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Physicochemical effects of varying fuel composition on knock characteristics of natural gas mixtures

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ABSTRACT

The physicochemical origins of how changes in fuel composition affect autoignition of the end gas, leading to engine knock, are analyzed for a natural gas engine. Experiments in a lean-burn, high-speed medium-BMEP gas engine are performed using a reference natural gas with systematically varied fractions of admixed ethane, propane and hydrogen. Thermodynamic analysis of the measured non-knocking pressure histories shows that, in addition to the expected changes arising from changes in the heat capacity of the mixture, changes in the combustion duration relative to the compression cycle (the combustion "phasing") caused by variations in burning velocity dominate the effects of fuel composition on the temperature (and pressure) of the end gas. Thus, despite the increase in the heat capacity of the fuel–air mixture with addition of ethane and propane, the change in combustion phasing is actually seen to increase the maximum end-gas temperature slightly for these fuel components. By the same token, the substantial change in combustion duration upon hydrogen addition strongly increases the end-gas temperature, beyond that caused by the decrease in mixture heat capacity. The impact of these variations in in-cylinder conditions on the knock tendency of the fuel have been assessed using autoignition delay times computed using SENKIN and a detailed chemical mechanism for the end gas under the conditions extant in the engine. The results show that the ignition-promoting effect of hydrogen is mainly the result of the increase in end-gas temperature and pressure, while addition of ethane and propane promotes ignition primarily by changing the chemical autoignition behavior of the fuel itself. Comparison of the computed end-gas autoignition delay time, based on the complete measured pressure history of each gas, with the measured Knock-Limited Spark Timing shows that the computed delay time accurately reflects the measured knock tendency of the fuels.

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1. Introduction

As a result of the globalization of the energy market and the drive towards sustainability, the chemical composition of gaseous fuels is becoming more diverse. For example, "rich" natural gases, which contain substantially higher fractions of non-methane hydrocarbons than the traditionally distributed pipeline gas, are being introduced into the gas infrastructure. Sustainable gases obtained from fermentation or gasification of biomass, which can contain substantial fractions of carbon dioxide, hydrogen and carbon monoxide are being considered for introduction into the gas supply. The different compositions of such "new" gases can impact the combustion behavior of end-use equipment. With an eye towards successfully incorporating this diversity of supply, it is necessary to assess the effects of the wider range of fuel compositions on end-use equipment quantitatively.

Gas-fueled reciprocating internal combustion engines are known to be sensitive to variations in fuel composition because of the possible occurrence of engine knock, caused by autoignition of unburned fuel–air mixture, the so-called end gas, ahead of the propagating flame in the cylinder. Mild engine knock increases fuel consumption and pollutant emissions, while severe knock can physically damage the engine [1], and as such should be avoided. The knock sensitivity of gas engines is a limiting design factor for power output, efficiency and the acceptable variation in fuel gas composition. Empirical methods analogous to the octane number for gasoline [2,3], such as a methane number [4], which often make use of a standard test engine, have been developed to classify natural gases with respect to their knock sensitivity. Since the autoignition behavior of fuels and the relative differences in autoignition

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between fuels depend strongly on the specific regime of temperature and pressure (e.g., [5–18]), the generality of the method for engine conditions other than those existing in the test engine is uncertain. Furthermore, empirical methods provide only limited insight in the physical/chemical origins of knock in engines, and are therefore of limited utility for the optimum design for knock-free engine operation when using a wide range of fuels. Elucidation of the microscopic details of the effects of fuel composition on cylinder processes can provide insight essential for engine design, and can also be used to derive a fundamentally sound method for determining the knock tendency of fuels.

Autoignition of the end gas is governed by chemical kinetics, and occurs when the rate of reaction and the rate of heat release in the end gas grow exponentially. The tendency of a fuel mixture to autoignite depends strongly upon the reactivity of the fuel itself, the equivalence ratio and the pressure and temperature conditions of the mixture. For example, studies performed in shock tubes and rapid compression machines, RCMs, (see, for example, [5,7–9,12–18]) showed that the autoignition delay time of methane-based fuels decreases significantly as a result of increasing the temperature and pressure, and the addition of higher hydrocarbons or hydrogen. A fundamental analysis of engine knock therefore requires detailed knowledge about the actual state of the end gas, as well as any changes in this state caused by varying composition. Since the state of the end gas is affected by the thermophysical properties of the mixture and rate of combustion [1,20], the trends observed in shock tubes and RCMs by themselves are insufficient to characterize changes in knock behavior with varying fuel composition. Furthermore, affected by mechanical compression and thermal compression caused by progressive consumption of the fuel–air mixture, the state of the end gas varies with time during the combustion cycle. To quantify the progress of autoignition under these conditions for different gas compositions, this temporal variation in the temperature and pressure of the end gas must be determined. Although the knock characteristics [19,20], combustion duration [21,22] and flame speed [23,24], of CH_4, C_2H_6, C_3H_6, H_2 and their mixtures have been studied individually, the available information is insufficient to assess the contributions of the individual changes in the knock behavior of the fuel.

