An Investigation of the Effect of Changes in Engine Operating Conditions on Ignition in an HCCI Engine

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The dependence of the ignition timing in an HCCI engine on intake temperature and pressure, equivalence ratio, and fuel species is investigated with a zero-dimensional model combined with a detailed chemical kinetics. The accuracy of the model is evaluated by comparing measured and computed results in a propane-fueled HCCI engine. It is shown that the peak pressure values are reproduced within 10% and ignition timing within 5° CA. The heat loss through the walls is found to affect significantly on the ignition timing for different inlet conditions. It is also shown that for the propane-fueled engine, the tolerance in intake temperatures is 20-25K and the tolerance in intake pressure is about 1 bar for stable operation without misfire or too early ignition. Comparison of propane and heptane fuels indicates that the tendency to misfire when heptane is employed as the fuel is less than that when propane is employed with the same wall temperature conditions. However, the heptane-fueled engine may have a lower compression ratio to avoid too early ignition and hence lower efficiency. For the selected set of engine parameters, stable operations might be achieved for the heptane-fueled engine with twice as much tolerance in intake temperatures as for the propane-fueled engine.

Key Words: Ignition, HCCI Engine, Fuel

1. Introduction

The continuing pressure to reduce particulate matters (PM) and NOx emissions simultaneously in Diesel engines while maintaining the high thermal efficiency is the motivating force behind efforts by designers to explore alternative designs and combustion strategies that may replace conventional Diesel engines. Most of the modifications in the case of Diesel engines that have been suggested to achieve the dramatic reductions in pollutants legislated by the U.S. EPA are based on achieving a certain degree of homogeneity of the fuel-air mixture in the chamber (Najt et al, 1983; Thring, 1989; Ryan et al 1996). It is well known that the homogeneous charge compression ignition (HCCI) engines have the potential to improve the fuel efficiency and to reduce exhaust emissions, especially PM and NOx, since they can operate with the extremely lean mixtures.

In the case of direct injection of the fuel into the combustion chamber, this requires a significant increase in the ignition delay so that there would be more time for mixing and homogenization. This increase may be brought about by early injection of the fuel or by late injection after top dead center (Takeda et al, 1996; Nakagome et al,

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1997 ; Shimazaki et al, 1999 ; Kimura et al, 2001). Introduction of the fuel into the intake port, as in spark-ignition engines, is another approach to achieve homogenous mixture distribution in the combustion chamber. In this approach, the fuel is introduced, often in gaseous form, into the intake port and premixed with the incoming air (Christensen et al, 1997 ; Christensen et al, 1998). Once the mixture starts to ignite, it may ignite at several points in the chamber almost simultaneously leading to rapid combustion without apparent flame propagation. While this concept is simple, it is challenging to implement in practice because of the high sensitivity of ignition to relatively small changes in load and intake conditions. Understanding this sensitivity, and controlling ignition, is essential if HCCI engines are to be developed successfully.

It is generally accepted that HCCI combustion is dominated by chemical kinetics (Najt et al, 1983). With the advances in the understanding of chemical reaction mechanisms for higher hydrocarbon chemistr rapid increase in computational powers, more researchers have begun to formulate theoretical description of HCCI combustion. An increasing number of papers on modeling HCCI engines have recently appeared in the literature (Aceves et al, 2000 ; Flowers et al, 2000 ; Kong et al, 2001). A zero-dimensional models can predict ignition timing and combustion with relatively simplicity and less computational time even though the heat release rate and CO and HC emissions cannot be predicted with sufficient accuracy due to their assumption of homogeneity in the physical properties of mixture in the cylinder. Therefore, it can be applied to the parametric study to investigate the effect of engine operating conditions on ignition delay and combustion duration for the understanding of the combustion controllability in HCCI engines.

2. Model

The model employed is a zero-dimensional version of the multidimensional engine code, REC (Magi, 1987). Kelly-Zion and Dec (Kelly-Zion et al, 2000) in their work considered the effect of changes in several initial conditions on ignition timing in an HCCI engine through a computational modeling study and showed that fuels that have minimum cool temperature chemistry may have less sensitivity to changes in operating conditions relative to those with two-stage ignition characteristics. This work differs from their work in that it is considered the effect of wall heat loss on the results. Another focus is also on identifying the range of intake parameters for which stable operation without misfire can be achieved. The assumption of zero-dimensionality is justified only if the reactions are homogeneous. However, even if the reactions are homogeneous, wall heat loss is likely to set up a temperature gradient in the chamber which will have an effect on location of ignition and possibly heat release rates. These concerns notwithstanding, the zero-dimensional model is employed to isolate some interesting trends. Wall heat loss rate, $\dot{q}_w$, is modeled with an Annand correlation which is expressed as (Heywood, 1988)

