Sub Topic: Internal combustion and gas turbine engines

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Effect of natural gas conditions on combustion characteristics and overall performance of a novel bimodal internal combustion engine

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Abstract: Abundant availability and potential for lower CO_2 emissions are drivers for increased utilization of natural gas in automotive engines for transportation applications. However scarce refueling resources for on-road vehicles impose an infrastructure limited barrier on natural gas use in transportation. A novel 'bimodal' engine which can operate in a compressor mode has been developed that allows on-board refueling of natural gas where available without the need for any supplemental device. Engine compression of natural gas however results in altering the initial state of the fuel with potential impact on combustion characteristics and overall engine performance. Increase in natural gas temperature and addition of oil are two key effects attributed to the onboard refueling process. A secondary effect is the presence of water in the natural gas supply line. This study aims to investigate these effects by coupling an upfront system model of the onboard refueling process with a thermodynamic model of the engine processes. Parametric studies will be undertaken to study the effects of variation in natural gas inlet temperature, oil and water content on ignition, flame propagation and auto-ignition processes. Inlet fuel temperature has a strong influence on unburned hydrocarbons released in the exhaust while presence of heavier hydrocarbons due to the oil content can influence auto-ignition characteristics. Another effect of implementing the onboard refueling setup is that it requires altering the spark plug placement in the cylinder head. The influence of this modification will be additionally studied through literature review. Overall, this work attempts to model the influence of the upstream natural gas refueling stage on downstream combustion processes to verify that engine metrics such as overall efficiency, coefficient of variation, and hydrocarbon emissions are maintained at an acceptable level to ensure clean combustion.
Keywords: Natural gas, Internal combustion engine, Auto-ignition, Chemical kinetics

1. Introduction

Natural gas has emerged as a leading alternative to petroleum-based liquid fuels for transportation applications in recent years. The rapid increase in production and unlocking of vast amounts of natural gas from shale deposits through the improvement of hydraulic fracturing or "fracking", and horizontal drilling technologies facilitated this transition. These discoveries and increased production have also led to a considerable decline in the price of natural gas. Natural gas production in the US is expected to grow by 56% from 2012 to 2040 with the contribution from shale gas increasing from 40% in 2012 to 53% in 2040 [1]. This increased

supply also means that the difference in retail price between gasoline or diesel and compressed natural gas (CNG) can be over $2 per equivalent gallon of gasoline (GGE) [2].

Beyond the economic benefits of utilizing natural gas in transportation applications, there are other benefits to be accrued as well. First, it reduces the reliance of the nation on the import of petroleum. In 2011, the US imported 28 quadrillion BTU of petroleum gallons of crude oil, 70% of which was utilized for transportation applications and 45% of which was imported [3]. This has significant economic and geo-political implications. Second, natural gas has a higher octane number facilitating the use of higher compression ratios in internal combustion (IC) engine applications giving a path to possible higher overall efficiency [4]. There are environmental benefits to be gained from natural gas use in transportation. Several studies have indicated a net reduction in exhaust gas emissions [5—7].

While there are highly persuasive arguments to utilize natural gas in transportation applications, two major barriers remain to be overcome. These relate to vehicle onboard storage of natural gas and refueling capabilities. Over 60 million homes and businesses are connected to the natural gas supply network [8]. However, as of 2012 only 700 public compressed natural gas (CNG) refueling stations are available in the US as compared to over 100,000 gasoline stations [9, 10]. The lack of refueling infrastructure is reflected in the low market penetration of commercially produced natural gas vehicles. Currently, few vehicles are manufactured and sold in the United States operating on natural gas. The onboard storage issue is chiefly due to the low density of natural gas as compared to liquid hydrocarbon fuels. Solutions to this issue include compressing or liquefying natural gas for onboard storage. However, liquefaction is a much more expensive and complex strategy as compared to natural gas compression. Unfortunately, refueling times for compressed natural gas can range on the order of hours depending on supply pressure, availability of an on-site compressor, and the associated cost.

A collaborative effort between Oregon State University's Energy Systems Laboratory and Czero [11] resulted in the development of a novel 'bi-modal' engine that, by cylinder deactivation, can utilize power supplied by firing engine cylinders to operate the non-firing cylinders in a compressor mode. Natural gas that enters the compressing cylinders at atmospheric or slightly boosted pressures is used to fill a storage tank to a pressure of 3600 psi. The firing cylinders provide the power required by the compressing cylinders and the system is completely self-contained. This eliminates the infrastructure-limited barrier to utilizing natural gas as well as makes it possible to refuel at any location where natural gas supply is available. This onboard refueling system is being implemented on a 6.2L, V8 Boss Ford production engine.

Onboard refueling of natural gas in this manner however results in some changes to the condition and composition of natural gas stored in the fuel tank. First, piston compression results in considerable heating of natural gas. Despite utilizing heat exchangers for inter-cooling, the final tank temperature could potentially be elevated, resulting in high temperature of natural gas entering the engine cylinder. Second, as the natural gas moves through the engine cylinders there is a high likelihood of lubrication oil being entrained. Third, pipeline natural gas can contain water [12] that would be carried through the system during the refueling process. The high gas temperatures will result in vaporization of water and possibly that of oil as well. This would make it difficult to separate water and oil using filters planned to be incorporated into the refueling system. It is quite likely that there will be some residual content of both present in the fuel tank that can make its way into the engine cylinders with natural gas during normal engine operation. In this context, it is important to understand the downstream effects of the refueling system on the in-cylinder combustion processes. This would enable the refueling system to be

tailored to prepare compressed natural gas in a manner that would not have any detrimental effects on engine operation, life or exhaust products.

