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Investigation of an Anti-Knock Index and Hydrocarbon Emissions of Various Natural Gas Blends

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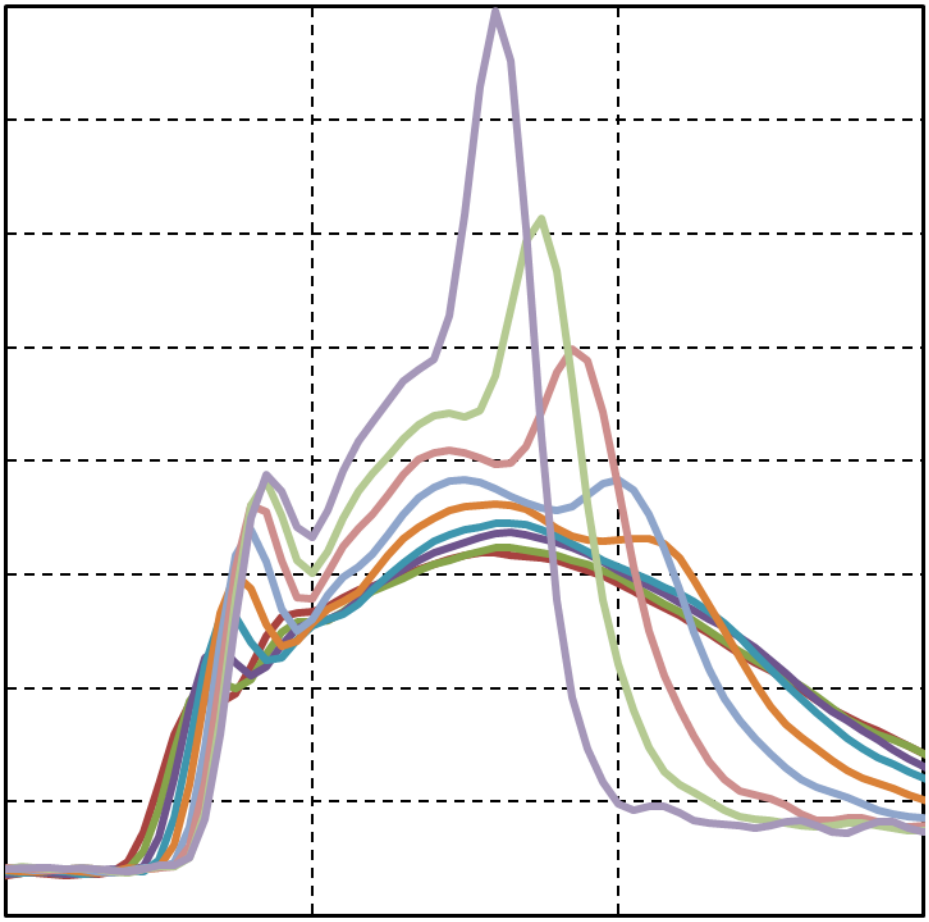

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13. ABSTRACT (Maximum 200 words)

The North American rail industry is examining the use of natural gas to reduce fuel costs for locomotives that are powered by dual fuel engines. This report evaluates the ability of an existing methane number algorithm to predict rapid combustion in a dual fuel engine. The Methane Number index, which quantifies the propensity of a gaseous fuel to autoignite, has the ability to well-characterize engine knock in spark-ignited combustion. However, the ability of the methane number, which was originally developed for spark-ignited engines, to predict a fuel's "knock" behavior in dual fuel combustion is not fully understood.

Specialized natural gas fuel blends are tested in a dual fuel engine and induced to rapid combustion. For fuels that should exhibit similar knock behavior, the transitions to rapid combustion occurred at significantly different conditions. This demonstrated that the existing methane number algorithm, while excellent for spark-ignited engines, did not fully predict the propensity for rapid combustion to occur in a dual fuel engine within the scope of this study. In its current form, a methane number algorithm can be used to conservatively rate dual fuel engines. It is possible that a new reactivity index for dual fuel combustion might allow ratings to be less conservative.

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1 gallon (gal) = 3.8 liters (l)	
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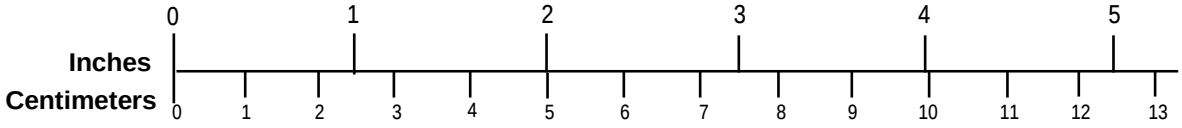

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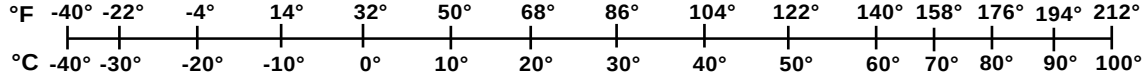

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Contents

Illustrations

Tables

Executive Summary

Low natural gas prices have made natural gas an attractive alternative to diesel and other common fuels, particularly in applications that consume large quantities of fuel. The North American rail industry is examining the use of locomotives powered by dual fuel engines to realize savings in fuel costs. This report documents efforts to evaluate the ability of an existing methane number algorithm to predict rapid combustion in a dual fuel engine.

Dual fuel engines can replace a large portion of diesel fuel with premixed natural gas and intake air. Traditional pre-mixed spark-ignited combustion can cause engine knock, which is undesirable but well characterized by the methane number index. This index, which was originally developed for spark-ignited engines, quantifies the propensity of a gaseous fuel to autoignite after a period of time at high temperature. However, the ability of the methane number index to predict a fuel's "knock" behavior in dual fuel combustion is not fully understood.

Sets of specialized natural gas fuel blends that should have similar knock characteristics (according to the Motoren-Werke Mannheim GmbH (MWM) methane number algorithm) were tested in a dual fuel engine and induced to experience rapid combustion. Test results and Computational Fluid Dynamics (CFD) analysis revealed that rapid or aggressive combustion rates happened late in the dual fuel combustion event with this engine hardware configuration. The transition from normal combustion to late rapid combustion was characterized by changes in the heat release rate profiles. In this study, the transition is also represented by a shift in the crank angle location of the combustion's peak heat release rate. For fuels of similar methane number that should exhibit similar knock behavior, these transitions occur at significantly different relative air-fuel ratios. This demonstrates that the existing MWM methane number algorithm, while excellent for spark-ignited engines, does not fully predict the propensity for rapid combustion to occur in a dual fuel engine within the scope of this study.

In its current form, a methane number algorithm can be used to conservatively rate dual fuel engines. However, physical and chemical phenomena present in rapid or aggressive dual fuel combustion processes may differ from those in knocking spark-ignited combustion. Perhaps a new reactivity index that better predicts rapid combustion behavior of the gaseous fuel in dual fuel combustion would allow ratings to be less conservative.

1. Introduction

This section introduces the concept of the methane number and describes the objective and scope of the research program.

1.1 Background

In the United States, horizontal drilling and hydraulic fracturing have produced an abundance of natural gas and reduced the fuel's price significantly. In many industrial sectors where fuel costs are significant, natural gas might be used as a low-cost alternative to traditional fuels. To take advantage of this fuel cost benefit, the North American rail industry is examining the use of dual fuel engine systems, which use a combination of diesel and natural gas to power the locomotive. In dual fuel combustion, a reduced injection of diesel fuel burns and ignites a premixed charge of natural gas and air in the cylinders. Current dual fuel engines in this size class can range from operating on diesel fuel only (0% substitution of fuel energy with premixed natural gas) to as high as 80% substitution of diesel with premixed natural gas.

If dual fuel engine technologies in the North American locomotive market are adopted, an industry-wide fuel standard for natural gas will be necessary. A critical part of the standard will be a method for specifying resistance to "knock" or rapid combustion required of the gaseous fuel. Knock in spark-ignited (SI) engines is the rapid, unintended, volumetric combustion of premixed fuel that can damage internal engine components. Knock in dual fuel combustion is distinctly different than knock in SI engines and not clearly defined in the current state of the literature. It is characterized by rapid or aggressive combustion rates during a portion of the combustion event, and many terms, including "knock" and "aggressive combustion", have been used to describe this. This study describes this duel fuel-related phenomenon as rapid combustion to avoid confusion and comparison to knock in SI engines.

