

Integration of Fuel Auto-ignition Characteristics and HCCI Engine Operation

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ABSTRACT

A recently improved Arrhenius fuel auto-ignition model was combined with a single zone explicit discrete Homogeneous Charge Compression Ignition (HCCI) engine model in order to investigate a wide range of combinations of fuel type with engine setup and operational configurations.

The engine model was validated using experimental data from a single cylinder variable compression ratio engine running in HCCI mode.

The model was used to identify promising and problematic areas for the combination of fuel properties, engine configurations and operational ranges. Insights regarding the interaction between trapped gas pressure and temperature histories and auto-ignition reaction rate surfaces in the pressure and temperature domain are presented.

INTRODUCTION

BACKGROUND & LITERATURE REVIEW

Homogeneous Charge Compression Ignition engines offer significant advantages in efficiency over spark ignition engines and engine out emissions advantages over diesel engines [1, 2]. However, due to wide range control and starting challenges HCCI operation is chiefly being developed as part of dual mode systems in spark ignition and diesel engines [1]. While HCCI combustion has been shown to be achievable using almost any hydrocarbon fuel, appropriate choice of fuel characteristics can help in optimising engine operation [1, 4]. This fuel characteristic optimisation is often hampered by the fuel characteristics required for dual mode operation due to the combustion requirements of the non-HCCI mode [1].

Hydrocarbon fuel auto-ignition characteristics can be divided into 2 classes: Single stage ignition fuels such as

methanol exhibit decreasing constant volume auto-ignition delay times with increasing temperature and increasing pressure [5-10]. Autoignition delay times of two stage ignition fuels such as n-heptane and iso-octane also decrease with increasing temperature and increasing pressure, with the exception of the "negative temperature coefficient" zone wherein autoignition delay times remain constant or increase with increasing temperature [5-10]. This NTC effect is associated with a cool flame heat release that precedes the main heat release. The cool flame timing and heat release magnitude are also strongly affected by temperature and pressure [5-10].

Fuel mixture composition also dramatically affects fuel autoignition behaviour. Air-fuel ratio, residual exhaust gas fraction and concentrations of oxygen, H₂O, CO and partially oxidised hydrocarbons all affect autoignition delay times [11, 12].

Fuel autoignition behaviour in an HCCI engine is therefore intimately connected with the particular trapped charge composition and thermodynamic history experienced by the charge. The charge's thermodynamic history is in turn a complex function of engine configuration parameters (e.g. compression ratio, combustion chamber wall temperatures, chamber size) and operational parameters (e.g. inlet heating, valve timing, inlet throttling/boosting).

All these factors influence fuel autoignition behaviour in HCCI engines and the complexity is greatly increased by the inter-connectedness of many of these parameters. For example, inlet heating reduces inlet gas density and results in increased exhaust gas fraction and reduced mass of the trapped charge, while compression ratio changes affect in-cylinder turbulence, residual gas fractions and therefore trapped charge composition and temperature [1, 13]. These interactions make research into direct cause and effect relationships in HCCI engines extremely difficult [1].

It has been noted in many studies that HCCI operation is typically limited in speed range due to combustion phasing requirements [1, 4, 14-16]. Combustion phasing is generally retarded to the point of instability at high speed operation limits and advanced to the point of excessive pressure rise rates and excessive pumping work at low speed operation limits unless phasing is corrected by changes to other parameters [17, 18]. However, it is also known that at low engine speeds, heat losses to the combustion chamber walls result in decreased peak pressures and temperatures [19, 20]. In the extreme isothermal compression case, autoignition would never take place due to insufficient temperature required to initiate combustion even within the time scales of the isothermal process. Since high engine speed results in retarded phasing, low speed in advanced phasing and ultra low speed in ultra retarded phasing, it stands to reason that there must exist a speed range where phasing is relatively independent of engine speed changes.

This speed convergence behaviour has been noticed in experimental work conducted by Sjöberg and Dec [19]. Detailed reasons for this behaviour were suggested and the following statement was made in reference to this unique operational zone:

“... we can conclude that the compression and combustion temperatures increase with engine speed in such a manner to almost perfectly compensate for the reduced “real” time available for both autoignition and for completion of the CO-to-CO₂ reactions, as observed for iso-octane.” - Sjöberg and Dec [19].

