Homogeneous Charge Compression Ignition Engine: Experiments and Detailed Kinetic Calculations


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ABSTRACT
Experiments have been performed on a Homogeneous Charge Compression Engine (HCCI) fuelled with natural gas. The in-cylinder pressure has been measured for different engine speeds and fuel-air ratios. Numerical simulations of the ignition process in the engine have been carried out using a detailed reaction mechanism for butane and lower alkanes. The effects of the engine speed and fuel-air ratio on autoignition have been calculated and compared with the measurements. In addition, calculations have been made of the ignition delay time sensitivity to changes in initial pressure, initial temperature, and quality of gas fuel. Excellent agreement with single-cycle measurements is obtained for the calculated temperature and pressure profiles. The single-cycle temperature simulations show good agreement with 100 cycle-averaged measurements as well, but cycle-to-cycle variations flatten out the averaged profiles, and the need for a PDF-based approach to achieve perfection is evident. Furthermore, it was found that the autoignition process in an HCCI engine is extremely sensitive to variations in initial temperature, whereas changes in pressure, fuel-air ratio and engine speed affects the ignition timing to a much lesser extent.

INTRODUCTION
The Homogeneous Charge Compression Ignition is a promising alternative to the existing Spark Ignition engine (SI) and Compression Ignition engine (diesel). The HCCI concept can be described as a hybrid of the SI and the diesel engine concepts. As in a diesel engine, the fuel is exposed to a sufficiently high temperature for auto ignition to occur, but in HCCI, a homogeneous fuel-air mixture is used. As in a SI engine, the homogeneous mixture is created in the intake system using a low-pressure injection system or a carburetor. No ignition system is necessary. To limit the rate of combustion, very diluted mixtures are used. A low fuel-air ratio and/or Exhaust Gas Recycling (EGR) may be used to achieve high dilution. If the mixture is too rich, the pressure rises too rapid and will generate knock-related problems. A too lean mixture will lead to incomplete combustion or misfire.

In SI engines, large cycle-to-cycle variations occur, since the early flame development varies considerably due to mixture inhomogeneities in the vicinity of the spark plug [1]. With HCCI, cycle-to-cycle variations of combustion are very small. Combustion initiation takes place at many points at the same time. The whole mixture burns almost homogeneously and unstable flame propagation is avoided.

Several studies have been performed on the HCCI engines [2,3,4,5,6] showing that both two stroke and four stroke HCCI engines are possible and that part load efficiency is dramatically increased. Comparisons between HCCI, CI, and GDI engines [7] show that the HCCI concept had the lowest fuel consumption, lowest NOx-, but highest HC-emissions. Honda has demonstrated a concept for HCCI combustion for a production two stroke engine [8][9] and proved the reliability of the concept by competing in the Granada-Dakar desert race with a pre-production motorcycle [10]. A scooter, Honda 125 Pantheon, equipped with HCCI-engine, is to be sold in Europe in the near future [11][12]. A pre-production two-stroke HCCI engine has also been shown by JIP [13].

Our previous research shows much higher indicated efficiency with HCCI than with SI operation at part load [14]. The low upper load limit (IMEP) attainable with naturally aspirated HCCI was improved by supercharging [15]. No combustion related problems in operating an HCCI under high pressure have been detected. Up to two bar of boost pressure can be applied by adjusting the inlet temperature accordingly. When running the engine on natural gas, the ignition timing is sensitive to the composition of the gas.

The aim of the current paper is to investigate effects of different parameters on the ignition timing. Experiments have been performed with natural gas as fuel. The crank-angle resolved pressure has been measured for a variety of engine speeds and fuel-air ratios. As the HCCI combustion process is mainly controlled by chemistry, the computer code used for simulations of the process uses detailed chemical kinetics, but neglects effects from transport phenomena. Homogeneous reactor calculations have been performed taking the compression of the gas by the engine into account.

EXPERIMENTS
A six-cylinder Volvo TD100 series truck diesel is used, modified for one-cylinder use, and converted to homogeneous charge compression ignition operation. The engine data are given in Table 1, additional details can be found in [13].
<table>
<thead>
<tr>
<th>Component</th>
<th>Mole-%</th>
<th>Mass-%</th>
</tr>
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<tbody>
<tr>
<td>Methane</td>
<td>91.3</td>
<td>81.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>5.0</td>
<td>7.9</td>
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<tr>
<td>Propane</td>
<td>1.8</td>
<td>4.2</td>
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<tr>
<td>n-Butane + higher</td>
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<td>4.7</td>
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<tr>
<td>Nitrogen</td>
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<td>0.9</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>0.6</td>
<td>1.2</td>
</tr>
</tbody>
</table>