Gaseous fuels for spark-ignited engines commonly use the "methane number," a measure that quantifies their tendency to knock. Existing methane number algorithms were developed for SI combustion of gaseous fuel as early as the 1970s [1]. Yet combustion in a dual fuel engine is unique and distinctly different than SI combustion. For example, the stoichiometric zones of the multiple diesel injection plumes burn and provide a very large, turbulent surface area for ignition and propagation of the combustion reaction through the premixed natural gas and air. In contrast, traditional SI combustion typically has just one distinct point of ignition. Then the flame front propagates outward from the single, initially slow-growing, kernel of reaction.

Since there fundamental differences in the combustion characteristics of SI and duel-fuel engines, it is not certain if the current methane number algorithms that can predict knock in SI combustion would also fully represent the rapid combustion behavior in dual fuel engines. This project evaluated the ability of an existing methane number algorithm to predict when rapid combustion would occur in the gaseous air-fuel mixture within a dual fuel engine.

Liquid hydrocarbon fuels have established indices for knock/auto-ignition performance, most notably the Octane Number for gasoline and the Cetane Number for diesel fuel They are standardized in both definition and testing method by American Society for Testing and Materials (ASTM) standards D2699/D2700 (Octane Number and D613 (Cetane Number). Gaseous fuels, on the other hand, have no standardized index or test for anti-knocking performance. Early studies found that the Octane Number scale (defined with two liquid

reference fuels) has limited applicability to gaseous fuels, especially in natural gas blends with more than 90% methane [2]. In 1971, researchers from **Anstalt für Verbrennungskraftmaschinen List GmbH** (AVL) introduced a anti-knock index named the Methane Number (MN) specifically for gaseous fuels [1]. Their seminal work led to a method to calculate the methane number of a gaseous fuel, primarily various types of natural gas, based on the molar composition of the fuel. The methane number scale is bounded by two gaseous reference fuels, namely hydrogen (0 MN, more likely to auto-ignite) and pure methane (100 MN, difficult to auto-ignite). Table 1 presents the components considered by the original AVL method when determining the methane number. The extensive experimental data collected by AVL was transformed into a series of two- and three-axis charts from which the methane number can be calculated from the gas composition.

Since the methane number and the AVL method were introduced, many efforts found similar results when testing the methane number of various natural gases or have proposed adjustments and corrections to accommodate additional species and wider composition ranges [3-5]. For example, Gersen et al. performed simulations and experiments to include the effects of carbon monoxide (CO) on the methane number by comparing the knock-limited spark timing [6]. Eventually, these efforts led to many marginally-similar algorithms being used across the industry to calculate a methane number.

Table 1: Species included in the original AVL method

Hydrocarbon Species	Other Species
Methane (CH_4)	Nitrogen (N_2)
Ethane (C_2H_6)	Hydrogen (H_2)
Propane (C_3H_8)	Carbon Dioxide (CO_2)
n-Butane (C_4H_{10})	Hydrogen Sulfide (H_2S)

Caterpillar Inc., like many other companies (including Waukesha, Cummins Westport, AVL, and MWM [3, 7-9]), used historical regression data to establish a proprietary Caterpillar methane number for a given fuel to which an SI engine must be calibrated and rated. The specific methane number algorithms of these companies are proprietary or are restricted by licensing, which has impeded efforts to standardize on any particular algorithm.

In contrast, a publicly available algorithm created by Ryan et al. at Southwest Research Institute that determines the methane number of a fuel given its composition [10]. First, the team induced 31 natural gas fuel blends to knock on a single cylinder SI engine by varying the compression ratio. The data was then fit using a 28-term algorithm to predict methane number based on species concentrations of methane, ethane, propane, butane, pentane, and carbon dioxide. The algorithm fit has an R2 value of 0.94 and a standard error of ±3.0 MN. Comparison of this calculation shows similarity with several proprietary company standards.

Figure 1 illustrates the variation in selected methane number algorithms for 25 natural gas fuel samples taken from pipelines and wellheads by the U.S. Bureau of Land Management between 2007 and 2008. It includes algorithms from MWM GmbH (now Caterpillar Energy Solutions GmbH), Cummins Westport Inc., Waukesha (owned by General Electric Co.), Ryan et al. from

Southwest Research Institute, and an updated algorithm from AVL GmbH. Comparison between the natural gas samples reveals that there are commonly as many as 10-15 units of methane number difference between the algorithms in use today.

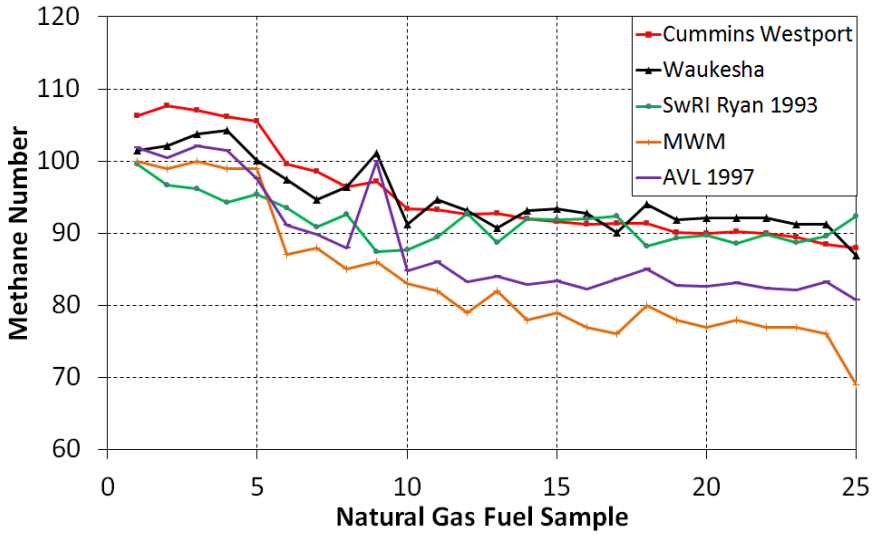

Figure 1: Methane number algorithm comparison using domestic pipeline and wellhead gas samples from the U.S. Bureau of Land Management

For the mobile machinery and transportation sectors, the variation in methane number calculation across the industry presents difficulties. According to one company's algorithm, fuel distributors may supply a natural gas fuel that has an acceptable methane number for use in specific locomotives, whereas that same fuel may have a methane number deemed unacceptable for another locomotive with a different engine system based on that manufacturer's algorithm. Beyond the algorithm itself, there is no mutually accepted value of methane number for the rail industry, such that engines must be calibrated to accept a wide variation in reactivity of the gaseous fuels. Creation of a fuel specification for dual fuel engines with an appropriate index or measure of fuel reactivity will allow further engine optimization, resulting in improved performance and wider acceptance of lower cost natural gas fuel.

1.2 Objectives

This project's goal is to evaluate the ability of an existing methane number algorithm to predict rapid combustion in a dual-fuel engine. If an existing methane number algorithm accurately represents the rapid combustion behavior of a dual-fuel engine, then recommend it for inclusion in a rail industry natural gas fuel standard. If not, future work could develop an index or metric specifically for dual-fuel combustion.

1.3 Overall Approach

This project's methodology employs engine testing, data analysis, and 3D CFD modeling. Several specialized and controlled natural gas fuel blends of different compositions are used to fuel the engine and knock (or rapid combustion) behavior is induced. Comparisons and analyses

of rapid combustion behavior is made for fuel blends with similar methane numbers. CFD modeling is used to enhance understanding of the in-cylinder process for dual-fuel rapid combustion.

1.4 Scope

The scope of this project is limited to commercial-grade natural gas in North America of ≥ 70 MN in a dual fuel engine. The scope is also limited to the specific hardware configuration and operating condition described throughout Section 2.

1.5 Organization of the Report

This report is organized to introduce the methane number of a fuel, describe the experimental testbed, outline the testing procedure, and describe the results and discussion. It ends with conclusions, recommendations, and an introduction of future research opportunities.