The above example is just one of a number of imaginable “sweet spots” or “convergence zones” where the complex interplay of system variables could result in independence of critical parameters such as engine speed, charge density and air-fuel ratio. Identifying these areas and enlarging them could offer an additional approach to other more complex HCCI combustion controls being researched such as charge stratification [21], thermal stratification [22] and exhaust recompression/rebreathing strategies [11, 12]. Development of this approach could prove helpful in the advance of HCCI technology.

AIM OF THIS STUDY

The aim of this work was to explore the complex engine-fuel interactions in an HCCI engine with a view to identifying and optimising the naturally occurring auto-compensation zones described above. This required the development of a single zone explicit discrete engine model capable of accurately simulating combustion chamber trapped gas thermodynamic histories and the effects of engine configuration and operational changes on these histories without the need for numerical solving techniques. These thermodynamic histories were used in an explicit discrete version of the Arrhenius form Auto-ignition Integral Model improved upon in [9]. The explicit

nature of the engine and autoignition model was imposed due to the requirements of demonstrating the effects of a very broad range of engine configuration and operational states simultaneously. The explicit formulation was also able to solve for initial conditions required in order to achieve desired combustion phasing. This enabled easy assessment of trends in effects and rapid identification of optimal configurations of the many variables. Such a model formulation cannot compete with the accuracy of CFD and detailed chemical kinetics models used in other studies [23, 24], but was merely aimed at identifying operational trends in HCCI combustion.

METHODS IN THE STUDY

ENGINE MODEL

The formulation of the engine model was aimed at being as generic as possible in order to be able to explore wide ranges of setup and operating conditions. The generic model was set up in Microsoft Excel and formulated to allow easy manipulation of conditions, multiple copies solving simultaneously and instant visual assessment of the effects of changes to conditions.

The variables used to define the setup condition were:

- cylinder swept volume
- compression ratio
- bore/stroke ratio
- connecting rod length/stroke ratio
- Fuel choice

The variables used to define the operational condition were:

- engine speed
- inlet charge temperature (mixture entering the cylinder)
- inlet charge P (mixture entering the cylinder)
- air fuel equivalence ratio
- residual exhaust gas pressure at exhaust valve closure.

Note that external residual exhaust gas recirculation was kept constant at zero and no chemical effects of exhaust gas residuals on autoignition were included. This was a recognised simplification in the modelling which is a planned future extension to this work.

Exhaust gas product species and mole fractions were calculated from stoichiometric and lean burn balanced chemical equations assuming no dissociation due to the typically low burned temperatures in HCCI combustion. Values for constant volume specific heat were calculated as a polynomial function of temperature using the JANAF thermodynamic tables (National Bureau of Standards, 1971). Exhaust valve closure was assumed to occur at TDC and residual exhaust gas temperature was assumed to be a linear function of equivalence ratio

as indicated by spark ignition engine exhaust temperature data in [13].

The calculated mass of trapped exhaust gas was adiabatically adjusted to the inlet gas pressure with the associated changes in volume and temperature. The inlet gas was assumed to fill the remainder of the volume to BDC at its inlet pressure and temperature. The moles of both mixtures were summed and the temperature and pressure of the mixture calculated for start of compression at BDC. Using the mole fractions and JANAF coefficients for specific heats of each component, the expression for gamma as a function of temperature for the specific mixture could be calculated. Values of gamma were related to an appropriate polytropic compression coefficient using a relationship derived from data showing speed effects on polytropic compression coefficient [13] and pressure data from a number of different engine sizes including very small displacement engines [25-29].

$$\text{Polytropic compression coefficient, } n = X_1 \gamma \quad (\text{Eq.1})$$

$$\text{Where } X_1 = 0.7 + 0.3 \left(1 - e^{-A_{\text{poly}} \text{ RPM}} \right) \quad (\text{Eq.2})$$

$$\text{And } A_{\text{poly}} = 0.000562 \ln(V_{\text{swept}}) - 0.000694 \quad (\text{Eq.3})$$

Where V_{swept} is the displaced cylinder volume in cm^3

And RPM is engine speed in revolutions per minute

This effectively simulated the effects of engine speed and displacement on heat loss during compression and associated effects on the compression pressure and temperature history. Temperature and pressure during compression were discretely calculated using this polytropic approximation, resulting in a pressure and temperature history showing sensitivity to inlet and exhaust boundary conditions, fuel type and equivalence ratio, engine speed, compression ratio and size.