$$\dot{q}_w = h_c A (T_g - T_w) \tag{1}$$

where h_c, the convective heat transfer coefficient, is given by

$$h_c = a\left(\frac{\rho \bar{S}_p B}{\mu}\right)^b \cdot \frac{k}{B} \tag{2}$$

A is the surface area of the combustion chamber, T_g is the gas temperature, T_w is the wall temperature, ρ is the density of the gas in the chamber, $\bar{S}_p$ is the mean piston speed, B is the bore, μ is the viscosity of the gas and k is its thermal conductivity. a and b are constants whose values are 0.46 and 0.7 respectively in our computations.

All properties of the gas are temperature dependent. Propane oxidation is modeled using a detailed mechanism (Konnov, 1998), that contains 121 species and 1027 reaction steps. The heptane oxidation is modeled using the mechanism proposed by Seiser et al. (Seiser, 2000). This consists of 159 species and 1546 reaction steps. In this case the NO is modeled using the reaction mechanisms based on GRI-Mech-3.0 (Smith et al, 1999).

3. Computational Conditions

The computations are carried out in an engine whose geometric parameters are given in Table 1. The engine is a derivative of a Cummins B-series engine whose piston has been modified so that the combustion chamber is disc shaped. Prior to employing the model to carry out parametric studies, comparisons of computed and measured results are carried out. The operating conditions for the three sets of experimental data employed in this work are indicated in Table 2(a). The cases reflect variations in speed, intake pressure and overall equivalence ratio. This experimental data has also been employed in reference (Aceves et al, 2000) to assess the accuracy of multidimensional modeling studies.

Table 1 Specification of the engine used in the experiment and computation

Displacement	1378cm^3
Bore	11.4cm
Stroke	13.5cm
Connecting rod length	21.6cm
Compression ratio	18 : 1
Intake valve opening	−370°BTDC
Intake valve closing	−146°BTDC
Exhaust valve opening	135°ATDC
Exhaust valve closing	370°ATDC
Swirl ratio	4.3
Combustion chamber shape	Disc type

4 Results and Discussion

The computed in-cylinder pressures were compared with the measured pressure trace from a HCCI engine for the three cases. Fig. 1 shows the comparisons for these three cases. The results are seen to agree within 10% in the magnitude of peak pressures and about 5° CA in the location of ignition which is indicated by a sudden change in the slope of the pressure-crank-angle curve. As the computations are zero-dimensional, the computed duration of combustion subsequent to ignition is only a measure of the completion of homogeneous reactions in a constant volume chamber. The rather close agreement in the slopes and peak values of the pressure curves following ignition is indicative that the combustion in the engine is homogeneous. All results henceforth will focus on ignition timing only. In order to achieve the agreement shown in Fig. 1, the set of initial and boundary conditions given in Table 2 (b) should be employed. Notice that these conditions are somewhat different from those in Table 2(a). The differences may arise from the zero-dimensional nature of the computations and also the fact that the flow in the intake and exhaust ports are not modeled. In the experiments, the intake conditions are measured in the intake port at some location upstream of the opening. In these computations the chemistry is active throughout the computational cycle. However, it is found that prior to 20-30°CA before top dead center (BTDC), the effect of chemistry is negligible. Fig. 2 shows the computed in-cylinder pressure when the chemistry is activated 20°CA BTDC and 30°CA BTDC in the computations. The close agreement of the computed pressures indicates that even at 20°CA BTDC the chemistry is relatively inactive.