2. Methane Number and Dual Fuel Combustion

This section presents the procedure, test results, analysis, and discussion of the findings.

2.1 MWM Methane Number Algorithm

The team chose to evaluate the MWM methane number algorithm and its applicability to dual fuel combustion for this study. The index is being adopted as the measure of knock propensity for SI engines in the European natural gas standard EN 16726 as recommended by the European Association of Internal Combustion Engine Manufacturers (Euromot) [11]. It is also recommended for inclusion in the ASTM natural gas standard under development in the United States. Due to its role in standardization and harmonization for SI engines, the MWM methane number algorithm has become publicly available for no charge.

The MWM methane number calculation accounts for 17 species, including both saturated (paraffins) and unsaturated (olefins, one diolefin) hydrocarbons, as well as other components as shown in Table 2. It is a complex algorithm that was based on the original AVL MN but has been modified over time to include several updates and corrections. Despite its complexity, it is implemented in a Microsoft Excel-based graphical user interface (GUI) that is simple to execute. Details of the algorithm are published in the annex of EN 16726.

Table 2: Species included in the MWM algorithm

Hydrocarbon Species	Other Species
Methane (CH_4) Ethylene (C_2H_4) Ethane (C_2H_6) Propylene (C_3H_6) Propane (C_3H_8) Butadiene (C_4H_6) Butene (C_4H_8) Butane (C_4H_{10}) Pentane (C_5H_{12}) Hexane+ (C_6 and above)	Nitrogen (N_2) Hydrogen (H_2) Oxygen (O_2) Carbon Monoxide (CO) Carbon Dioxide (CO_2) Water Vapor (H_2O) Hydrogen Sulfide (H_2S)

2.2 Experimental Testbed

Testing of different natural gas fuel blends using the MWM methane number algorithm was performed on a Navistar Maxxforce 13L dual fuel engine at Southwest Research Institute in San Antonio, Texas. Specifications for the engine are presented in Table 3. This testbed was chosen for its dual fuel configuration, external boosting capability, and access to a specialized fuel blending system.

Table 3: Engine testbed specifications

Engine Family	MaxxForce 13 (Model A410)
Cylinder Arrangement	Inline 6
Bore	126 mm
Stroke	166 mm
Displacement	12.4 L
Compression Ratio	18:1
Valvetrain	4 Valves/cylinder, DOHC
Rated Speed	1700 rpm
Peak Torque Speed	1000 rpm
Maximum BMEP*	23.4 bar
Turbomachinery	Sequential 2-stage turbochargers, external boosting capability
Diesel Injection System	2200 bar common rail
Natural Gas Fuel System	Fumigation post-compressors
Natural Gas Fuel	On-site fuel blending

* BMEP - Brake Mean Effective Pressure

This experimental test engine uses a dual fuel combustion system, which is similar to other systems that are being implemented for Environmental Protection Agency (EPA) Tier 4 compliant locomotives. It is a single-point fumigation system that mixes natural gas into the intake air after the turbocharger compressors but before it reaches the intake manifold, driving a premixed charge into the cylinder. A direct-injection common rail fuel system injects diesel fuel into the cylinder near or before top dead center (TDC). The compression-ignited diesel injection burns and in turn ignites the natural gas and air mixture.

The testbed also has a unique external boosting capability. An electrically-driven compressor can provide additional pressurized air flow to the intake system in a controlled manner. This additional degree of freedom enables the air-fuel ratio of the engine to be varied independently of other control actuators. This is used to perform the sweeps of the relative air-fuel ratio that are used to induce rapid combustion.

A specialized fuel blending system enables evaluation of the MWM methane number algorithm for various blends of natural gas. On site at Southwest Research Institute is a large metal sphere that can be charged with precise amounts of individual fuel components to create a well-controlled fuel blend. Then the large sphere is connected to the test engine and it supplies the gas fumigation system for the duration of the test. Though the composition of natural gas from a pipeline can vary with time (sometimes acutely), this fuel blending capability allows for testing of precise mixtures that do not change with time.

2.3 Procedure

Methane number and knock/rapid combustion testing can be approached in many different ways. Cooperative Fuels Research (CFR) engines with variable compression ratios were used in some of the earliest methane number testing for SIs [1-4]. The engine would run a test fuel and the compression ratio would be increased until light knock was observed. While conditions were held constant, blends of pure methane with increasing amounts of hydrogen (the two reference

fuels for the methane number scale) would be run until enough hydrogen was added to induce a light knock of the same intensity again. At this point, the amount of pure methane in the blend defined the methane number of the test fuel. For example, if a blend of 85% CH_4 and 15% H_2 transitioned to SI knock at the same conditions the test fuel did, the test fuel would be designated as 85 MN.

Since subsequent studies did not use a CFR engine and varied blends of hydrogen and pure methane, they employed other methods to induce knock (or rapid combustion) and correlate to the methane number scale. Other methods for inducing knock besides increasing an engine's compression ratio, include advancing spark timing (SI engines), advancing the diesel start of injection (dual fuel engines), enrichening the air-fuel ratio, increasing the load, or increasing the intake manifold temperature. Less common ways include varying the Exhaust Gas Recirculation (EGR) flow, using residuals in the cylinder, and manipulating fuel reactivity.

In this study, the air-fuel ratio is varied to produce favorable engine conditions for rapid combustion. In this process, the relative air-fuel ratio, also known as lambda (λ), is swept from lean conditions (typical for dual fuel engines) to increasingly fuel-rich conditions until rapid combustion is observed.

This study performed lambda sweeps for different fuel blends. If the MWM methane number algorithm fully represents dual fuel combustion, the sweeps should have exhibited the same rapid combustion behavior. There are many different gas compositions that can result in the same methane number rating. These different compositions are tested in the engine and rapid combustion is observed. If different blends have the same methane number transition to rapid combustion at the same point in the lambda sweep, it will show that the MWM methane number algorithm accurately predicts fuel reactivity in the dual fuel engine. If the fuel blends of the same methane number exhibit different transitions to rapid combustion, it will be evident that within the limited scope of this study, the traditional methane number algorithm is less capable of predicting the occurrence of rapid combustion in dual fuel engines and that other phenomena are present in rapid dual fuel combustion that are distinct from knocking SI combustion.

A total of ten natural gas fuel blends were used to rigorously test the MWM methane number algorithm. In this study, three different 70 MN fuel blends are made using methane, propane, and butane. One blend is a methane-propane mixture, another is a methane-butane mixture, and the last includes methane, propane, and butane together. These three blends have distinctly different compositions but are all rated at 70 MN and thus should exhibit similar rapid combustion behavior if the MWM algorithm is well suited to represent fuel reactivity in dual fuel combustion systems.

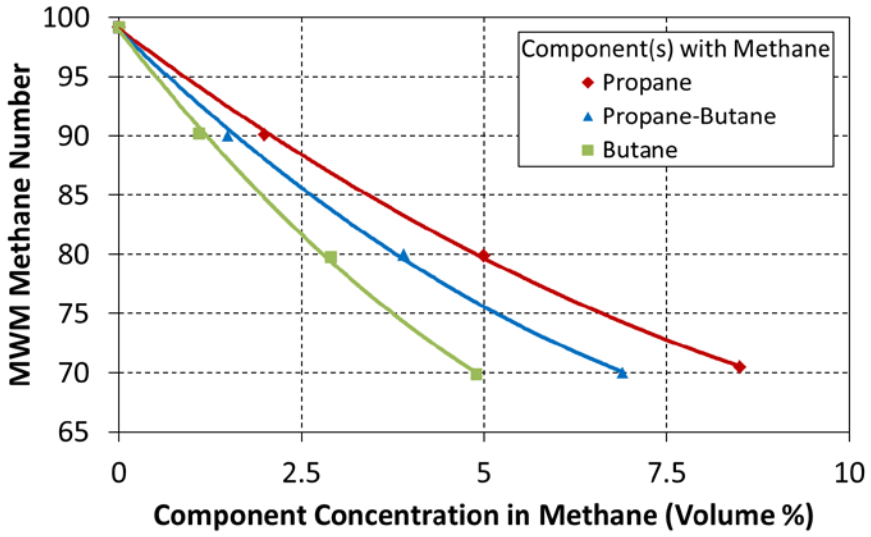

Figure 2: MWM MN for test blends of methane with propane and/or butane

Another three blends of methane, propane, and butane were made at 80 MN, and yet another three were made at 90 MN. The final blend of test fuel is nearly pure methane at 98 MN. This MN span represents the range of North American commercial-grade fuel that may be used in locomotives. Figure 2 charts the MWM methane number of the test fuels versus component concentration in methane for the test fuels, and Appendix A contains detailed composition data of the test fuels . Note that some of the methane that was used to make the blends contained small amounts of ethane, which is taken into account as the MWM methane number is calculated.