High natural gas temperature could potentially lead to auto-ignition events in the engine that are detrimental to engine life due to the high rates of pressure rise associated with such events. The likelihood of this is increased in natural-gas-fueled engines which utilize higher compression ratios (e.g., 10—12) due to the higher octane number of natural gas. Several research studies have associated pre-ignition events with presence of oil in the engine cylinder [13—15]. This has been a limiting factor for engine compression ratio due to the destructive nature of pre-ignition events also known as 'super-knock'. Finally water content in the fuel can affect engine combustion through thermal and kinetic mechanisms. While water content can reduce combustion temperatures it can also play a key role in suppression of NO_x as has been discussed in previous works [16—17].

This work presents a parametric study looking at the effects of natural gas temperature, water and oil content on auto-ignition processes and key chemical kinetic parameters such as ignition delay, and laminar flame speed. These studies are performed utilizing numerical simulations incorporating detailed chemistry of the fuel-air mixture. The paper is laid out as follows. First, the onboard refueling system and the engine under consideration are described in brief. Next, the numerical simulation tools used to investigate the different kinetic effects are described along with the chemical reaction mechanisms. Following this, simulation results are presented and discussed for each phenomenon investigated in this work. Finally, conclusions are presented and discussed.

2. Engine and onboard refueling system

The engine used in this work is an 8 cylinder Ford 6.2 L Boss engine. It has an overhead valve arrangement with two valves per cylinder as well as two spark plugs per cylinder. Table 1 gives a brief summary of the important specifications of the stock engine. The engine is used on several light duty trucks manufactured by the Ford motor company including the Ford F-Series.

Table 1: Engine specifications and operating parameters.

Parameter	**Value**	**Units**
Displacement	6210	cc
Bore	102	mm
Stroke	95	mm
Compression ratio	9.8	
Peak power	385	hp
Peak torque	405	ft-lb
Speed range	1000-5500	RPM

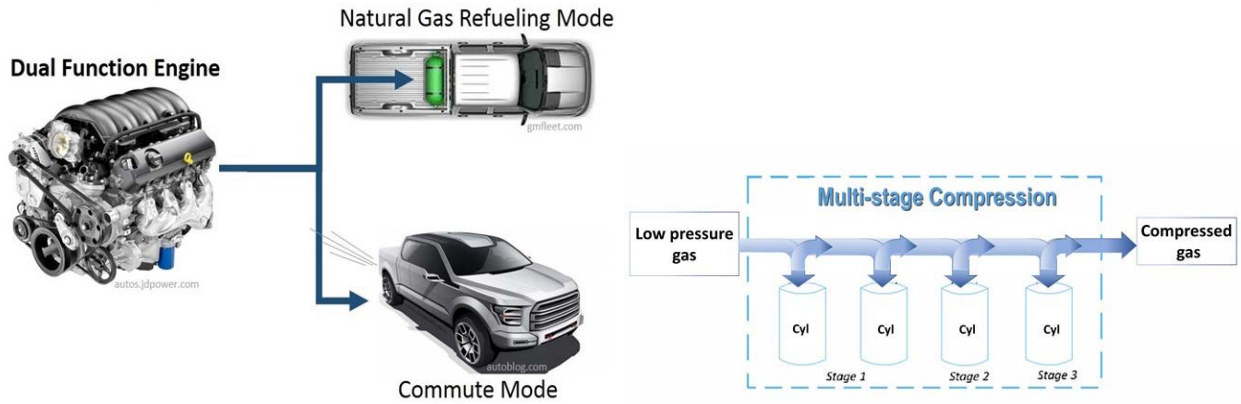


Figure 1: Schematic showing the dual-function mode of the engine as well as the compression process used to generate high pressure natural gas for tank storage.

Figure 1 shows a simple schematic illustrating the "bi-modal" engine functionality [11, 18]. During normal operation all eight cylinders produce power while in the refueling mode some of the engine cylinders compress natural gas while the remaining cylinders provide power required to perform this work. The engine is slated to run in an idling mode during the refueling operation. As seen in Fig. 1, the compression is performed in stages with inter-cooling provided by heat exchangers. The final temperature of the gas stored in the tank depends on the compression process and can potentially be as high as 200°C. The high pressure gas is expanded through a pressure-reducing valve before being introduced into the intake port similar to gasoline in the stock engine.

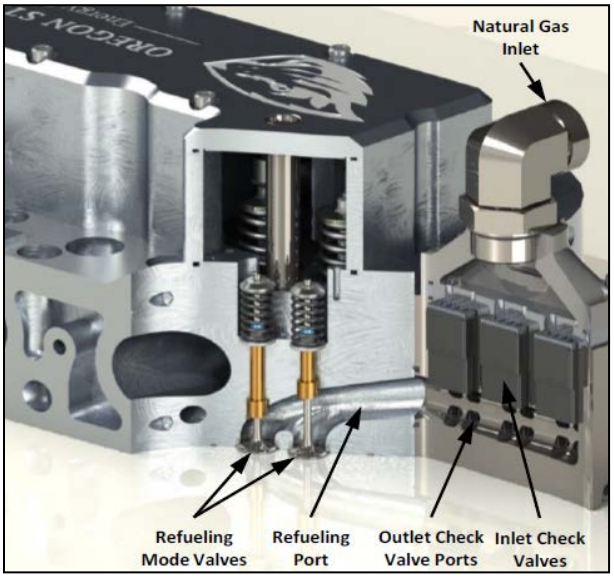


Figure 2: CAD drawing of the modified cylinder head from an earlier version of the onboard refueling setup (*rendering courtesy of Czero*).