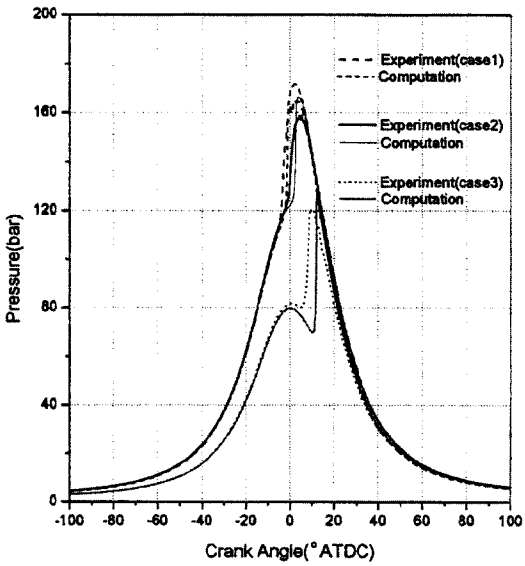

Fig. 1 Computed and measured in-cylinder pressure traces for case 1～3

Table 2(a) Operating conditions for the experiment

	Case 1	Case 2	Case 3
Engine speed (rpm)	1000	1000	1800
Intake temperature (K)	352.3	340.2	341.6
Intake pressure (bar)	2.72	2.75	1.88
Equivalence ratio	0.165	0.167	0.36
Fuel	Propane		

Table 2(b) Operating conditions for the computation

	Case 1	Case 2	Case 3
Engine speed (rpm)	1000	1000	1800
Intake temperature (K)	377	365	365
Intake pressure (bar)	2.64	2.68	1.81
Equivalence ratio	0.165	0.167	0.36
Fuel	Propane		

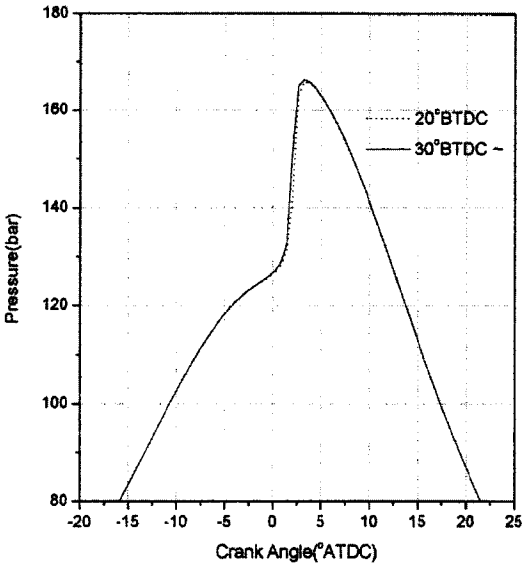

Fig. 2 Computed in-cylinder pressure traces for different timings to activate chemical kinetics

Figure 3 shows the computed in-cylinder pressure for a case where the engine speed (N) is 1000rpm, intake pressure (P_I) is 1 bar, wall temperature (T_w) is 450K, and equivalence ratio (ϕ) is 0.5. Results are shown for several values of intake temperature T_I in the range of 395K to 425K. When the T_I=425K, it may be seen that ignition occurs at about 2°CA BTDC. Increasing T_I further leads to advanced ignition which results in a drastic loss in engine efficiency. When the T_I= 400K, ignition occurs at about 7°CA ATDC. If the intake temperature is reduced further for this case, misfire occurs as shown for the case where T_I=395K. In this case, we identify the range of stable operation to be 400-425K.

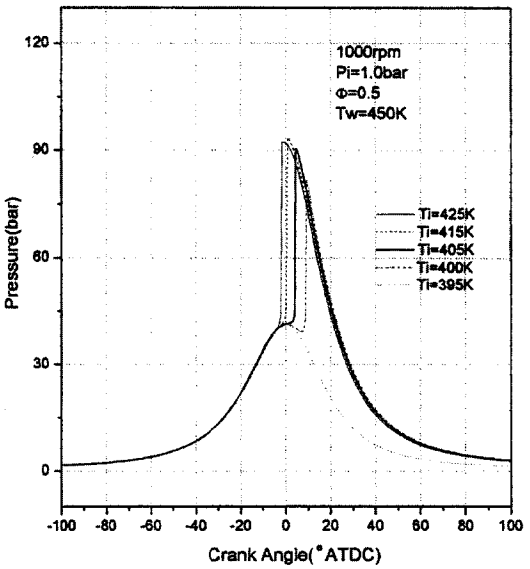

Fig. 3 Comparison of combustion pressure traces for different intake temperatures

Figure 4 shows consolidated results for the range of stable operation for several wall temperatures and intake temperatures when N=1000rpm, P_I=1bar and ϕ=0.3. It may be seen that with an assumption of T_w=410K, the range of operation is T_I of 425-450K, i.e. a variability of about 25K. As wall temperatures are increased, the compressed gas temperatures would increase, and the engine can operate with lower intake temperature. When T_w=450K, the range of T_I is from 395-420K, i.e. about 25K. Of course, the wall temperature is not a variable that can be readily varied in an engine and, hence, the effect of the wall temperature is presented only to show the dependence of the results on its specified value in the model. However, since the wall temperature can be varied with engine operating conditions, especially during engine warm up, the understanding of the effect of wall temperature on ignition trend is necessary to control the ignition