Testing of the blends was performed at 1300 rpm with the load held at 13 bar BMEP. The proportion of diesel to natural gas was held constant at 73% of the fuel energy on a lower heating value basis. The start of the diesel injection is constant at 8° crank angle (CA) BTDC, the intake manifold temperature is held constant at 40°C, and no EGR is used. Although data is collected on all six of the cylinders, the data presented here is from cylinder 3 only as it is always the first to experience rapid combustion under these conditions. The data is averaged over 300 engine cycles. Note that the lambda values reported below are calculated for just the natural gas and air, which is more representative of the mixture in the unburned zones where rapid combustion can occur.

2.4 Results & Discussion

Sweeps of lambda for all ten of the test fuels, from lean to rich, were performed at the previously described conditions. Figure 3 displays the apparent heat release rate (AHRR) as a function of crank angle for the lambda sweep of the 80 MN methane-propane mixture. There is a local peak in heat release rate shortly after TDC, due to combustion of the premixed portion of the diesel injection, and then the burn rate increases again as the premixed natural gas and air ignite and burn. The leanest case ($\lambda = 2.78$) shows the premixed diesel peak and then a normal, smooth heat release rate with no knock or rapid combustion. As the mixture becomes gradually more fuel-rich, a small increase in heat release rate is observed near the end of the combustion event,

signifying that a small amount of fuel is beginning to burn rapidly. The first instance of this light, late rapid combustion occurs for the λ = 2.22 case at roughly 17°CA after top dead center (ATDC). Becoming even more fuel-rich, the magnitude of the late rapid combustion event grows aggressively until it becomes the dominant feature of the heat release rate profile, as seen in the richest case of λ = 1.68.

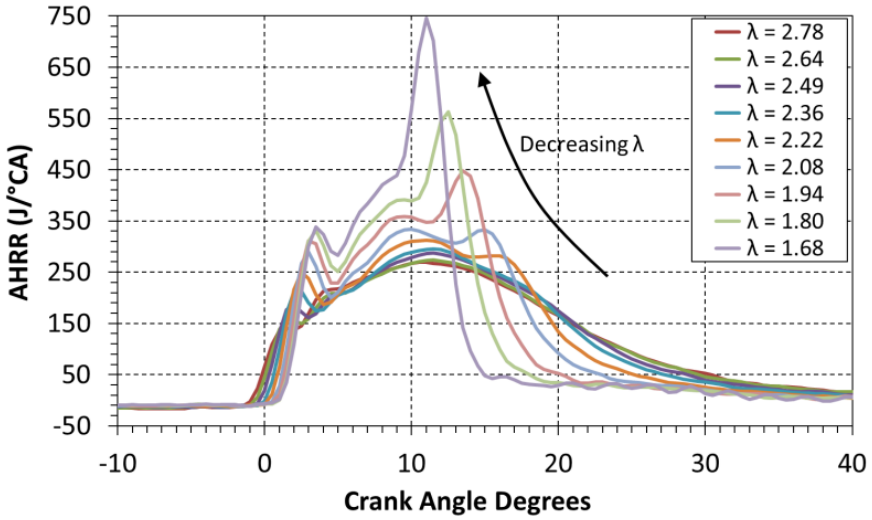

Figure 3: Lambda sweep of 80 MN methane-propane mixture showing AHRR vs. crank angle

Lambda sweeps for the other fuels exhibit similar behavior, and rapid combustion occurs near the end of each combustion event. Combustion CFD results for this hardware set at 1300 rpm, 18 bar BMEP, λ = 1.67, and 70% substitution by energy provide insight. The test engine has a wide, spherical bowl in the pistons. The CONVERGE combustion CFD results presented in Figure 4 show equivalence ratio and chemical heat release rate at four crank angle locations. The first case at 4°CA ATDC shows the well-developed diesel injection with heat release at the stoichiometric boundaries of the plume. The second case at 10°CA shows the reaction now propagating away from the diesel spray into the premixed natural gas-air mixture, already well into the squish area and near the crevices, while a significant unburned zone exists in the bottom center of the piston bowl.

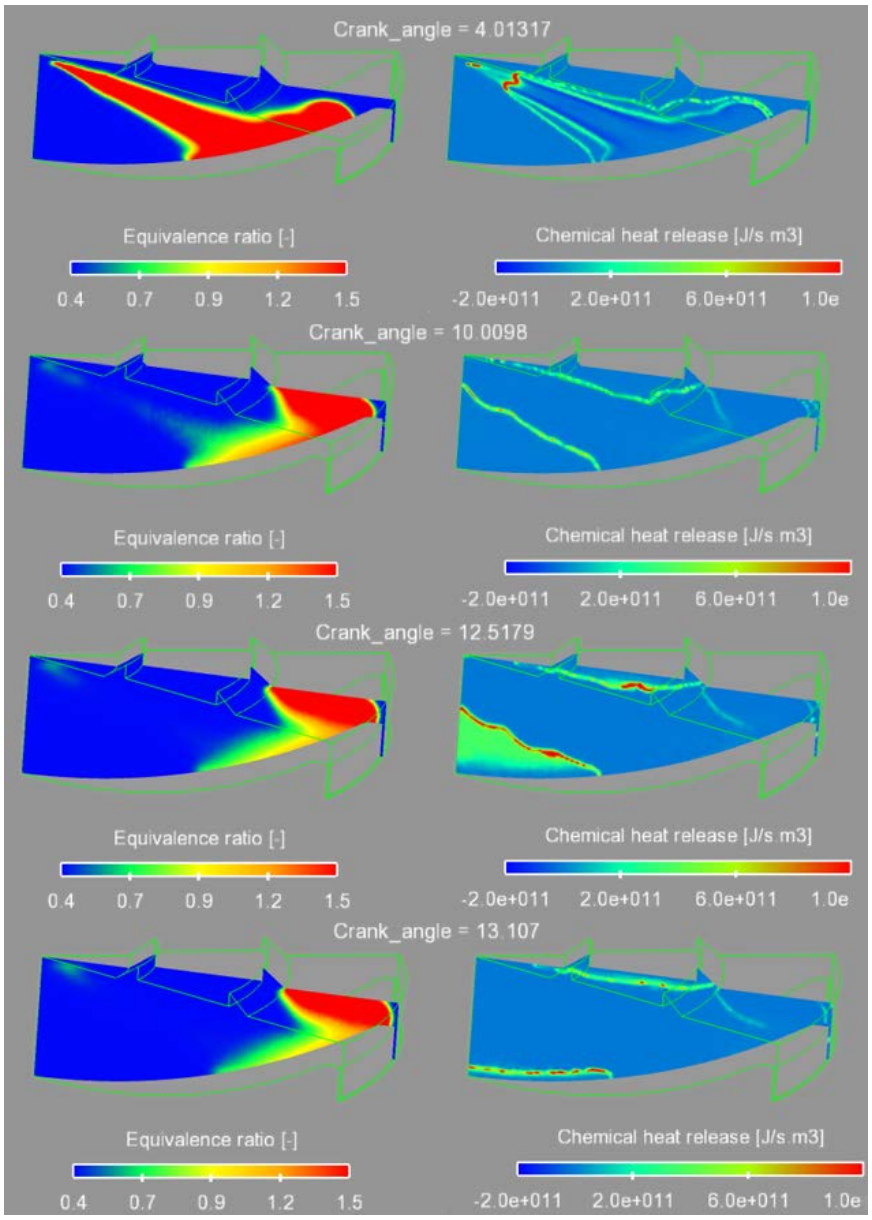

Figure 4: Combustion CFD results for equivalence ratio and chemical heat release rate at 4, 10, 12.5, and 13.1°CA ATDC

The third case at 12.5°CA shows the mixture at the bottom of the bowl starting to react, and the fourth case at 13.1°CA shows nearly all of the remaining mixture in the bowl being burned. In just 0.6°CA the significant unburned zone in the bottom of the bowl reacts rapidly, creating the large, late spike in heat release rate observed for the lambda sweep in Figure 3. The combustion CFD results show that the repeatable, late timing of the peak in heat release rate is due to rapid combustion in the bottom center of the piston bowl, attributed to the spray targeting and combustion chamber geometry of this hardware set.