Figure 2 shows a CAD drawing of a modified similar head from a configuration that was implemented on an earlier engine [2, 11]. The modifications to the current engine to incorporate the onboard refueling process are anticipated to result in a slightly different setup. In the current system designed by Czero, the intake and exhaust valves are outfitted with custom cylinder

deactivation but are otherwise left untouched while two additional poppet valves along with check valves are introduced to facilitate the intake and exhaust of natural gas. During the refueling process, the compressing cylinders operate essentially in a two-stroke mode. The cylinder is filled with natural gas during the downward stroke that is compressed and exhausted during the upward stroke. The process continues until the required pressure is achieved in the fuel tank.

3. Simulation methods

The numerical simulations conducted in this work were carried out using CHEMKIN version 10131 [19], a suite of reaction-kinetic tools developed by Reaction Design Inc. Different tools were used to investigate auto-ignition phenomena, ignition delay, and laminar flame speed. These tools and the reaction mechanism used in this work are described briefly in the following sections.

3.1 Auto-ignition phenomena

An internal combustion engine model is used to study auto-ignition phenomena. Inputs for key engine parameters are used with piston-crank relationships [20] to describe the cylinder volume as a function of time during engine operation. The cylinder volume is treated as a single homogeneous volume. In all the simulations performed here, adiabatic processes are assumed and no heat transfer to the cylinder walls is modeled. Conservation equations are solved for mass, species, and energy. The production rates for different species that appear in the energy equation are computed using a detailed reaction mechanism for natural gas combustion as described in Section 3.4. The simulations are carried out from 180°BTDC (before top dead center) to 180°ATDC (after top dead center). The cylinder is treated as a closed volume throughout the simulation with the initial conditions set by the equivalence ratio (φ), pressure, and temperature specified at the beginning of the simulation at 180°BTDC.

3.2 Ignition delay

Ignition delay is computed using a closed homogeneous reactor model. Conservation equations for mass, species, and energy are solved utilizing the detailed reaction mechanism to estimate species production rates.

3.3 Laminar flame speed

A premixed laminar burning velocity is estimated using the one-dimensional premixed laminar flame model. The same conservation equations as before are solved. Transport properties are calculated using the mixture-averaged formulation. Radiation heat losses are neglected in this study.

3.4 Reaction mechanism

The primary reaction mechanism used in this work is GRI-Mech [21]. The reaction mechanism consists of 53 species and 325 elementary chemical reactions. This mechanism is optimized for methane and natural gas as fuel for the temperature range 1000—2500 K, pressures between 10 torr—10 atm, and equivalence ratios between 0.1—5 for premixed systems.

4. Results and Discussion

The goal of this work was to study the effects of the onboard refueling strategy implemented on the modified engine on the downstream combustion phenomena occurring in the engine cylinder. To accomplish this, a parametric analysis was performed utilizing the simulation tools described

in Section 3. The chief parameters that were studied in this work are water content in the fuel, oil content in the fuel, and initial gas temperature. Water content was varied between 1—5 % by volume of the fuel content. Correspondingly fuel (CH_4) content was varied between 99—95%.
In the relatively simple zero-dimensional configuration used in this work, it is difficult to study the effects of oil on reaction chemistry. The first step in having oil molecules participate in the gas-phase chemistry is for them to vaporize. This can be difficult given the low volatility of lubricant components. The next step is for gas—phase chemistry of oil molecules to be described accurately. Again, due to the complicated molecular structure of these species, there do not appear to be any accurate descriptions of the gas—phase chemistry of oil molecules. As an alternative, an approach similar to that pursued by Maas et al. [22] has been pursued in this work. Maas et al. modeled the oil molecule as *n*-hexadecane whose physical properties are similar to that of lubricant oil. This allows for a better description of the vaporization of the oil molecule. In the gas—phase, reaction chemistry of the oil molecule is taken to be similar to that of *n*-heptane. This is justified by the fact that ignition delay times of linear *n*-alkanes from *n*-heptane to *n*-hexadecane are similar [23]. In this work, it is assumed that the oil molecules are vaporized given the relatively high temperature of the fuel and, similar to Maas et al., the gas—phase chemistry of oil is prescribed to be the same as that of *n*-heptane. *N*-heptane gas—phase chemistry is incorporated using a reaction mechanism from the Lawrence Livermore National Laboratory [24]. The following sections discuss the results from the various analyses.

4.1 Auto-ignition phenomena

The different parameters investigated in this study are summarized in Table 2. The temperature and pressure at BDC (bottom dead center) correspond to the temperature and pressure at the start of the simulation. The parameter T_{min} is defined as the minimum temperature required to achieve auto-ignition. Occurrence of auto-ignition in this interpretation is indicated by a rapid rise in temperature and pressure accompanied by complete conversion of the fuel in an instantaneous manner.

Table 2: Range of parametric values studied in the auto-ignition simulations.