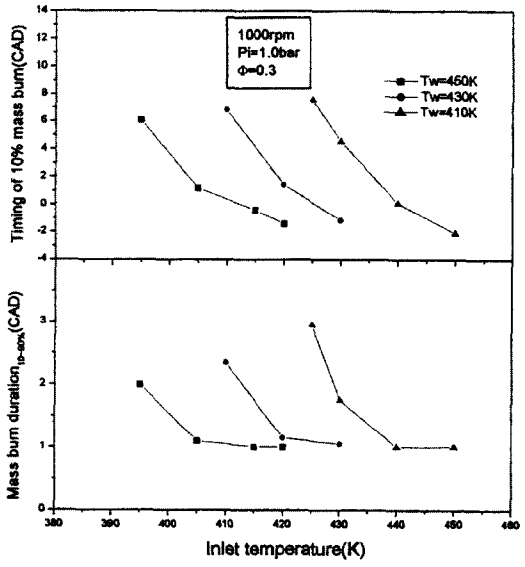

Fig. 4 Effect of intake temperature and wall temperature on combustion duration (propane)

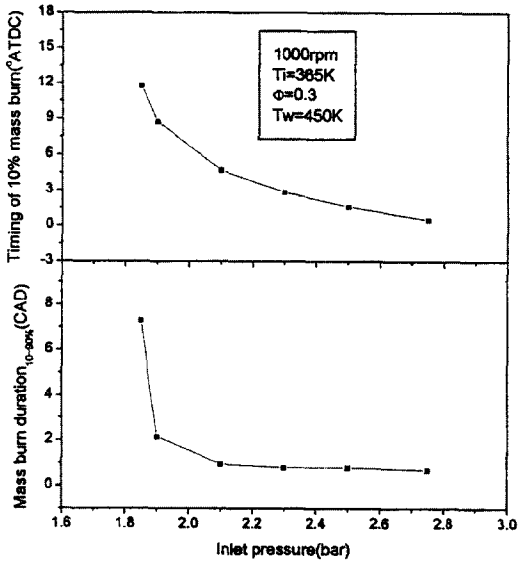

Fig. 5 Effect of intake pressure on combustion duration (propane)

in HCCI engine during transient operation. The important point about this set of results is that the variability of intake temperature for stable operation of the engine is about 25K. Fig. 5 shows the corresponding results where P_i is varied. For this case N=1000rpm, T_i=365K, ϕ=0.3 and T_w= 450K. It may be seen that stable operation is achieved in the range of P_i=1.8~2.8bar. This range would depend on the values of the other selected parameters.

The dependence of ignition timing on equivalence ratio, as predicted by the model, is very interesting. There are at least three factors to be considered : (1) As equivalence ratio is increased, peak pressures and temperatures would increase reflecting a higher engine load and this generally leads to increased wall temperature; (2) For hydrocarbon fuels, reacting in a constant volume chamber, chemical kinetics may lead ignition to occur sooner as equivalence ratio is increased provided the mixture temperature is kept unchanged ; and, (3) As the equivalence ratio increases, the specific heat of the mixture decreases and hence the compression temperature reduces. These three factors play a role in determining the outcome when the equivalence ratio is changed. Fig. 6 shows the ignition timing as a function of equivalence ratio for N=1000rpm. These results were obtained with the wall temperatures scaled with the maximum in-cylinder temperature after combustion. In this case, the increase in wall temperature with equivalence ratio leads to earlier ignition. However, if fixed wall temperatures are used, a different trend is obtained. Fig. 7 shows

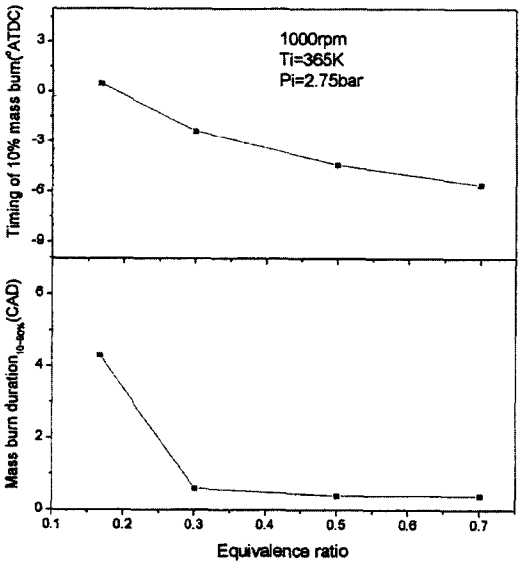

Fig. 6 Effect of equivalence ratio on combustion (propane)