In this paper we analyze the changes in autoignition delay time of the end gas caused by the changes in the reactivity of the fuel itself and those arising from changes in in-cylinder pressure and temperature experienced by the end gas upon changing gas composition. The changes in in-cylinder conditions are studied both theoretically and using data obtained from a practical engine fueled with a variety of (simulated) natural gases. The fractions of ethane, propane and hydrogen in the gases are varied systematically to illustrate the underlying principles. In addition, the gases studied have been ranked for knock resistance based on the experimental determination of knock and on an analysis using computed end-gas autoignition delay times. The ultimate goals of this work are to provide insight into the physical and chemical processes governing the effects of fuel composition on engine knock and to rank gases for knock resistance based on a physically correct representation of these effects.

2. Experimental procedure

A lean-burn, high-speed, turbo-charged, intercooled 6-cylinder gas engine (MAN) for combined-heat-and-power applications (CHP) was used in this study. Table 1 lists the key specifications of this engine. We remark here that this CHP system maintains constant equivalence ratio, engine speed and power output. The engine management system and further instrumentation allowed for precise adjustment, monitoring and acquisition of power output, fuel consumption, exhaust gas emissions, ignition timing, air–fuel-ratio and other relevant engine parameters.

The in-cylinder pressures in all cylinders were measured with Kistler type 6052 piezoelectric pressure sensors and a Kistler type 5011 charge amplifiers connected to a Smetec Combi-Pro indication system. A crankshaft-mounted pulse generator provided 0.1 °CA resolution for the cylinder pressure data acquisition. The Combi-Pro system was also used for knock detection through monitoring of the maximum amplitude of pressure oscillations in the high-pass-filtered cylinder pressure data in a window of consecutive cycles. Threshold settings used were 2 bar for the amplitude and 30 cycles for the window. For knock-limited spark timing (KLST) experiments ([20], see below), the knock limit was arbitrarily chosen to be one knock event or cluster of knock events within a 15 min steady-state test run. The Combi-Pro system also provided analyses of the combustion process, such as the phasing of the heat release, based on the pressure trace.

During the experiments, fuel for the test engine was delivered by a gas mixing unit. This unit allows on-stream variation of the fuel gas composition by independent adjustment of the flow rates of up to six source gas streams, with a maximum capacity of 4 MW. The fuel compositions used in the experiments consist of Dutch natural gas (DNG) mixed with increasing fractions of ethane and/or propane (Table 2), or hydrogen (Table 3). All mixture compositions were verified by gas chromatography.

Once the composition of the fuel/air mixtures at equivalence ratio $\varphi = 0.67$ and the other relevant cylinder parameters are set (Tables 2 and 3), the pressure traces of the gases under non-knocking condition are measured at a constant spark timing of 14° before top dead center (BTDC). Subsequently, the spark timing was gradually varied up to the point of the onset of borderline knock to determine the KLST.

3. Simulation procedure

Since knock in spark-ignited engines is an autoignition phenomenon, we simulate engine knock by modeling autoignition of the compressed end gas during the cycle using the SENKIN code [25], in the CHEMKIN II library [26]. To predict the occurrence of engine knock accurately, it is necessary to account for the effects of the piston motion and flame propagation on the pressure and temperature history of the end gas in the simulations. Since we focus here on gaining insight into autoignition during the engine cycle, we avoid complex calculations of flame propagation for the present, and derive the pressure and temperature history of the unburned end gas from the experimental engine measurements. As successfully applied previously [27,28], we assume that knock occurs in an adiabatic core of the unburned end gas. As shall be seen below, the engine results themselves point to challenges for the simulation of burn cycle that are necessary to predict engine knock, a priori. For each simulation we derive the specific volume of the end gas from a measured non-knocking pressure history, using

$$\int_{T_i(t_0)}^{T(t)} \frac{\gamma}{\gamma-1} d\ln T = \ln \frac{P(t)}{P_i(t_o)}, \tag{1}$$

and

$$\ln(CR(t)) = \ln\left(\frac{V_i(t_0)}{V(t)}\right) = \int_{T_i(t_0)}^{T(t)} \frac{1}{\gamma-1} d\ln T, \tag{2}$$

where T_i and P_i are the measured intake temperature and pressure, respectively, while V_i is the specific volume of the unburned gas at the start of the compression stroke, derived from T_i and P_i; $P(t)$ is the measured pressure of the unburned gas mixture, $T(t)$ is the temperature of the unburned gas mixture, and $V(t)$ is the time-varying

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