N_2 \quad (6)$$

This regression appears to more accurate than equation 5. However, both equations 5 and 6 should be considered to be general approximations based on the small sample size used in their generation. Based on these limitations, it is not recommended that these equations be used.

The second MON method is based on a correlation of measured MON to the reactive hydrocarbon/carbon ratio (H/C).

$$MON = -406.14 + 508.04 H/C - 173.55 (H/C)^2 + 20.170 (H/C)^3 \quad (7)$$

There are two different regression equations identified by Kubesh to convert MON to MN:

$$MN = 1.624 MON - 119.1 \quad (8)$$

And

$$MN = 1.445 MON - 103.42 \quad (9)$$

Equation 8 is based on a regression of calculated MN from a model and measured MON¹⁰ while equation 9 is based on measured MN and measured MON numbers.

There are a number of technical limitations to the Kubesh paper:

- The analysis is limited to 12 gas samples tested plus two tests performed by others on propane and ethane only gases.
 - Of the 12 tests, three samples had to be excluded because the measured MON on the reference engine were above the maximum scale of the test engine.
 - Table 1 of the paper shows the same gas composition for Blends 6 and 7. The listed composition for Blend 6 is incorrect.¹¹
- To correlate MON to MN, only eight compositions were used (the first six of the twelve plus only propane and only ethane). These compositions were used because they had measured methane numbers.
- The measured MN for the only methane composition measured 94 when it should have measured 100 by definition indicating a possible calibration error.
- Using equation 8, a pure methane gas yields a MN of 108.4 vs. the 100 it should be by definition. By comparison, equation 9 yields a MN of 99.0 for a pure methane gas.
- These methods are not reliable for compositions that contain >1% hydrogen or contains any hydrogen sulfide in the fuel gas.

¹⁰ Based on the information provided in the paper, equation 8 could not be reproduced. The regression based on modeled MN was recalculated as $MN = 1.558 MON - 112.5$. Based on the new regression, a pure methane gas would have a MN of 105.8 (vs. the 108.4 obtained by equation 8). In Figure 4, this alternate fit is shown as the CARB' method.

¹¹ By comparison to Table 4 and back calculation of the MON, the correct values for Blend 6 was determined to be 83.3% methane, 3.0% ethane, 11.9% propane, 0.8% butane, 0.3% carbon dioxide, and 0.7% nitrogen.

- None of these methods are not reliable for compositions that contain >3% carbon dioxide. The analysis in this paper shows that the addition of diluent in the fuel increase the MON but the method excludes the impact of diluents.

Of the methods presented by Kubesh, equation 7 appears to be the best model for MON and equation 9 should be used to convert MON to MN.

Because these formulas are relatively straight forward, they can be readily implemented in engine control systems. However, these equations should be used with caution because they were based on limited gas compositions. These methods should not be used if the sum of ethylene, propylene, carbon monoxide, hydrogen, hydrogen sulfide, and helium exceeds 1%; alarm flags are used to indicate when the gas compositions are outside of these bounds.

ISO15403-1

ISO Standard 15403-1 [19] includes a discussion on MN and includes a calculation method based on equations 7 and 9 of the GRI/SwRI methods. The standard does not list the limits of the method. In Figure 4, this method is identified as *ISO*.

ISO/TR 22302

The MN in the technical report *ISO/TR 22302 Natural gas - Calculation of methane number* reference equations 5 and 7 of the GRI/SwRI methods to calculate MON and then use equation 9 to convert MON to MN. The standard recommended that if the calculations between the two methods are different by more than 6, the calculations should be considered to be in doubt and a test method should be used rather than the results of the calculation. The document also references the AVL method in passing stating it can be used to calculate MN but the exact algorithm is confidential to AVL. [20] [21]

CARB Method

The California Air Resources Board (CARB) method [22] was derived from the GRI/SwRI methods using equations 7 and 8. The paper specifies that the method adopted by CARB should not be used for reactive hydrogen/carbon ratios less than 2.5 or where inert concentrations are “greater than the typical 1-5 percent range.”