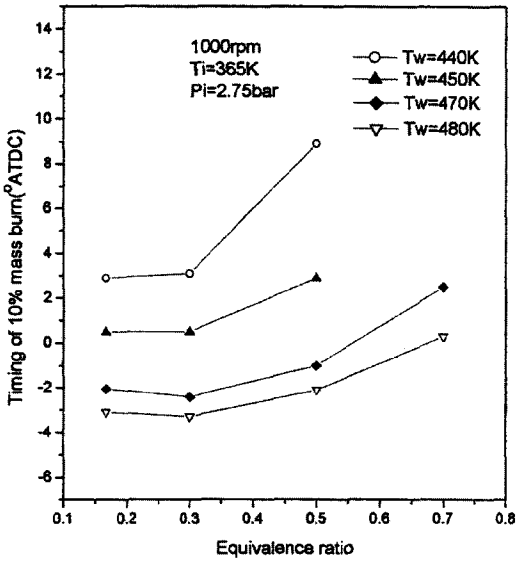

Fig. 7 Effect of equivalence ratio on combustion (propane) for fixed wall temperatures

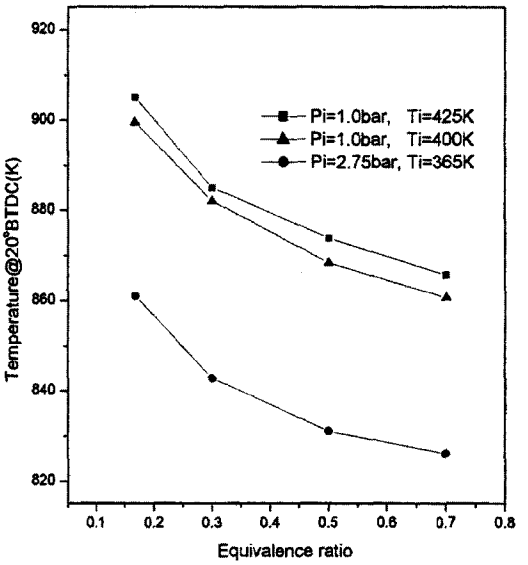

Fig. 9 Minimum compression temperature at 20° BTDC for autoignition (propane ; 1000rpm)

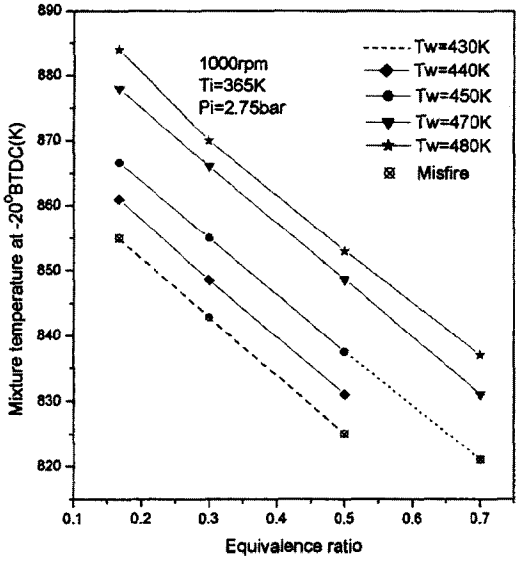

Fig. 8 Effect of equivalence ratio and wall temperature on compressed mixture temperature (propane)

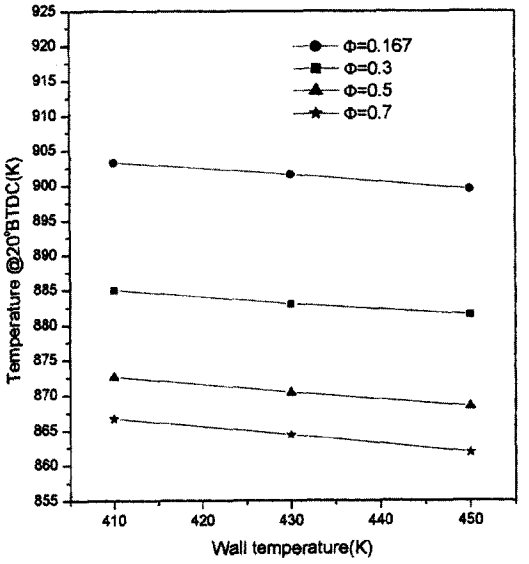

Fig. 10 Minimum compression temperature to autoignite at 20°BTDC for wall temperatures (propane ; 1000rpm and P_i=1bar)