FUEL AUTO-IGNITION MODEL

The Arrhenius form auto-ignition integral model used in this study was originally proposed in [30]. The model was further improved in [5-7], incorporated into a discreet implicit HCCI engine model and compared with experimental HCCI test results in [8]. The model was further improved in [9] to incorporate predictions of cool flame ignition delay and heat release magnitude (for 2 stage ignition cases) in addition to the main heat release timing prediction, and effects of air-fuel ratio were incorporated. The model form and coefficients used were taken directly from [9]. Since the AI model was applied in a discrete engine model, the AI integral calculations were used in their discrete form. A summary of the discrete formulation of the model is given in the appendix.

The cool flame and peroxide heat release rates were modelled using a Wiebe burn function. Some effort was spent formulating an empirical model to describe the burn durations for the cool flame and peroxide reactions using the underlying Chemkin simulation data used to formulate the autoignition model in [9]. However, when these burn durations were compared with typical durations during the experimental validation, it was found that the real burn durations were more than an order of magnitude longer. It was therefore deduced that the burn durations were completely dominated by physical effects such as thermal profile and since the burn duration values were very similar throughout the limited range of validation, constant crank angle degree burn durations of 9 and 16 CAD were used for the cool flame and peroxide burn durations respectively.

RESULTS

EXPERIMENTAL VALIDATION

Limited experimental validation was done using a 507cm^3 displacement, single cylinder, variable compression ratio engine. The naturally aspirated engine had been modified to incorporate a port fuel injection system and inlet air was heated to 313K to aid fuel evaporation. Geometric information for the engine is given in Table 1 below.

Engine description:	Research test engine
Number of cylinders:	1
swept volume:	507 cm^3
Cylinder bore size:	76.2 mm
Piston stroke length:	111.1 mm
Connecting rod length:	241.3 mm
compression ratio	variable 6:1 – 20:1

Table 1: test engine geometry

The engine was run using n-heptane at 600, 1200 and 1800 rpm and lambda values of 2.0, 2.5, 3.0, and 3.5. The higher engine speeds caused knocking and instability at the lower lambda values, so not all points the test matrix could be achieved. In each test, the HCCI combustion phasing was varied by compression ratio adjustment to produce peak pressure at 10-13 degrees after TDC. Combustion phasing retarded to this range has been shown to optimise efficiency, combustion stability, peak heat release rates and emissions [1, 31].

Representative pressure traces from each test condition were compared to those predicted by the engine model. The polytropic compression and cool flame phasing

correlated reasonably well, assuming a fixed inlet mixture temperature rise of 60°C due to heat transfer from the inlet manifold, port, valve and combustion chamber walls. The cool flame temperature rise was slightly under-predicted. The phasing of the main heat release in the model was slightly retarded compared with experimental results. An attempt was made to rectify this problem by scaling the X factor in the autoignition model, and it was found that multiplying the X factor by 2.0 gave good correlation across the admittedly small range of experimental results. Comparison of resulting pressure traces are shown below in figure 1.

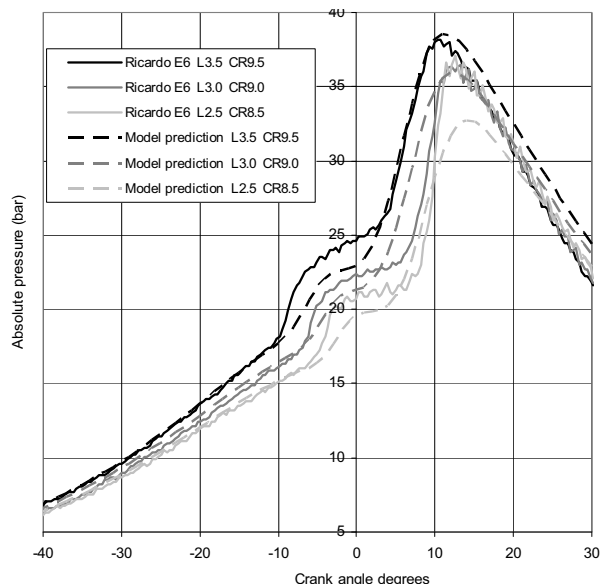


Figure 1: Comparison of experimental and modelled pressure traces at 1200rpm with "X factor" multiplied by 2 (note: combustion phasing controlled by CR adjustment).