**Table 2: The natural gas components**

The engine was run on natural gas at fuel-air ratios of $\phi = 0.30$–$0.45$. Four different engine speeds were used: 800, 1000, 1200 and 1400 rpm. These engine speeds were chosen, as representative for normal use, considering that maximum torque for a normal CI-operating TD100-series diesel is achieved at 1400 rpm and the engine idle speed is 475–525 rpm. During the experiments, measurements were made on pressure and emissions of NOx and THC. Then the temperature profile was calculated from the measured pressure profile and other engine parameters, using a numerical code. Details about the code and measurement techniques are available in ref. [16]. The calculated temperature is highly dependent on the inlet-pipe pressure immediately before the inlet valve closes. Therefore, it is essential to determine the inlet manifold pressure accurately.

Engine run measurements show that ignition time measured in Crank Angle Degrees (CAD) decreases with increased fuel-air-ratios and increases with increased engine speed. The duration time (measured in CAD) of main combustion decreases with increased IMEP and increased engine speed. The in-cylinder pressure time-gradient decreases with increased engine speed and increased fuel-air ratio.

**MODELING**

The computer code used for simulating the engine combustion process is basically a set of zero-dimensional time dependent differential equations. The energy conservation and mass conservation balance for each chemical species is solved with Newton’s method and the time is resolved with higher order backward differential functions. The detailed kinetic mechanism used for the simulation of the ignition process contains 72 species and 864 reactions [17].

The main characteristics of the program have been discussed previously [18,19]. The HCCI engine simulations require only a few specific differences in calculation approach. The initial pressure and the temperature are taken from the experiments at a specified crank angle position. The volume decrease and consequently the pressure increase due to the piston movement can easily be calculated [20]. Thus the total pressure is calculated as the sum of inlet pressure, the pressure increase caused by piston movement, and the pressure increase due to chemical reactions. The conservation equation for the chemical species is given by:

$$\frac{dY_j}{dt} = \frac{M_j}{\rho} \sum_{k=1}^{N} \frac{\xi_k}{\rho} V_{j,k} \omega_k$$  \hspace{1cm} (1)

And the energy conservation equation is given by:

$$m \sum_{j=1}^{N} \left( h_j - \frac{RT}{M_j} \right) \frac{M_j}{\rho} \sum_{k=1}^{N} \frac{\xi_k}{\rho} V_{j,k} \omega_k + p \frac{dV}{dt} + m(C_p - \frac{R}{M}) \frac{dT}{dt} = 0$$  \hspace{1cm} (2)

The instantaneous volume is calculated from [20]:

$$V = V_c + \frac{\pi B^2}{4} \left( l + a - a \cos \Theta + (l^2 - a^2 \sin^2 \Theta)^{1/2} \right).$$  \hspace{1cm} (3)

The pressure is then calculated from the equation of state:
\[ p = \rho \frac{RT}{M} \]  

(4)

RESULTS AND DISCUSSION

Simulations of the autoignition process in the HCCI-engine were made using initial values obtained from the experiments at 60 CAD before Top Dead Center (BTDC), as given in Table 3. The results from these calculations are shown in Figures 1 and 2 in comparison with the corresponding experiments. The speed of the engine has been varied between 800 and 1400 rpm and the fuel-air equivalence ratio between \( \phi = 0.304 \) and \( \phi = 0.453 \). In principle the fuel-air equivalence ratio for the higher speeds was increased to achieve shorter ignition delay times. Efforts were made to keep the experimental temperature and the pressure at 60 CAD BTDC constant for each engine speed. The compression ratio was only slightly changed from CR = 17.10 to 17.30.

<table>
<thead>
<tr>
<th>CASE</th>
<th>( \phi )</th>
<th>CR</th>
<th>( T )</th>
<th>( P ) [BAR]</th>
<th>SPEED [RPM]</th>
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<tbody>
<tr>
<td>1</td>
<td>0.304</td>
<td>17.10</td>
<td>761</td>
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<td>800</td>
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<tr>
<td>4</td>
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<td>17.30</td>
<td>814</td>
<td>4.40</td>
<td>1000</td>
</tr>
<tr>
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<td>17.30</td>
<td>815</td>
<td>4.40</td>
<td>1000</td>
</tr>
<tr>
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<td>0.414</td>
<td>17.30</td>
<td>818</td>
<td>4.42</td>
<td>1000</td>
</tr>
<tr>
<td>7</td>
<td>0.371</td>
<td>17.15</td>
<td>733</td>
<td>3.87</td>
<td>1200</td>
</tr>
<tr>
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<td>0.400</td>
<td>17.15</td>
<td>735</td>
<td>3.87</td>
<td>1200</td>
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<tr>
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<td>736</td>
<td>3.88</td>
<td>1200</td>
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<tr>
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<td>1400</td>
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<tr>
<td>12</td>
<td>0.412</td>
<td>17.30</td>
<td>740</td>
<td>4.14</td>
<td>1400</td>
</tr>
</tbody>
</table>