the computed ignition timing as a function of equivalence ratio for several fixed wall temperatures. It may be seen that as the equivalence ratio increases, the ignition timing is retarded. This trend is obtained because the mixture temperature that results from compression decreases as the equivalence ratio increases which result in an decrease in the specific heat. This trend can be applied to the control strategy in HCCI engine during transient operation with different equivalence ratios. Fig. 8 shows the mixture temperature at 20°CA BTDC for the different cases plotted in

Fig. 7. It may be seen that if the wall temperature is assumed to be 430K, misfire results as the compression temperature is not sufficient to bring about ignition. It is possible, based on the results above, to identify a minimum compression temperature at 20°CA BTDC which would result in ignition and stable operation. Fig. 9 shows this minimum temperature plotted as a function of equivalence ratio for three values of T_i and two values of P_i. In the case of $\phi=0.5$ with an intake pressure of 1.0 bar and temperature of 425K, the minimum temperature at 20°CA BTDC is about 875K. When the intake temperature is lowered to 400K, the minimum temperature is about 870K. This means that lowering of the minimum temperature occurs as a result of greater mass of charge being present in the chamber and hence higher pressure when the intake charge temperature is lowered. This trend is confirmed by the third case where the intake pressure is increased to 2.75bar and the intake temperature is reduced to 365K. It is possible that changes in the selected wall temperature may influence these results of minimum temperature required for ignition when the temperature is identified at 20°CA BTDC. Fig. 10 shows the minimum temperature at 20°CA BTDC required for ignition plotted as a function of wall temperature for different equivalence ratios. It may be seen that the tolerances in the value of minimum temperature that leads to ignition are about 4-5K for a change in wall temperature of about 40K.

Heptane is also applied to gain some insight into the range of values of the operating variables and compare the range with that obtained with propane as the fuel. Heptane has different ignition characteristics relative to propane. Most importantly, heptane ignites more readily compared to propane and hence, intake conditions remaining the same, the compression ratio of the engine has to be lowered. Based on initial studies carried out, the compression ratio is set as 13 for the heptane-fueled engine instead of 18 for the propane fueled engine. Heptane also has a two-stage ignition characteristic whereas propane has single-stage ignition. Fig. 11 shows the mass burn fraction curve for heptane for several values of T_i. The two

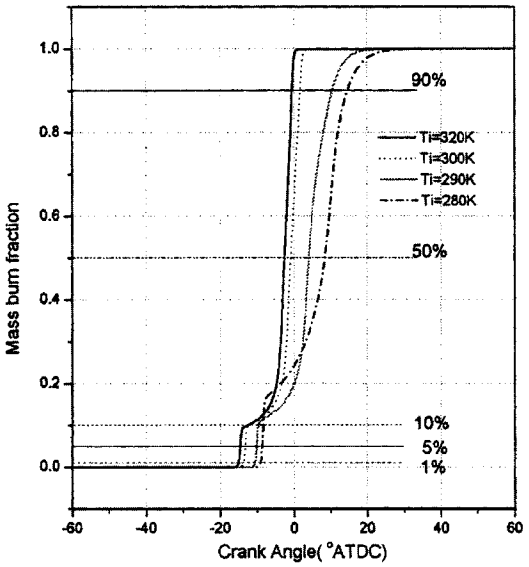

Fig. 11 Typical mass burn fraction profile of n-heptane for different intake temperatures

stages of ignition may be clearly identified. In this case, the crank-angle corresponding to 10% mass burn fraction appears to indicate the end of the first stage of ignition or some fraction of burned mass during the first stage. Unlike in the case of propane, it is not an indicator of ignition that would lead to significant heat release and rise in in-cylinder pressure. Hence, the crank angle at which 50% of mass is burned is selected as an indicator of ignition timing for heptane.