The combustion CFD results provide another vital insight. Methane number algorithms for SI combustion are developed to predict knock in the unburned end gas (a mixture of the gaseous fuel and air). In a dual-fuel combustion system, over-penetration of the diesel injection could lead to unreacted diesel fuel mixing into the unburned natural gas-air mixture, altering the chemical kinetics and progression to knock or rapid combustion. Altered chemical kinetics like this are not captured by existing methane number algorithms. Fortunately, the progression of equivalence ratio plots in Figure 4 reveals that the equivalence ratio increase from the diesel injection does not penetrate or mix into the bottom center of the bowl where the late rapid combustion occurs, leaving the natural gas-air mixture intact.

Comparison of the lambda sweeps of three different fuel blends of similar methane number requires two steps. First, the transition from normal to rapid combustion must be characterized. Second, the lambda values where this transition occurs, termed the critical lambda (λ_{cr}), are compared. Again, if the critical lambdas are close for fuels of similar methane number, their reactivity is similar and the MWM methane number captures it well. If the critical lambda values are dissimilar, more complex combustion phenomena are present and the existing MWM algorithm, while excellent for SI combustion, does not fully capture all of the effects.

Characterizing the transition to rapid combustion is a challenge, as no universal definition of knock exists, particularly for dual fuel combustion. Combustion parameters are used to emulate the transition to rapid combustion in the lambda sweeps, including the maximum in-cylinder pressure rise rate (bar/°CA) and knock intensity (KI) as

$$KI = \int_{-10}^{+90} HPF(P, 3.5kHz)^2$$

where HPF is a high pass filter at 3.5 kHz and P is the in-cylinder pressure signal. Neither of these two parameters gives a clear indication of the transition to rapid combustion. In addition, a threshold using the maximum in-cylinder pressure rise rate will not scale well to other engine speeds given that the time-crank angle relationship and variation in the early diesel premixed burn spike will influence the knock intensity calculation and make them both unfavorable candidates. Yet understanding the late location of the rapid combustion as seen in Figures 3 and 4 provides another parameter for consideration. As the increasingly rapid combustion burns faster and shortens the end of the combustion event, the 50-90% burn duration will be influenced.

Figure 5 presents the 50-90% burn duration for the lambda sweeps of all ten fuel blends. As the lambda is swept from lean to rich, all fuel blends shortened the 50-90% burn duration. This is consistent with increasing magnitudes of late rapid combustion. However, all of the trends are monotonic in nature and none show a clear or distinct transition to rapid combustion. Characterizing or defining a threshold at which these fuels transition from normal to significant rapid combustion is difficult, given the gradual increase in magnitude of the late rapid combustion in the lambda sweeps. Beyond this, Figure 5 displays significant variation in combustion rates among similar fuel blends. For example, the three red curves in Figure 5 represent the three 80 MN fuel blends. The window where the 50-90% burn duration falls between 10 and 12°CA occurs at largely different values of lambda (nominally 2.3, 2.7, and 3.3 λ), highlighting differences in the combustion processes at these specific conditions.

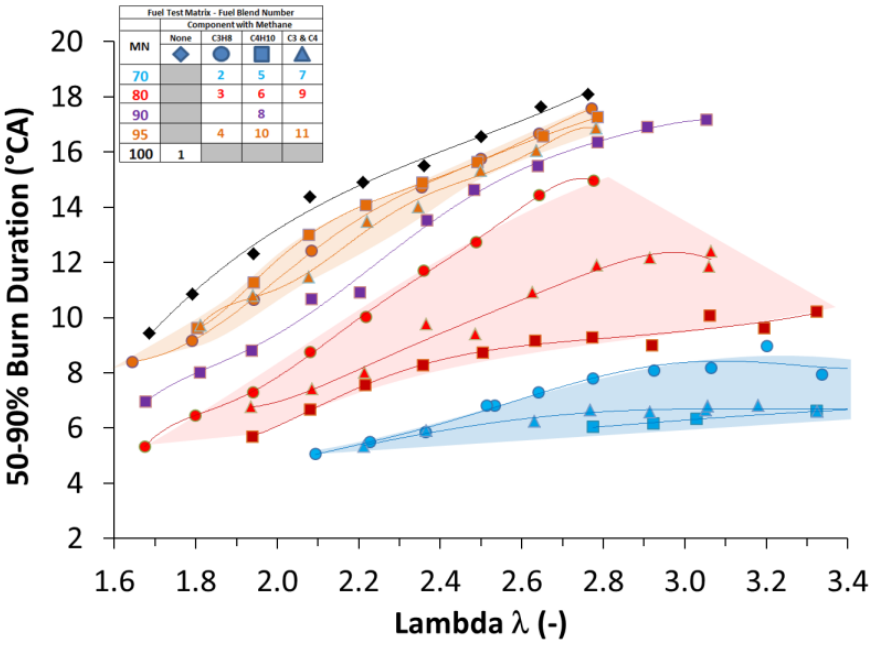

Figure 5: 50-90% burn duration vs. lambda for all ten fuel blends

Further analysis shows that transition to rapid combustion can be represented by a shift in the crank angle location where the peak heat release rate occurs. In Figure 3, it is seen that the peak heat release rate occurred in one of three features—in the early diesel premixed burn spike, in the middle of the normal (non-rapid) burn, or in the late rapid combustion event. At leaner lambda values, the combustion is not rapid and the location of the peak heat release rate was centered in the main burn. Once the late rapid combustion becomes significant, the location of the peak heat release rate shifted as much as 4°CA later to the late rapid combustion event, designating a distinct transition from normal to rapid combustion. Figure 6 presents this for the three 70 MN fuel blends. Inherent in this definition is that the threshold for significant rapid combustion to occur is when the late, rapid burn becomes large enough in magnitude to have higher heat release rates than the main burn of the combustion event.

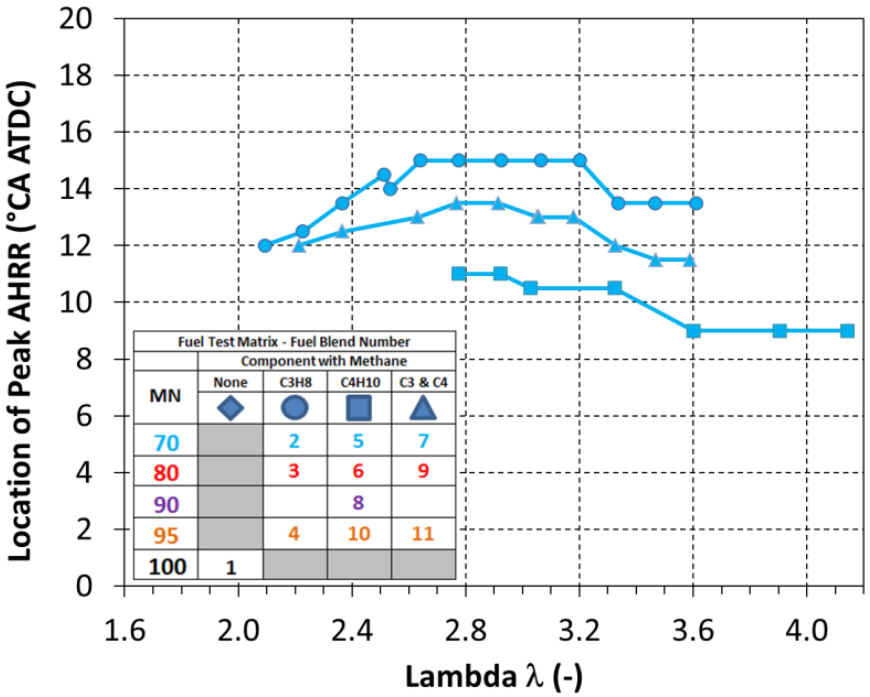

Figure 6: Location of peak AHRR vs. lambda for the three 70 MN fuel blends

The lambda sweeps in Figure 6 show the locations of peak heat release rate shift later when the late rapid combustion became dominant (λ = 3.2 to 3.6), even though most of the data points with these lower methane number fuels already experienced some level of rapid combustion. After the transition, further richening lambda increased the magnitude of the rapid combustion, which shortened the 50-90% burn duration and caused the location of peak heat release rate to gradually move earlier again as it remains with the late rapid combustion event.