	T_{BDC} (K)	P_{BDC} (bar)	φ	Engine speed (RPM)	Water content (%)
Range of variation	T_{min} to 800	1	0.7,1,1.2	1200,3000,5000	1,2,3,4,5

T_{min} was determined by sweeping through a range of inlet temperatures and checking for auto-ignition via pressure rise. Figure 3 shows a plot of burned fraction of fuel as a function of intake temperature for a case with engine speed of 1200 RPM, φ=1.0, and water content of 1%. For this particular case, a T_{min} of 567 K is required to achieve auto-ignition.

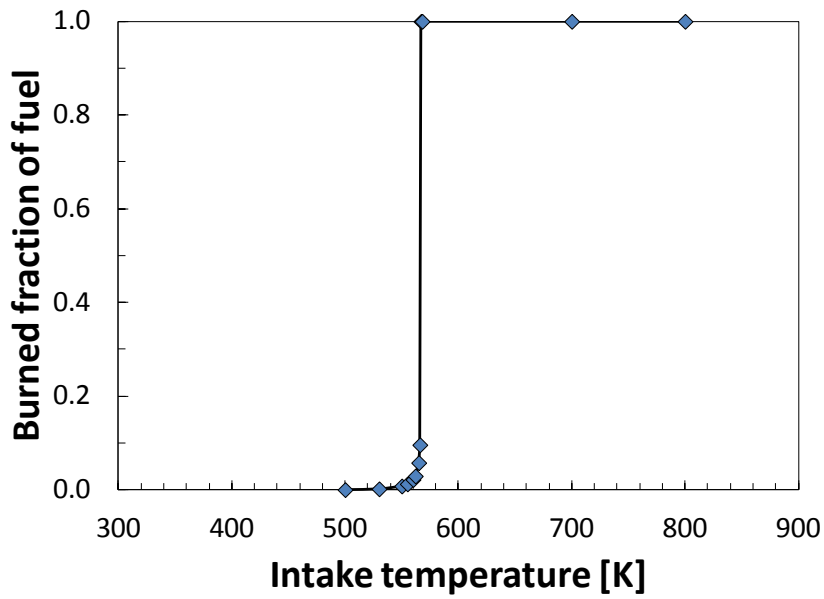


Figure 3: Burned fraction of fuel (CH_4) as a function of intake temperature for an engine speed of 1200 RPM, φ=1.0, and 1% water content.

Table 3 summarizes T_{min} as a function of engine speed for water content values of 1% and 5%, and engine speeds varying from 1200-5000 RPM at φ=1. Water content was found to have a negligible effect on T_{min}. However T_{min} increased with increasing engine speed. This is primarily attributed to the progressive decrease in residence time with increasing engine speed. As a result a progressively higher inlet temperature is required to initiate auto-ignition.

Table 3: Minimum intake temperature required for auto-ignition as a function of engine speed and water content.

Water content [%]	Engine speed [RPM]	T_{min} [K]
1	1200	567
	3000	611
	5000	639
5	1200	567
	3000	612
	5000	639

Table 4 shows the effect of φ and water content while keeping the engine speed constant at 1200 RPM. As before, changing water content between 1—5% was found to have a negligible effect on T_{min}. However T_{min} decreased as the mixture became progressively leaner. The increase in T_{min} for leaner mixtures is primarily due to the decrease in the ratio of specific heat ratios as observed in previous work [25]. Since fuel has a lower ratio of specific heats, addition of more fuel results in a lowering of the overall ratio of specific heats of the mixtures. This results in a progressively lower temperature at the end of compression requiring a higher inlet temperature to cause auto-ignition.

Table 4: Minimum intake temperature required for auto-ignition as a function of equivalence ratio and water content.

Water content [%]	φ	T_{min} [K]
1	0.7	547
	1	567
	1.2	580
5	0.7	547
	1	567
	1.2	580

Changing the intake temperature also affects the auto-ignition delay. Figure 4 shows cylinder pressure as a function of crank angle rotation for different values of initial/intake temperatures. The results are presented for an engine speed of 1200 RPM, φ=1.0, and water content of 1%. A minimum temperature of 567 K is required to cause auto-ignition. As expected, increasing intake temperatures beyond 567 K results in the ignition timing being advanced. The figure also shows different peak cylinder pressures being achieved depending on auto-ignition location. The peak cylinder pressure did not change significantly with changes in water content between 1—5 %.