The CARB report is widely available via the internet and has been adopted by others [2] [23 p. 76] [24 p. 2] [25 p. 30] [26 p. 67] et al. Due in part to its public availability, this method has been adopted by some engine manufacturers. [27] However, the method does not appear to be accurate enough to be used for many gas compositions. The CARB method should only be used on existing engines that have adopted its use. In Figure 4, this method is identified as *CARB*.

AVL METHANE Method

The AVL method employs a series of ternary diagrams to estimate the MN using patented techniques. [28] These methods have been compiled into an application named METHANE. It should also be noted that this application treats all hydrocarbons that are pentane and higher as butanes. Some engine manufacturers exclude nitrogen when calculating the MN using the AVL application. The application also performs calculations on gas components not typically found in natural gas, including carbon monoxide, ethylene, and propylene.

The application appears to be reasonably accurate but the MN is over predicted if the gas contains >5% carbon monoxide. This calculation method is only available in compiled code format and thus is not suitable for direct usage in engine control systems. In Figure 4, this method is identified as *AVL*.

DGC Method

The Danish Gas Technology Centre (DGC) developed a method to calculate MN using interpolated AVL ternary diagrams. There is some error in the interpolation, especially with respect to hydrogen due to its nonlinear nature. The estimated uncertainty is ± 3 MN. [29 p. 11] The calculation methods are hosted on a DGC server and are available for use on a fee based subscription. [30] As such, the DGC method is not suitable for use in engine control systems.

E.ON GasCalc

The E.ON GasCalc application calculates MN in addition to other gas calculation properties. [13] The application is only available in compiled code format but appears to be based on the DGC/AVL methods. Because the application is only available in compiled format, it is not suitable for direct usage in engine control systems.

Caterpillar GERP Method

The specific methods used in Caterpillar's Gas Engine Rating Pro application [31] to calculate MN are unknown. However, the results produced are similar to those calculated by the AVL METHANE application with the exception that the application treats pentane and higher hydrocarbons differently than butane. As a result, gas compositions that have significant quantities of pentane and higher should be more accurately calculated with this tool than the AVL method. The application also performs calculations on gas components not typically found in natural gas, including carbon monoxide, ethylene, and propylene.¹² Because the application is only available in compiled format, it is not suitable for direct usage in engine control systems. In Figure 4, this method is identified as *CAT*.

Waukesha Knock Index

The Waukesha Knock Index (WKI) [32] uses a hybrid method employing curve fit equations for some gas composition ranges and a hydrogen/carbon ratio method (similar to the GRI/SwRI methods) for other compositions. Adjustments are made for inert gases. The curve fit equations apply and accommodate alkanes up to hexane.

The WKI method is unique in that it recognizes that isomers (e.g., iso-butane and iso-pentane) have different knock characteristics than their normal counterparts. This is addressed by assigning 58% of the iso-butane concentration to propane, the balance to normal butane and 68% of the iso-pentane concentration to normal butane and the balance to normal pentane. The model is stated to be valid for gases that are within the following concentrations:

- Methane 60-100%
- Ethane 0-20%
- Propane 0-40%
- Normal butane 0-10%

¹² The Wobbe Index as calculated by the Caterpillar method appears to be based on the lower heating value of the gas while the common convention calculates it based on the higher heating value. [24] In addition, the higher and lower heating values are only applicable for a base pressure of 14.696 psia. The most common base pressure for pipeline companies is 14.73 psia.

- Normal pentane 0-3%
- Hexane+ 0-2%
- Nitrogen 0-15%
- Carbon dioxide 0-10%

The WKI does not appear to work for gas compositions that have any significant concentrations of hydrogen or hydrogen sulfide. With the exception of pure methane, the WKI will generally calculate a higher value than either the AVL or Caterpillar method. [33 p. Fig. 9] The program is only available in a compiled format and thus is not suitable for direct usage in engine control systems.

Direct Measure Instruments

There are some instruments that directly estimate the MN based on measuring gas parameters such as the speed of sound and thermal conductivity. These instruments include the GasPT2 by CUI Inc., Elster Instromet Gas-lab Q1, and gasQS by MEMS AG. These devices have a stated accuracy in the range of ± 3 MN and have a faster response to changing gas compositions when compared to gas chromatographs. The range of gas compositions for the stated accuracy is not specified. These devices could be interfaced directly with engine control systems.