Figure 7 presents the location of peak heat release rate vs. lambda for the three 80 MN fuels. The shifts in the location of the peak heat release rate that represent the transitions to rapid combustion are clearly seen. Given that butane has the highest reactivity of the three components, the transition to rapid combustion for the methane-butane mixture presumably has already occurred at λ > 3.4. The second most reactive blend is the methane-propane-butane mix, which transitions next at roughly λ = 2.7. The methane-propane mixture is the last to transition to rapid combustion (as expected), which occurs at a significantly richer relative air-fuel ratio of λ = 1.95. Although the sequence in which these 80 MN blends transition to rapid combustion occurs as expected according to the individual components' reactivities, the transitions to rapid combustion happen at significantly different values of critical lambda. As these three fuels were predicted to have similar knock behavior by the MWM methane number algorithm in an SI sense, this is an indication that the SI-based methane number may not capture all of the phenomena that influence rapid combustion behavior of premixed fuels in this type of dual fuel combustion system.

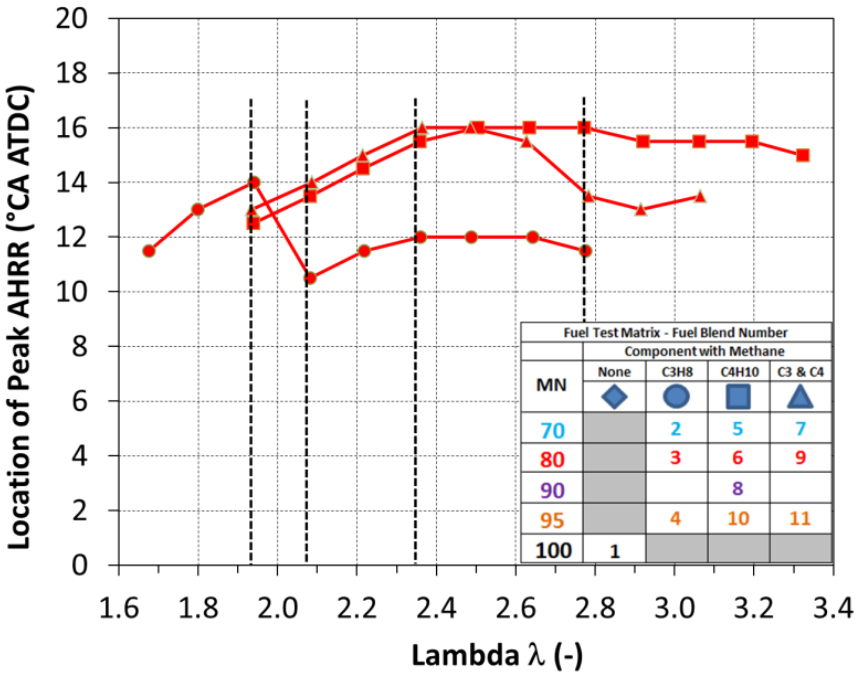

Figure 7: Location of peak AHRR vs. lambda for the three 80 MN fuel blends (four vertical dashed lines indicate lambda values for AHRR data shown in Figure 8)

For a more focused view of the 80 MN blends shown in Figure 7, Figure 8 compares the AHRR curves that correspond to four different lambda values (designated by the vertical lines in Figure 7). Starting from the lean side of the lambda sweep, the AHRR curves for $\lambda = 2.8$ show the three blends exhibiting three distinct conditions. The methane-propane blend experiences a normal, non-rapid heat release rate, the methane-propane-butane blend is starting the transition to late rapid combustion, and the methane-butane mix is already experiencing some amount of the fuel burning in late rapid combustion. Moving more rich to $\lambda = 2.4$ it is seen that the methane-propane blend continues to show no rapid combustion, the methane-propane-butane mix has fully transitioned to include some late rapid combustion, and the rapid combustion of the methane-butane blend increases in magnitude. Richer yet at $\lambda = 2.1$ shows the methane-propane blend now in its transition to late rapid combustion while both the methane-propane-butane and methane-butane blends exhibit even faster late rapid combustion. At $\lambda = 1.9$ all three blends have transitioned and experience late rapid combustion but of varying magnitude.

At all four of these lambda conditions, note that the early regions of AHRR curves are nearly identical between fuel blends and the differences in combustion rates primarily manifest later in the burn duration, indicating the effects that drive the transition to rapid combustion in these cases are most likely a characteristic of the premixed natural gas and air regions as opposed to the early diesel premixed burn.

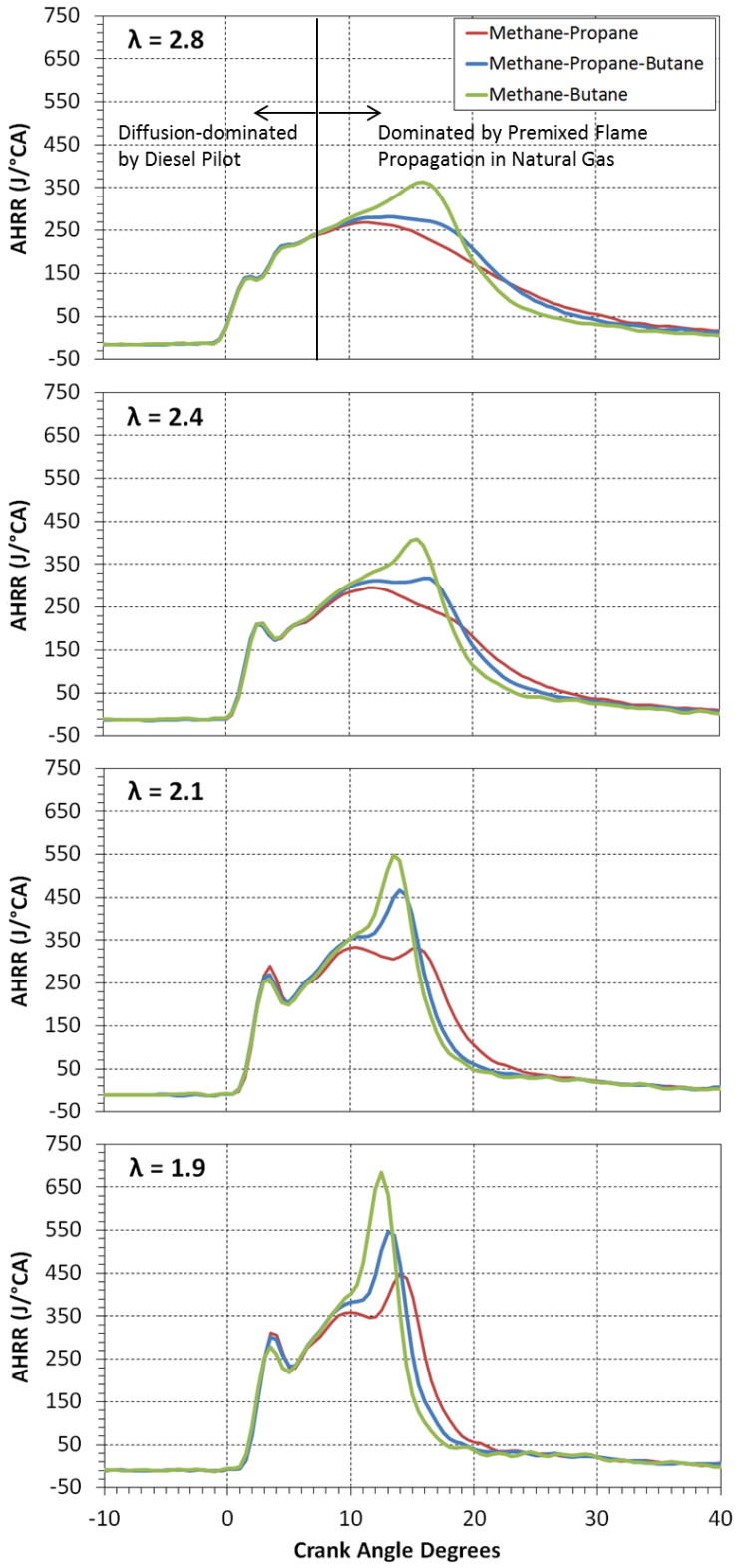

Figure 8: AHRR curves of the three 80 MN blends corresponding to four lambda values as indicated in Figure 7