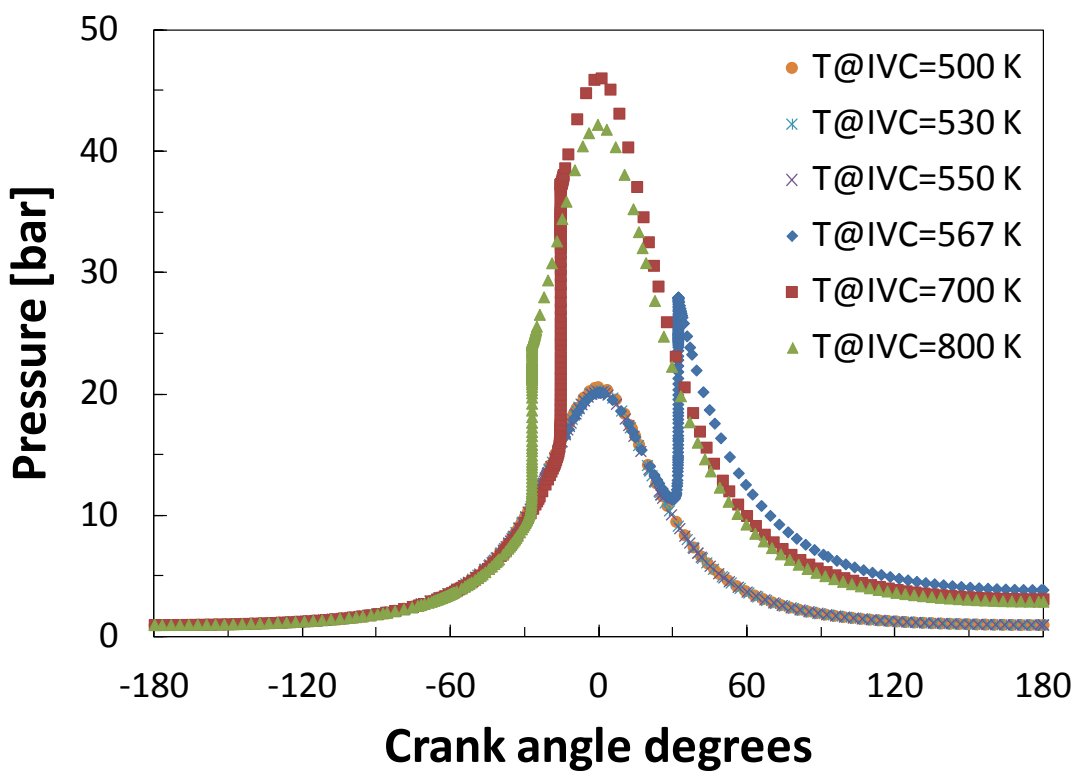


Figure 4: Cylinder pressure as a function of crank angle for different values of intake temperature.

4.2 Ignition delay

Ignition delay calculations were performed for a fixed pressure of 30 bar, varying initial gas temperatures, varying water content (1—5 % by volume), and varying φ (0.7-1.2). Figure 5 shows a plot of ignition delay as a function of inverse of temperature for water content of 1 %,

three different values of φ, and a fixed initial pressure of 30 bar. The initial pressure was set based on the pressures observed in the IC engine simulations at TDC (top dead center). As expected, ignition delay decreased with increase in initial temperature. Only slight differences in ignition delay are observed with change in φ.

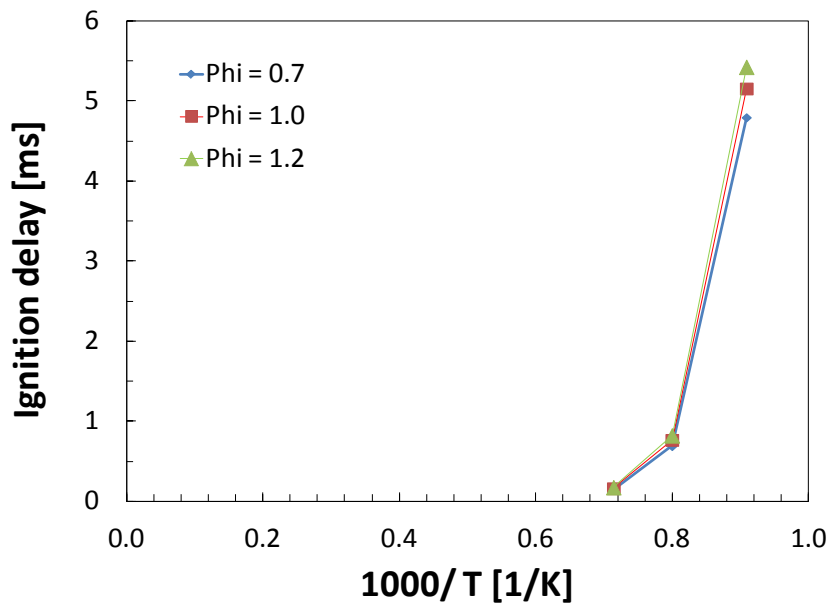


Figure 5: Ignition delay as a function of inverse of temperature for different φ for a water content of 1% and a fixed pressure of 30 bar.

Figure 6 shows the variation in ignition delay as a function of inverse of temperature for different water contents in the fuel for φ=1.0. Changing the water content between 1—5% is found to have a negligible effect on ignition delay.

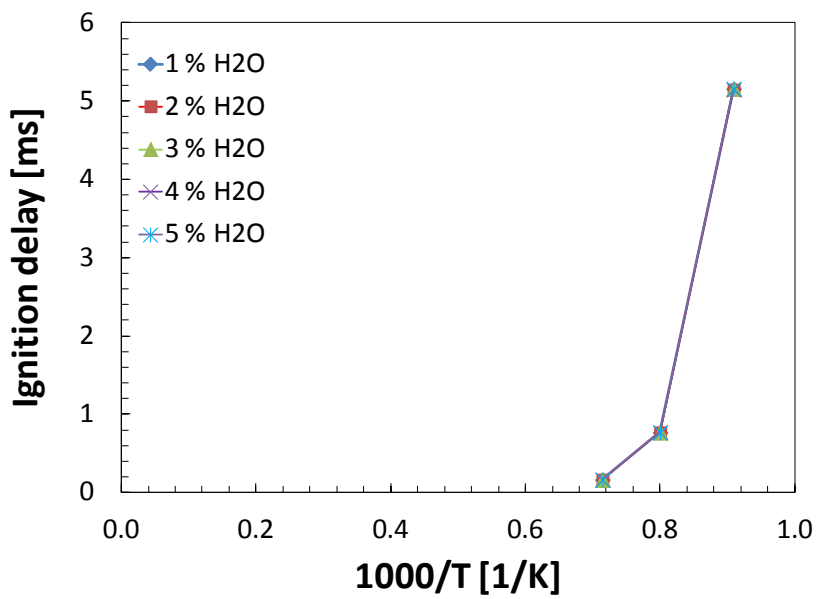


Figure 6: Ignition delay as a function of inverse of temperature for different water contents from 1-5% at φ=1.0 and a fixed pressure of 30 bar.