There are similar devices that don't directly infer MN that calculate the heating value and specific gravity which can be used to estimate MN using the methods outlined below.

MN Approximation

Based on the literature review performed for this effort and MN calculations on the gas composition data set, the following MN estimation method has been developed:

$$MN = MN_{Raw} + H2S_{Adj} + CO2_{Adj} - 100 H2 \quad (9)$$

Where

$H2S_{Adj}$ is an adjustment for hydrogen sulfide

$CO2_{Adj}$ is an adjustment for carbon dioxide

And MN_{Raw} is calculated by:

$$MN_{Raw} = 34.26 HCR_{Adj} + 2.944 \cdot 10^{-9} SG_{Adj} (21.31 HCR_{Adj}^2)^{HCR_{Adj}} - 59.2 \quad (10)$$

Where

HCR_{Adj} is the hydrogen to carbon ratio for only combustible components (renormalized to 100%) with H2 treated as C1

SG_{Adj} is the specific gravity for only combustible components with H2 treated as C1

And $H2S_{Adj}$ is calculated by:

$$H2S_{Adj} = -14.83 H2S - 1.048 H2S^{0.002036} \quad (11)$$

Where

$H2S$ is the fraction of hydrogen sulfide by volume¹³

¹³ Hydrogen sulfide is commonly measured in grains per 100 cubic feet. To convert from grains to fraction, multiply by 0.000016.

And

$$CO2_{Adj} = 57.094 CO2^2 MN_{Raw} + 1.161 \cdot 10^{-6} CO2 MN_{Raw}^4 - 0.0811 - 45.208 CO2 - 2153.39 CO2^2 - 253.97 CO2^3 - 0.3377 CO2^2 MN_{Raw}^2 \quad (12)$$

For the $CO2_{Adj}$ calculation, the MN_{Raw} value should be clamped to a minimum value of 70 (if the calculated value of MN_{Raw} is less than 70, use a value of 70 for equation 12).

This method provides reasonable results when compared to the AVL and Caterpillar methods. Unlike the AVL method, this method treats C5+ components differently than butane but they do not reduce the MN as aggressively as the Caterpillar method does. This method is not suited for compositions with >1% ethylene, propylene, or carbon monoxide. This method could be employed in engine control systems. In Figure 4, this method is identified as *Est*.

Four Component Estimation

For four component gas compositions, the MN_{Rawj} used in the MN Estimation method (equation 9 above) can be approximated by estimating HCR_{Adj} and SG_{Adj} :

$$SG_{Adj} = \frac{(28.964 SG - 44.01 CO2 - 28.013 N2)}{28.964 (1 - CO2 - N2)} \quad (13)$$

$$HCR_{Adj} = 1.8002 + \frac{1.2164}{SG_{Adj}} \quad (14)$$

With only four component data, the carbon dioxide content is known but hydrogen content is not therefore the calculations for $CO2_{Adj}$ are performed the same as the full composition method but $H2$ in equation 9 is set to zero.

This method will not be reliable if the sum of ethylene, propylene, carbon monoxide, hydrogen, hydrogen sulfide, and helium exceeds 1%. This method could be employed in engine control systems. In Figure 4, this method is identified as *Est4*.

CONCLUSIONS

Calculation of SAFR is an important parameter for managing engine control and is relatively straight forward to calculate. A four component method has been generated that is suitable for many natural gas compositions.

Methane number can be an important tool in engine optimization. Observations on MN from this effort include:

- If an engine manufacture uses a specific method to calculate MN, that same method should be used to evaluate the fuel gas for its applicability to that engine. Should the fuel gas have constituents that are not suitable for that method, they should consult the engine manufacture for assistance.