OPERATIONAL PARAMETRIC STUDY

A parametric study was conducted using the engine model to predict the inlet charge temperature required to obtain complete combustion and peak pressure at ten degrees after TDC for a very wide range of engine speeds, compression ratios, inlet gas pressures and equivalence ratios. The combustion phasing was chosen as 10 CAD ATDC for reasons stated earlier. This was done for 3 fuels and 3 engine displacement sizes. The fuels used were n-heptane, iso-octane and methanol. The 3 engine displacements were chosen according to 3 HCCI engines currently being studied:

- a research test engine (507 cm^3),
- a small commercial utility engine (25 cm^3)
- a model aeroplane engine (6.5 cm^3).

For each engine and fuel combination, attention was directed towards compression ratios that yielded practically attainable initial temperatures and pressures.

Attention was directed towards areas where engine speeds converged, implying speed insensitivity to combustion phasing. Within these areas, attention was directed towards zones that exhibited load (equivalence ratio and/or initial pressure) insensitivity to combustion phasing.

These areas were then investigated for running stability by assessing the effect of small changes in initial temperature and/or engine speed on combustion phasing. Areas that exhibited high phasing sensitivity to these changes were deemed unstable operating points and therefore of little practical value, while areas that exhibited low sensitivity were deemed to be practically achievable and therefore of value. Pressure rise rate limits were not regarded as a limiting factor in this study since many researchers have attained extremely high load operation with corresponding high pressure rise rates and ringing intensities without evidence of engine damage [4, 16]. This is particularly interesting in the light of the modes of auto-ignition damage shown by [32, 33]. In addition, very small engines with large in-cylinder thermal gradients appear to operate at high loads completely free of knocking limitations [25-29]. However, care was taken to steer clear of lean misfire and emissions limits shown by [19, 21, 34]

PARAMETRIC STUDY RESULTS

Parametric study results using n-heptane and the 507 cm^3 research engine configuration, a typical set of initial pressure and charge temperature curves are shown in figure 2 below.

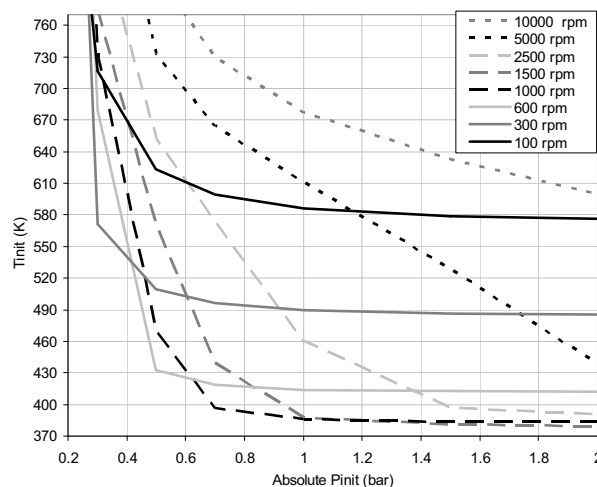


Figure 2: Curves of initial pressure and charge temperature for 507 cm^3 engine at $\text{CR} = 8$ and $\phi = 0.35$, using n-heptane.

A number of interesting features can be seen in figure 2:

1. Typical cranking engine speeds (300 rpm or less) require high initial temperatures in order to overcome the significant heat losses. High

engine speeds also require high initial temperatures in order to achieve short enough ignition delay times for appropriate combustion phasing.

2. For this particular set of conditions, there is a converging of the speed contours at around 1500 rpm for unthrottled ($P_i > 1\text{ bar}$) operation. This means that for changes in speed between 1000 and 1500rpm, very little change in the initial temperature of 380K is needed to maintain correct combustion phasing.
3. The lower speed curves flatten out at higher initial pressures. For example, there is almost no change in the initial temperature of 380K required to maintain correct combustion phasing at 1000rpm as the initial pressure is increased from 1bar to 2bar.