Ignition delay calculations were also performed with 'simulated' oil content (1—10 % by volume) with a fixed water content (1%). Figure 7 shows the effect of simulated oil addition on ignition delay for different values of φ, an initial temperature of 1100 K, and pressure of 30 bar. As discussed previously, oil is assumed to be vaporized and fully mixed with its gas—phase chemistry being described by that of *n*-heptane. As seen in Fig. 7, addition of oil from 1—10 % resulted in a progressive decrease in the ignition delay time. For 10 % oil addition, up to 75% reduction in ignition delay was observed for a given value of φ. However, as the oil content progressively increased, the reduction in ignition delay decreased and appears to reach a plateau beyond 10 %.

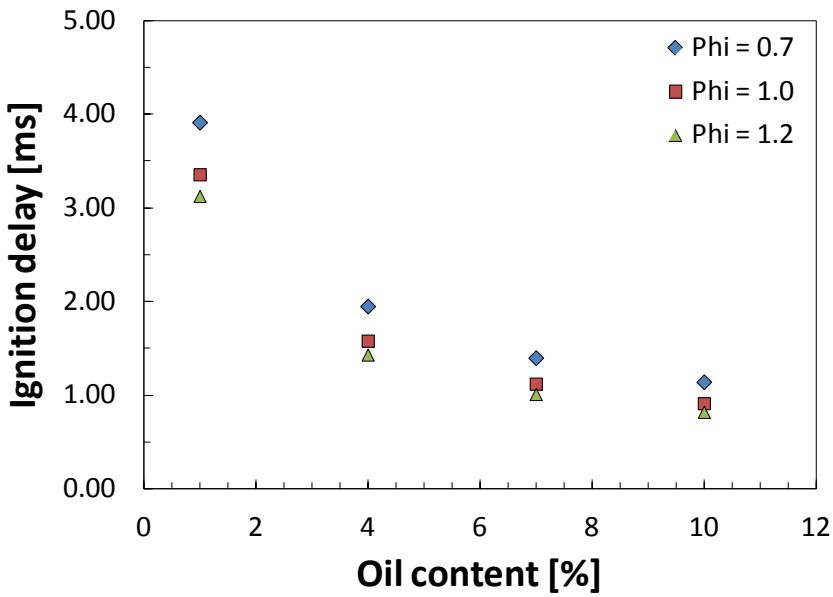


Figure 7: Ignition delay as a function of oil content for different values of φ for an initial temperature of 1100 K and a pressure of 30 bar.

Figure 8 shows the effect of simulated oil addition on ignition delay for different initial temperatures, at φ=1, and an initial pressure of 30 bar. As seen in Fig. 8, addition of oil from 1—10 % resulted in a progressive decrease in the ignition delay time. This effect decreases as the inlet temperature is increased since the effect of temperature on ignition kinetics overshadows that of oil addition.

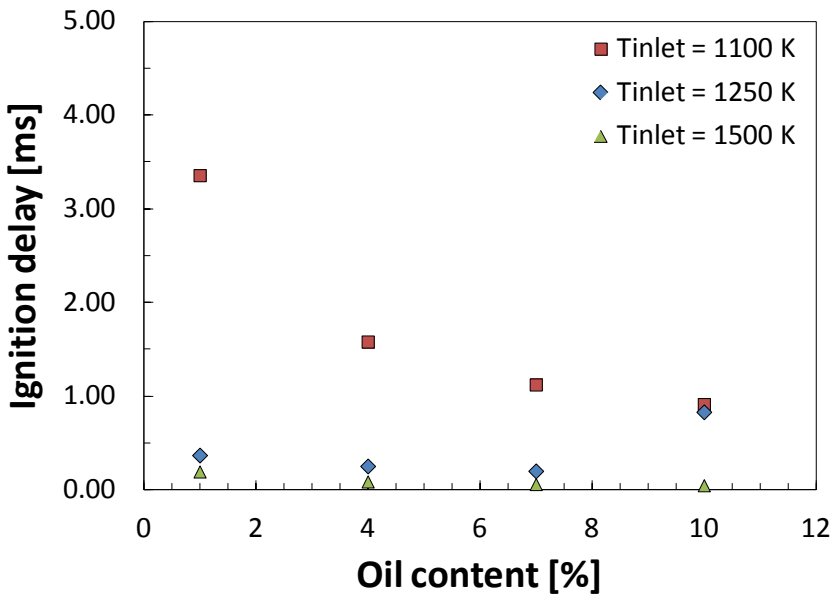
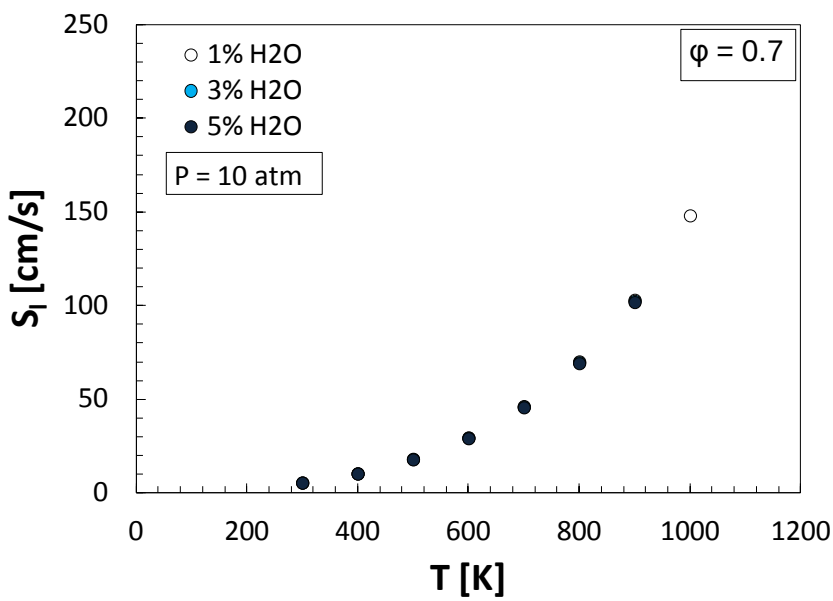