Table 3: initial values for the simulation of the engine cases 1–12 *at 60 CAD BTDC

It can be seen from Figs. 1 and 2 that the ignition delay time of the gas mixture could be calculated in good agreement with the experiments. However the pressure rise, during the auto-ignition process is steeper than in the experiments. This is due to the fact, that in experiments an average of 100 cycles was calculated. The small cycle to cycle variation lead to the observed flattening of the pressure rise. This evident from Fig. 3, where the calculation is compared with the temperature and pressure of one measured HCCI cycle. Here, the calculated temperature and pressure rise is in excellent agreement with the experiment.

Figure 1a: measured (solid lines) and calculated (dashed lines) gas temperature as a function of crank angle at a speed of 800 rpm

Figure 1b: measured (solid lines) and calculated (dashed lines) gas temperature as a function of crank angle at a speed of 1400 rpm

Sensitivities of the HCCI process to variations of the fuel-air ratio, engine speed, the initial pressure and the initial temperature at 60 CAD BTDC have been calculated for Case 5 in Table 3. This is shown in Fig.5. As can be seen, temperature has a dramatic impact on the ignition timing. In the given example, 5 K (0.6%) increases in the temperature at 60 CAD BTDC promote the ignition with almost one crank angle degree. An increased fuel-air ratio also has an ignition-promoting effect in this lean mixture region, but in this case a
10% variation of the fuel-air ratio is needed to give the same changes. Naturally, the predominant effect from raising the fuel-air ratio is higher power. Pressure was shown to have a rather low impact on ignition. Changing the pressure with as much as 0.5 bar (11%) at 60 CAD BTDC changed the ignition time by slightly more than one crank angle degree.

Assuming all parameters except engine speed are kept constant, the ignition delay time measured in CAD must increase with an increased engine speed, which also is the calculated result. The ignition-promoting effects of higher hydrocarbons, in this case ethane, propane and butane, have been discussed in a previous paper [15]. It was found that the existence of higher hydrocarbons in natural gas in some cases, e.g. close to the ignition limit, was sensitive to the timing and/or occurrence of ignition. Figure 4 shows calculations from two different inlet temperatures, where the composition of a gas fuel is varied. In both cases, ignition does not occur in pure methane gas. At the higher temperature, 2 mole-% butane gives an ignition point at 8 CAD ATDC, at the lower temperature, as much as 10 mole-% butane is required to give the same point of ignition.
CONCLUSION

Experiments have been performed in a Homogeneous Charge Compression Engine (HCCI) fuelled with natural gas. The in-cylinder pressure has been measured for different engine speeds and fuel-air ratios. It has been shown that the ignition process of the HCCI cycles can be simulated by a homogeneous reactor calculation. The effects of the engine speed and fuel-air ratio on autoignition have been calculated in agreement with the measurements. A sensitivity analyses of important engine parameter has shown how sensitive the HCCI process is for small changes in the initial temperature, where changes in initial pressure or fuel-air ratio affect the ignition less.

Simulations of how the natural gas quality affect ignition, show that the ignition process under some circumstances may be highly affected by a relatively small content of higher hydrocarbons. Simulations show that gas quality has a big impact on ignition at a higher temperature.

When temperature was lowered 30 K, ignition was much less affected by gas quality. Apparently, gas composition has a high impact on the HCCI combustion only when the engine works under conditions that are close to ignition limit. It must be noted however, that the engine quite often works close to ignition limit. As a consequence, the ignition promoting effects from higher hydrocarbons can not be neglected.

As the composition of natural gas varies from one gas source to another, the calculations clearly show the necessity of using standardized or octane-rated gas fuel, when running an HCCI-engine on natural gas. The calculations also suggest the possibility of using small amounts of higher, gaseous hydrocarbons, as fuel additives to promote ignition. Thereby, the area of possible working conditions for HCCI-combustion would be extended.
The use of a homogeneous reactor program for simulating the HCCI process allows to apply all features that such programs commonly offer, e.g. to perform a detailed sensitivity analyses to the reaction coefficients of a detailed reaction mechanism or to perform a detailed reaction flow analyses. The results presented show some interesting characteristics of the Homogeneous Charge Compression Ignition concept. The usefulness of this engine concept however involves, that more detailed information about the autoignition processes of more complex fuels for fuel lean conditions at high pressures is needed in the future.

ACKNOWLEDGEMENTS

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