- Unless used by the engine manufacture, only equations 7 and 9 of the GRI/SwRI methods should be used. Care must be employed to use these equations on gases with low hydrogen and inert content.
- The MN is measured under stoichiometric conditions. Additional model refinement should estimate the effects of variable air/fuel ratio.
- Current MN calculations do not alter the MN based on water content in either the fuel or the air. Additional research may be warranted to evaluate and quantify this effect.
- There is very little by way of actual measured MN data in the public domain. The development of robust MN models for broader fuel ranges may require additional measured MN data, especially with respect to C5+ components.
- The flame speeds and autoignition temperatures of the iso and normal components appear to be very different. Additional research may be of interest to better delineate the impact to the MN by these subspecies.
- New methods have been developed for MN calculations that are comparable to the results from the AVL and Caterpillar methods. These methods are available as open source VB.NET code: <https://github.com/gchoquet/EngineControlSoftware>.
- Reasonable approximations for MN can be produced from a four component gas analysis for many gas compositions provided the compositions contain no hydrogen.

ACKNOWLEDGMENTS

Special thanks to Dr. Daniel Olsen, Dr. Jacob Klimstra, and Dr. Ghazi Karim for providing reference material and analysis tools and Jacob Hedrick for his review and comments.

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NOMENCLATURE

<i>C1</i>	Mole fraction of methane
<i>C2</i>	Mole fraction of ethane
<i>C3</i>	Mole fraction of propane
<i>C4</i>	Mole fraction of normal and iso butane
<i>C5</i>	Mole fraction of normal and iso pentane
<i>C6</i>	Mole fraction of hexane
<i>C7</i>	Mole fraction of hexane
<i>C8</i>	Mole fraction of octane
<i>CO2</i>	Mole fraction of carbon dioxide
<i>C_{Mol}</i>	Composition weighted carbon content
<i>H2</i>	Mole fraction of hydrogen
<i>H2S</i>	Mole fraction of hydrogen sulfide
<i>HHV</i>	The higher heating value of the gas
<i>H_{Mol}</i>	Composition weighted hydrogen content
<i>MN</i>	Methane number
<i>MN_{Adj}</i>	Base methane number adjustment
<i>MON</i>	Motor octane number
<i>N2</i>	Mole fraction of nitrogen
<i>N_{Mol}</i>	Composition weighted nitrogen content
<i>O_{Mol}</i>	Composition weighted oxygen content
<i>SAFR</i>	Stoichiometric air/fuel ratio in lb air/ lb fuel
<i>SG</i>	Specific gravity of a gas relative to air
ϕ	Equivalence ratio (actual fuel/air times <i>SAFR</i>)

APPENDIX A – Gas Properties for Key Natural Gas Components

Component	Mole Wt	Hydrogen atoms	Carbon atoms	Cp	HHV	LHV	Auto Ignition Temp °F	Flame Speed @ ϕ (in/s)				
								0.6	0.8	1.0	1.2	1.4
H2	2.0159	2	0	3.4010	324.2	273.9	752	31.74	56.10	78.99	93.75	106.30
C1	16.0430	4	1	0.5266	1009.7	909.1	999	3.83	10.95	14.65	12.54	5.67
C2	30.0690	6	2	0.4080	1768.7	1617.8	959	4.49	11.12	15.91	16.32	10.40
C3	44.0960	8	3	0.3887	2517.2	2315.9	871	5.36	11.48	15.53	15.42	9.51
IC4	58.1220	10	4	0.3867	3252.6	3001.0	864	6.34	12.58	17.39	18.04	13.67
NC4	58.1220	10	4	0.3951	3262.0	3010.5	761	5.03	10.50	14.44	13.89	7.87
IC5	72.1510	12	5	0.3829	3999.7	3697.9	788					
NC5	72.1510	12	5	0.3880	4008.7	3706.8	496					
C6	86.1780	14	6	0.3857	4756.1	4403.9	433					
C7	100.2050	16	7	0.3842	5502.8	5100.3	433					
C8	114.2320	18	8	0.3831	6248.9	5796.1	428					
H2S	34.0760	2	0	0.2370	586.7	637.0	500					

Notes:

1. Specific heat (Cp) at constant pressure conditions near atmospheric
2. Heating values in BTU/SCF at 14.696 psia, 60 °F, and uncorrected for compressibility from GPA 2545-09
3. Auto ignition temperatures from Flammability Characteristics of Combustible Gases and Vapors [34]
4. Laminar flame speed from University of Southern California Combustion Kinetics Laboratory [35]