Figure 12 shows the ignition timing plotted as a function of intake temperature for three values of wall temperature. For these cases, N=1000rpm, P_i=1bar and $\phi=0.3$. Fig. 12 may be compared with Fig. 5 for propane. In the case of heptane, the variability in intake temperature ranges for which stable operation may be achieved is about 50K as compared to 25K for propane. The actual value of the intake temperature may be seen to be lower for heptane than for propane but this is likely to depend on the compression ratio. The result that the variability in intake temperature ranges for which operation may be achieved is greater when heptane is employed as the fuel instead of when propane is employed as the fuel is somewhat surprising and may appear to contradict the conclusion of Kelly-Zion and Dec

Nakagome et al., 1997 that fuels with two-stage ignition characteristics are more sensitive to changes in operating conditions. Heptane has a lower tendency to misfire than propane when intake temperatures are reduced. Table 3 summarizes the computed results of range of operation for the engine when propane and heptane are employed as the fuel. Fig. 13 is a bar plot illustrating the operating temperature ranges for the two fuels and for different equivalence ratios and wall temperatures. For propane, with increasing equivalence ratio the range of intake air temperature decreases. The increase in the range of values as the equivalence ratio is reduced may, in part, result from chemistry effects which cause the fuel to autoignite later as equivalence ratio is

Table 3 Operating inlet temperature ranges (K) for different operating conditions at $P_i = 1.0$ bar

	Propane			Heptane
Wall temperature (K)	ϕ=0.167	ϕ=0.3	ϕ=0.5	ϕ=0.3
410	430~475	425~445	435~450	365~405
430	415~460	410~430	415~435	345~390
450	400~450	395~415	400~420	330~370

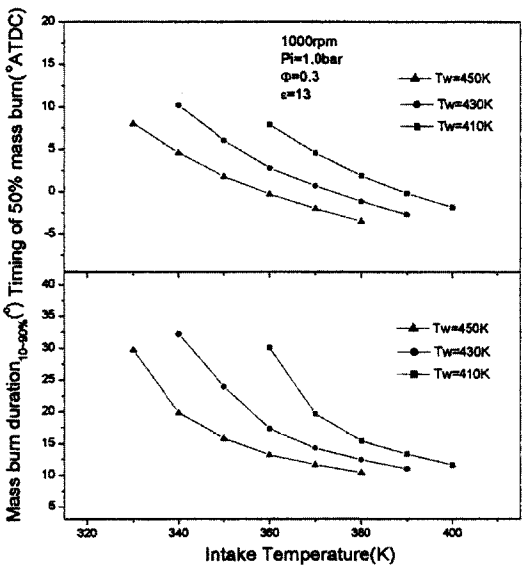

Fig. 12 Effect of intake temperature and wall temperature on combustion (n-heptane)

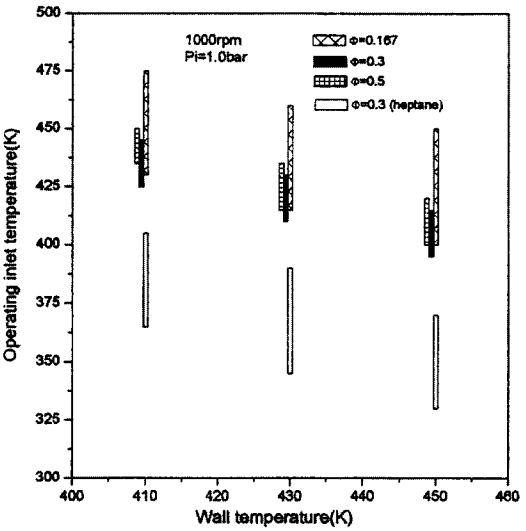

Fig. 13 Operating inlet temperature ranges for different equivalence ratios and wall temperatures (propane)

reduced. This implies that the chamber gas becomes less susceptible to autoignite as intake temperature is increased. There is an opposing trend in that compression temperatures increase as equivalence ratio is decreased. But, the former effect appears to dominate in this case. Heptane has a wider range of operation than propane.

7. Conclusion

In this work, a zero-dimensional model is employed to study ignition behavior in an HCCI engine. The accuracy of the model is assessed by comparing measured and computed results which show that peak pressures are reproduced within 10% and ignition timing within 5°CA. The optimum compression ratio for the heptane-fueled engine is lower (CR=13) than that of the propane-fueled (CR=18) engine as heptane has a greater tendency to autoignite compared to propane, which results in lower thermal efficiencies. The main contribution of this work is in identifying stable operating ranges of intake temperatures for the HCCI engine when propane and heptane are employed as fuels. This range is bounded on the lower end by the misfire limit and the upper end by the tendency to ignite early. It is shown

that the stable operating range for the heptane-fueled engine is broader than for the propane-fueled engine as the tendency to misfire is less when heptane is employed as the fuel. The effect of wall temperature on ignition shows a certain trend with different equivalence ratios and wall temperatures, which can be applied to the control of ignition during transient operation, especially warm up period. It is also shown that assumptions made about wall temperatures, which can change the value of wall heat transferred, may affect the trends. In this respect, full three-dimensional computations which compute intake processes, spatial inhomogeneities in gas temperature and species distribution, may be necessary to sort out the ambiguities.