Figure 8: Ignition delay as a function of oil content for different initial temperatures for φ=1.0 and a pressure of 30 bar.

4.3 Laminar flame speed



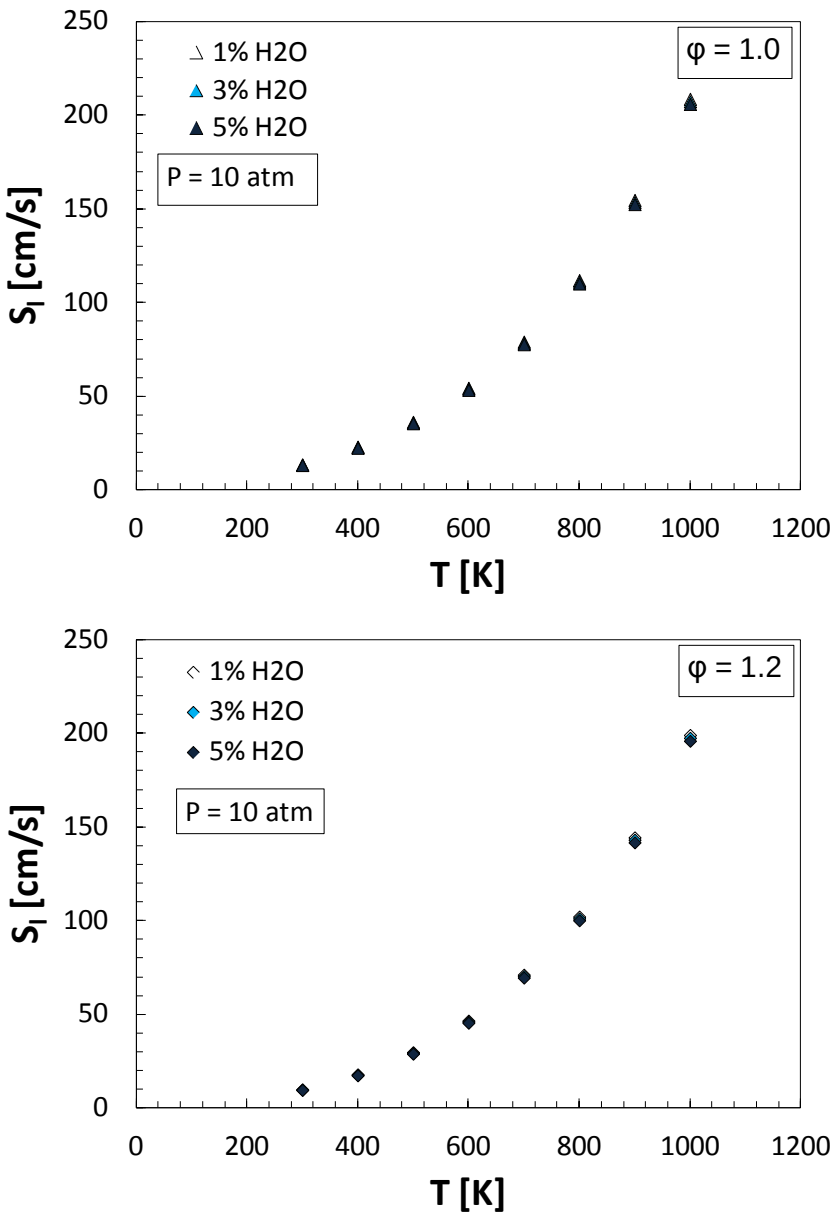


Figure 9: Laminar flame speed as a function of unburned gas temperature for different water contents from 1-5% at a fixed pressure of 10 atm for different values of φ.
a) φ=0.7; b) φ=1.0; c) φ=1.2.

Laminar burning velocity calculations were performed for a fixed pressure of 10 atm, varying unburned/initial gas temperatures, varying water content (1—5 % by volume), and varying φ (0.7-1.2). Figures 9(a)—9(c) shows variation in laminar flame speed (S_l) as a function of unburned gas temperature for different water contents ranging from 1—5 %, a fixed initial pressure of 10 atm and three different value of φ (0.7, 1.0, and 1.2). Flame speed increased with increasing unburned gas temperature of the mixture as expected. The highest values of flame speed are found for φ=1.0, with decreases as the mixture is made richer or leaner. Water content between 1—5 % in the fuel is found to have a negligible effect on flame speed at all conditions. Figure 10 shows the effect of addition of 'simulated' oil on the laminar burning velocity of CH_4

for a fixed pressure of 10 atm, unburned gas temperature of 300 K, 3% water content and φ=1. A 20 % change is observed in the burning velocity by increasing oil content from 1 to 7 % by volume.