This also raises a consideration of what reactivity index might be most suited to indicate a fuel's propensity to develop late rapid combustion in dual fuel engines. As noted, two of the 80 MN fuels transition to rapid combustion at critical lambdas roughly 0.75 units apart, which is a significant range. There can be large differences in performance and emissions for combustion that occurs between $\lambda = 1.95$ and $\lambda = 2.7$. Without having a fully validated measure for a fuel's reactivity as it relates to rapid combustion in dual fuel engines, manufacturers calibrate engines conservatively to accept the worst-case or most-reactive fuels anticipated in a specific application.

The locations of peak heat release rate for the lambda sweeps of the four higher methane number fuels is shown in Figure 9. In an effort to conserve the specialized fuel, the three 90 MN blends were in practice mixed to be 95 MN. These higher methane number blends do manifest the shift of location of peak heat release rate but at much smaller magnitudes. They appear to transition to rapid combustion in the range of $\lambda = 2.5$ to $\lambda = 2.8$. These transitions occur in a narrower range of critical lambda than the 80 MN fuels, showing additional similarity in their combustion behavior and reactivity. However, given the small changes experienced in the combustion process, higher resolution and more fuel-lean data is required.

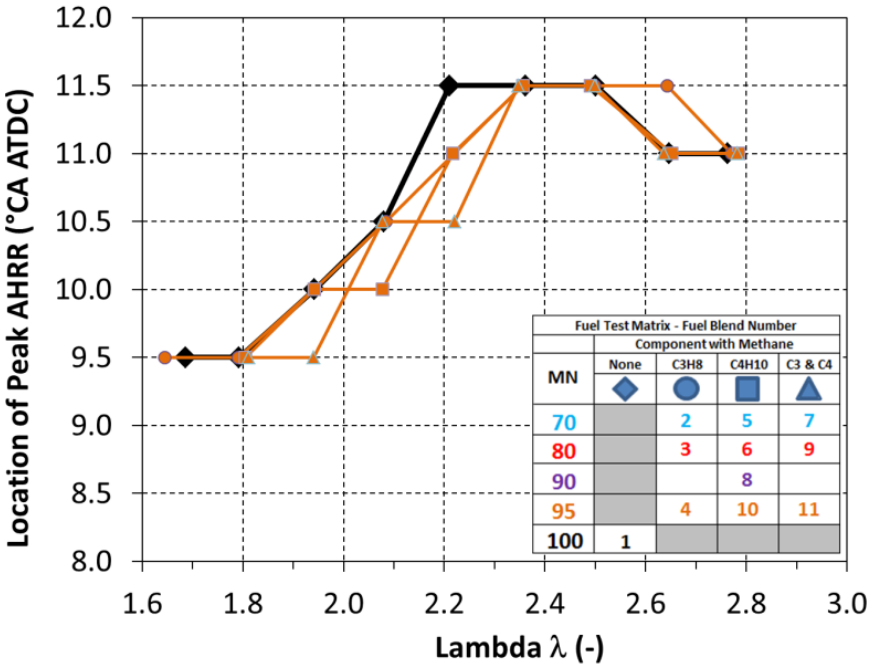

Figure 9: Location of peak AHRR vs. lambda for the three 95 MN and one 98 MN fuel blends

Since there are many chemical and physical phenomena that make rapid combustion in dual fuel engines distinctly different from knock in premixed spark-ignited combustion, ultimately dual fuel calibrations based on the SI methane number are required to be more conservative. One possible factor that makes dual-fuel rapid combustion distinct from SI knock is, as mentioned

previously, ignition and flame propagation in the premixed natural gas. Whereas spark-ignition creates a single, slow-growing kernel of reaction that needs turbulence to propagate the flame front, the burning diesel plumes in dual fuel combustion provide many large and spatially distributed surface areas that allow ignition and propagation of reaction in the premixed natural gas and air from many locations. The end gas in SI combustion experiences compression and preheat from one advancing flame front yet in dual fuel combustion several turbulent premixed flame fronts originating from different diesel plumes can interact with the same region of unburned mixture. For example, consider the bottom center of the piston bowl in this test engine, where the late knock occurs. Given the diesel injector's multi-hole nozzle, multiple premixed flame fronts will propagate outward from the plumes through the natural gas-air mixture. Portions of the multiple flame fronts will extinguish near the cylinder head and crevices while other portions eventually converge on the volume in the bottom center of the bowl, all providing heat addition to the unburned mixture there. Effects like this can certainly influence dual fuel combustion behavior to be unique from traditional SI behavior.

Another possible factor that makes dual fuel rapid combustion different from SI knock could be a change in chemical oxidation pathways associated with the two types of engines. While spark-ignited engines have relatively low compression ratio and hence lower compression temperatures, dual fuel engines typically have higher compression ratios with higher post-compression temperatures in the cylinders. Higher temperatures may allow the longer hydrocarbon chains to transition from primarily chain-propagating reactions to chain-branching reactions as the primary pathway for oxidation, in a similar way to the low, medium, and high temperature oxidation regimes observed for homogeneous charge compression ignition (HCCI) combustion [12]. This mechanism shift could also contribute to the distinct knock or rapid combustion behavior of dual fuel engines.

3. Conclusion

In this work, the MWM methane number algorithm is rigorously tested with ten specialized fuel blends of methane, propane, and butane to determine if it represents fuel reactivity and rapid combustion behavior specific to a dual fuel engine. The engine is operated very lean and gradually richened to induce rapid combustion for each fuel blend. Analysis of combustion CFD results and engine experiments concludes that:

1. There are undoubtedly many physical and chemical phenomena that make the dual fuel combustion process unique from SI combustion. The large surface areas of the burning diesel plumes create many ignition locations and premixed flame fronts that interact with the end gas. The higher compression ratios and temperatures in dual fuel engines can activate alternative chemical mechanisms and can even shift the reaction kinetics into a different combustion regime altogether.

2. Knock in this dual fuel configuration manifests as rapid heat release near the end of the combustion event (termed late rapid combustion), in which a significant mass of natural gas-air mixture in the bottom center of the piston bowl burns exceptionally fast.

3. No over-penetration or mixing of unburned diesel fuel is present in the region of the combustion chamber where the late rapid combustion event occurs.

4. The location of peak heat release rate can identify the transition from normal combustion to rapid combustion in a relative air-fuel ratio sweep. For natural gas blends of similar methane number, the critical lambda values where this transition occurs can be significantly different, indicating that there may be improved methods to characterize fuel reactivity and rapid combustion in dual fuel engines than the existing SI-based MWM methane number algorithm.

5. The need for a metric or index that rates the propensity of the gaseous fuel to reach rapid combustion in dual fuel combustion systems with a high degree of certainty means engine manufacturers must alternatively calibrate in a conservative manner with existing methane number algorithms to account for the worst-case fuel blends anticipated in a specific application. The variance in rapid combustion behavior for the fuel blends of similar methane number, in particular the 80 MN blends of Figure 7, illustrates that a less conservative calibration and improved performance can be gained by development of a new index.