The base of the speed converged T_i - P_i curves tends to slope upward for higher equivalence ratios and downward for lower equivalence ratios than the $\phi = 0.35$ condition shown in figure 2.

Similar curves can be calculated illustrating the effects of equivalence ratio on initial charge temperatures required for correct combustion phasing. A typical set is shown in figure 3 below.

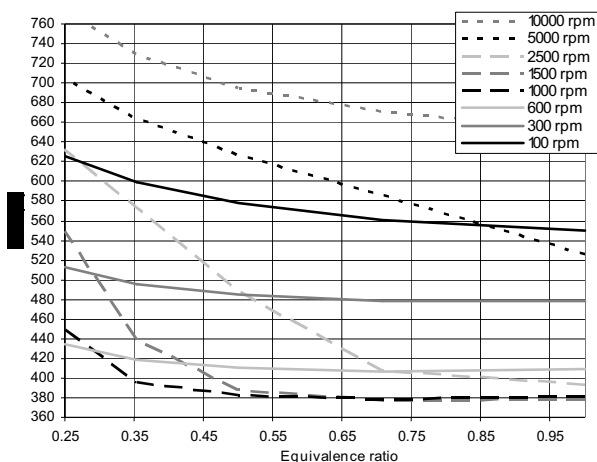


Figure 3: Curves of equivalence ratio and charge temperature for 507 cm³ engine at CR = 8 and $P_i = 0.7$ bar, using n-heptane.

A number of interesting observations can be made from the T_i - ϕ curves shown in figure 3:

1. The convergence of speeds can also be observed in the equivalence ratio dimension at an inlet charge temperature of 380K and occur in a similar speed range (1000-1500rpm) to that seen in figure 2.

2. The curves flatten out at higher equivalence ratios. For example, there is almost no change in initial temperature of 380K required to maintain correct combustion phasing at 1000rpm as the equivalence ratio is increased from 0.5 to 1.0.

Note that the base of the converged T_i - ϕ curves tends to slope upward for higher initial pressures and downward for lower initial pressures than the $P_i = 0.7$ bar condition shown in fig 3.

Increasing compression ratio results in inlet charge temperature convergence over a wider range of engine speeds. This means that inlet heating is not desirable, since it reduces the compression ratio needed to achieve correct combustion phasing.

For n-heptane in the 507 cm³ engine without inlet air heating, inlet charge temperatures (including port heating of 60 K) were kept constant at 360 K. This allowed the following operation while maintaining peak pressure phasing of CAD 10 ± 1 ATDC:

- For $P_i = 1.5\text{ bar}$ and $\phi = 0.5$ a speed range of 950 – 2600 rpm.
- At 1500 rpm and $\phi = 0.5$ an inlet pressure from 0.6 bar upwards (upper boost pressure limit would be limited by peak cylinder pressures and intercooling requirements)
- At 1500 rpm and $P_i = 1.5\text{ bar}$, equivalence ratio $\phi = 0.2 - 0.75$

A stability analysis was conducted on these conditions by testing the phasing sensitivity to small changes in initial conditions. Peak pressure phasing can be seen as a function of inlet charge pressure and temperature in figure 4 below.

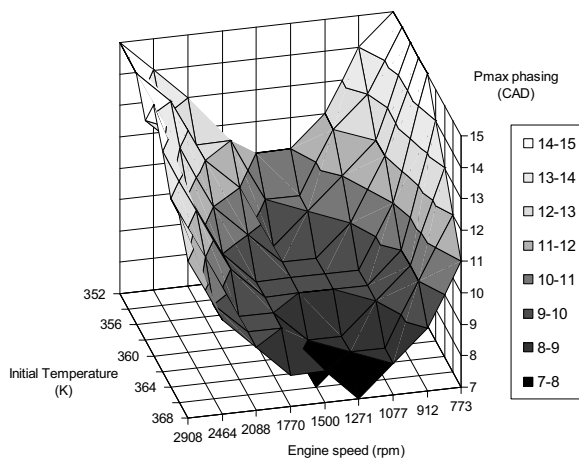


Figure 4: Peak pressure phasing surface showing engine speed and charge temperature effects on