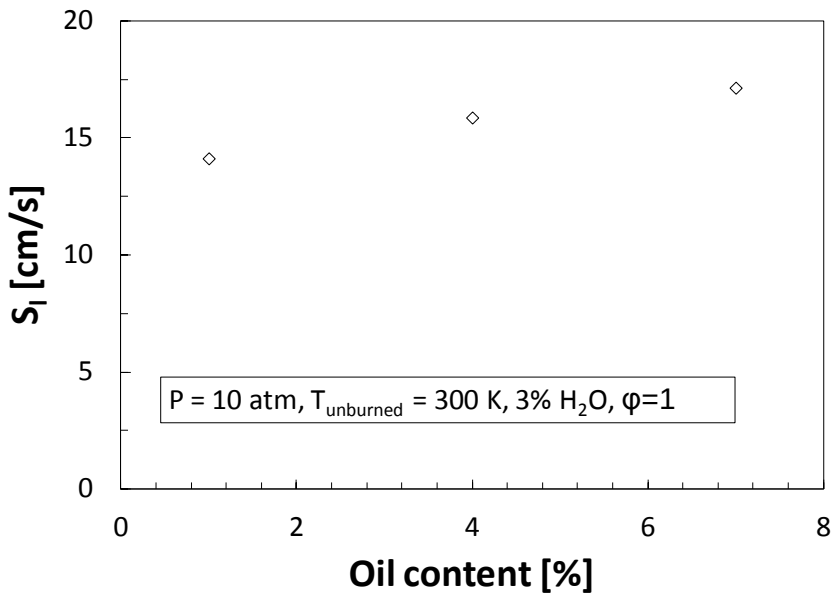


Figure 10: Laminar flame speed as a function of oil content for a fixed pressure of 10 atm, unburned gas temperature of 300 K, 3% water content and φ=1.

4.4 Spark plug placement

An additional consideration investigated in this work is the effect of spark plug placement on engine operation. This is motivated chiefly by the fact that the cylinder head modifications to incorporate the onboard refueling strategy results in elimination of one of the spark plugs in the stock cylinder head. This is required due to the limited space available in the modified cylinder head. A literature study was undertaken to investigate the effects of this change on engine operation. Primarily it is found that multi-ignition strategies facilitate in extending the lean-operating limit of spark-ignited gasoline engines [26]. Under lean operating conditions having multiple spark plugs would allow for improved flame initiation and improve burning rates of natural gas. This would result in reduced torque fluctuation, improved brake specific fuel consumption (BSFC), and reduced emissions. Since the engine under consideration would operate primarily under stoichiometric mixture conditions, operating with a single spark plug should not produce any significant changes in engine combustion. Another study performed by Johansson et al. [27] investigated the effects of changes in piston geometry and also concluded that no significant changes in engine performance were noticed unless the spark-ignited gasoline engine was operated at a very lean air-fuel mixture ratio. In summary, the removal of one of the spark plugs is not expected to cause any performance degradation during normal engine operation. This issue will be further investigated during actual experimental engine tests.

5. Conclusions

A parametric study is undertaken to investigate the effects of natural gas conditions produced in a novel “bi-modal” engine on the chemical kinetic phenomena taking place during normal engine

combustion operation. Specifically the effects of increase in fuel temperature, water and oil content are investigated with the aid of numerical simulation tools and a detailed description of gas phase fuel-air chemistry. Fuel-air equivalence ratio and engine speed are found to have a strong influence on the minimum temperature required to cause auto-ignition for the engine under consideration. Water addition of 1—5 % by volume is found to not have any significant effect on the temperature required to cause auto-ignition. Ignition delay calculations conducted in a closed homogenous reactor show similar results. Ignition delay is affected strongly by initial mixture temperature, only slightly by equivalence ratio and by a negligible amount by changing water content from 1—5 %. Addition of oil from 1—10 % by volume results in a 75% reduction in ignition delay. The oil is assumed to be vaporized and show similar chemical kinetics as *n*-heptane in gas phase. Increasing oil content more than 10% results in negligible change in ignition delay. Laminar flame speed is found to increase with unburned gas temperature as expected. Water addition of 1—5 % by volume is found to have a negligible effect on laminar burning velocity. Oil addition by 1—8 % is found to produce a 20% change in laminar burning speed. In summary, water addition to natural gas by 1—5 % does not result in any major changes in the combustion processes. Oil content on the other hand has a strong influence on ignition delay as well as on laminar burning speed with the effects diminishing with increasing oil content. Initial air-fuel mixture temperatures of higher than about 550 K are required for the onset of auto-ignition phenomena in the engine under consideration. Given peak fuel temperatures of about 200°C in the fuel tank, it is unlikely that any auto-ignition phenomena would result from routine engine operation as a result of the onboard refueling process. Finally, based on literature review, removal of a spark-plug from the stock engine is not anticipated to cause any performance degradation during normal engine operation. This issue will be further investigated during engine dynamometer tests.

6. Acknowledgements

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