The authors caution that the results and conclusions in this study are for a specific hardware configuration at one speed-load condition and one natural gas substitution level. While these conclusions may be applicable to other operating conditions and other dual fuel engine hardware and platforms, an exhaustive experimental and analytical study with varying fuel blends is

needed to fully characterize the relationship between fuel reactivity and rapid combustion in dual fuel engines.

As a result of this study, two specific recommendations are made to the Federal Railroad Administration. First, consider supporting future efforts to develop a reactivity index specifically for dual fuel combustion in locomotive engines. It is clear that development of this metric will enable increased engine efficiency, performance, and gas substitution rate, as well as broader acceptance of natural gas as a fuel. Secondly, in the interim, and although it is conservative for dual fuel engines, define the MWM MN algorithm as the standard MN calculation method in any rail industry natural gas fuel specification. It is an excellent candidate for standardization due to its accuracy, large number of fuel species included, easy to use Excel-based GUI, and availability at no cost. The MWM MN algorithm is currently in the process of being adopted in natural gas fuel specifications by the European Committee for Standardization (CEN), ASTM, and the California Department of Food and Agriculture.

4. Future Research Opportunities

Future research opportunities may include fuel blend testing at additional speed-load points, with some of the throttle notch conditions specified for locomotive engine performance. Lower substitution rates of 25% and 50% natural gas by energy could reveal more insight into the location and magnitude of dual fuel knock. Other dual fuel configurations, such as port injection or direct injection of the natural gas, could be considered. These studies and a larger bore engine may be used to investigate and develop a new fundamental reactivity index to quantify the rapid combustion propensity of fuels for dual fuel combustion of diesel and natural gas.

Development of a new reactivity index specifically for dual fuel combustion could be completed in the following phases:

1. Phase I: Evaluate fuels of varying composition over the speed-load map with fixed gas substitution rate of 75%; investigate flame speed effects of the fuel compositions
2. Phase II: Evaluate fuels of varying composition over the speed-load map at additional gas substitution rates of 25% and 50%
3. Phase III: Develop a dedicated dual fuel reactivity index from analysis and experimental data taken in Phases I and II
4. Phase IV: Investigate the effect of natural gas port injection mixing differences on rapid combustion performance relative to fumigation of natural gas (optional)

5. References

1. Leiker, M., Christoph, K., Rankl, M., Cartellieri, W., and Pfeifer, U., "The Evaluation of the Antiknocking Property of Gaseous Fuels by means of the Methane Number and its Practical Application to Gas Engines." 9th International Congress on Combustion Engines, Stockholm Sweden, 1971.

2. Kubesh, J. and King, S.R., "Effect of Gas Composition on Octane Number of Natural Gas Fuels." SAE Technical Paper 922359, 1992.

3. Sorge, Gregory W., Kakoczki, Richard J., Peffer, John E., "Method of Determining Knock Resistance Rating for Non-Commercial Grade Natural Gas." United States Patent Number 6,061,637, May 9, 2000.

4. Malenshek, Martin, and Olsen, Daniel B., "Methane number testing of alternative gaseous fuels." Fuel volume 88, pgs. 650-656, 2009.

5. Andersen, Paw. "Algorithm for methane number determination for natural gases." Danish Gas Technology Centre a/s, file number 719.45, 1999.

6. Gersen, S., Rotink, M.H., van Dijk, G.H.J., "A new experimentally tested method to classify gaseous fuels for knock resistance based on the chemical and physical properties of the gas." International Gas Union Research Conference, 2011.

7. *Cummins Westport Fuel Quality Calculator*, 2015. Web: http://www.cumminswestport.com/fuel-quality-calculator.

8. *AVL Methane Number Version 3.10a*, 1997. Software: AVL List GmbH.

9. *MWM Methane Number Calculation*, 2015. Software: Caterpillar Energy Solutions (formerly MWM GmbH).

10. Ryan III, T.W., Callahan, T.J., and King, S.R., "Engine Knock Rating of Natural Gases – Methane Number." ASME Journal of Engineering for Gas Turbines and Power, Volume 115, pgs. 769-776, 1993.

11. European Committee for Standardization (CEN), “Gas Infrastructure – Gas Quality – H Gas.” European Standard prEN 16726, 2015.

12. Pilling, M.J., “Low-Temperature Combustion and Autoignition, Volume 35 (Comprehensive Chemical Kinetics).” ISBN 0 444 82485 5, 1997.

Appendix A.
Detailed Analysis of Fuel Compositions Tested

LNG	Fuel					1 - LNG
	Calc MWM MN					98
	nitrogen					0.18
	methane					99.29
	ethane					0.49
	propane					0.04
	butane					0.00
Propane Blends	Fuel	2 - 70 MN C3H8	3 - ~80 MN C3H8		4 - ~94 MN C3H8	
	Calc MWM MN	69	82.6		93.6	
	nitrogen	0.14	0.09		0.11	
	methane	90.25	95.00		98.61	
	ethane	0.86	1.45		0.36	
	propane	8.73	3.44		0.92	
	butane	0.00	0.00		0	
Butane Blends	Fuel	5- 70 MN C4H10	6 - 80 MN C4H10	8 - 90 MN C4H10	10 - 95 MN C4H10	
	Calc MWM MN	69	79.4	89.2	95	
	nitrogen	0.09	0.09	0.23	0.11	
	methane	94.80	96.94	98.52	99.54	
	ethane	0	0	0	0	
	propane	0	0	0	0	
	butane	5.1	2.97	1.25	0.35	
Propane/Butane Blends	Fuel	7 - 70 MN C3&C4	9 - 80 MN C3&C4		11 - 94 MN C3&C4	
	Calc MWM MN	68.7	80.5		93.6	
	nitrogen	0.08	0.11		0.15	
	methane	93.01	96.26		99.02	
	ethane	0	0		0	
	propane	4.20	2.22		0.51	
	butane	2.72	1.41		0.32	

Abbreviations and Acronyms

AHRR	Apparent Heat Release Rate
ASTM	American Society for Testing and Materials
ATDC	After Top Dead Center
AVL	Anstalt für Verbrennungskraftmaschinen List GmbH
BMEP	Brake Mean Effective Pressure
BTDC	Before Top Dead Center
CA	Crank Angle
CEN	European Committee for Standardization
CFD	Computational Fluid Dynamics
CFR	Cooperative Fuels Research
CO	Carbon Monoxide
DOHC	Dual Overhead Camshafts
EGR	Exhaust Gas Recirculation
EPA	Environmental Protection Agency
GUI	Graphic User Interface
HCCI	Homogeneous Charge Compression Ignition
HPF	High Pass Filter
KI	Knock Intensity
MN	Methane Number
MWM	Motoren-Werke Mannheim GmbH
SI	Spark-Ignited
SwRI	Southwest Research Institute
TDC	Top Dead Center
US	United States

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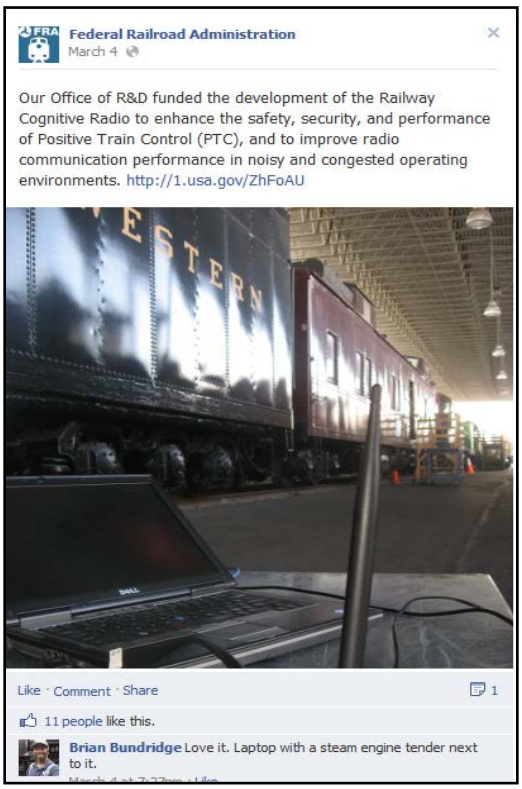

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