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References

Aceves, S. M., Flowers, D. L., Westbrook, C. K., Smith, T. R., Pitz, W., Dibble, R., Christensen, M. and Johansson, B. 2000, "A Multi-Zone Model for Prediction of HCCI Combustion and Emissions," *SAE Paper* 2000-01-327.

Aceves, S. M., Flowers, D. L., Martinez-Frias, J., Smith, J. R., Westbrook, C. K., Pitz, W. J., Dibble, R., Wright, J. F., Akinyemi, W. C. and Hessel, R. P. 2000, "A Sequential Fluid-Mechanic Chemical-Kinetic Model of Propane HCCI Combustion," *SAE paper* 2000-01-1037.

Christensen, M., Johansson, B., Amneus, P. and Mauss, F. 1998, "Supercharged Homogeneous Charge Compression," *SAE Paper* 980787.

Christensen, M., Johansson, B. and Einewall, P. 1997, "Homogeneous Charge Compression Ignition (HCCI) Using Isooctane, Ethanol, and Natural Gas-A Comparison," *SAE Paper* 97 2874.

Heywood, J. B. 1988, "Internal Combustion Engine Fundamentals," *McGraw-Hill*, pp. 670~678.

Kelly-Zion, P. L. and Dec, J. E. 2000, "A Computational Study of the Effect of Fuel Type on Ignition Time in Homogeneous Charge Compression Ignition Engines." *Proc. Combust. Inst.*, 28 :1187-1194.

Kimura, S., Aoki, O., Kitahara, Y. and Aiyoshizawa, E. 2001, "Ultra-Clean Combustion Technology Combining a Low-Temperature and Premixed Combustion Concept for Meeting Future Emission Standards," *SAE Paper* 2001-01-0200.

Kong, S.-C., Marriott, C. D., Reitz, R. D. and Christensen, M. 2001, "Modeling and Experiments of HCCI Engine Combustion Using Detailed Chemical Kinetics with Multidimensional CFD," *SAE Paper* 2001-01-1026.

Konnov, A. A. 1998, "Detailed Reaction Mechanism for Small Hydrocarbons Combustion.," Release 0.4 http://homepages.vub.ac.be/~akonnov/.

Magi, V. 1987, "A New 3-D Code for Sprays and Combustion in Reciprocating and Rotary Engines," Technical Report, *Mechanical and Aerospace Engineering Report No. 1793*, Princeton University, Princeton, NJ.

Najt, P. and Foster, D. E. 1983, "Compression-Ignited Homogeneous Charge Combustion," *SAE Paper* 83 0264.

Nakagome, K., Shimazaki, K., Niimura, K. and Kobayashi, S. 1997, "Combustion and Emission Characteristics of Premixed Lean Diesel Combustion," *SAE Paper* 97 0898.

Ryan, T. W. and Callahan, T. J. 1996, "Homogeneous Charge Compression Ignition of Diesel Fuel," SAE 961160.

Seiser, R., Pitsch, H., Seshadri, K., Pitz, W. J., and Curran, H. J. 2000, "Extinction and Autoignition of N-Heptane in Counterflow Configuration," *Proceedings of the Combustion Institute*, 28 :2029-2037.

Shimazaki, N., Akagawa, H. and Tsujimura, K. 1999, "An Experimental Study of Premixed Lean Diesel Combustion," *SAE Paper* 1999-01-0181.

Smith, G. P., Golden, D. M., Frenklach, M.,

Moriarty, N. W., Eiteneer, B., Goldberg, M., Bowman, C. T., Hanson, R. K., Song, S., Gardiner Jr., W. C., Lissianski, V. V., and Qin, Z. 1999. http://www.me.berkeley.edu/gri_mech/.

Takeda, Y., Nakagome, K. and Niimura, K. 1996, "Emission Characteristics of Premixed Lean Diesel Combustion with Extremely Early Staged Fuel Injection," *SAE Paper* 96 1163.

Thring, R. H. 1989, "Homogeneous Charge Compression Ignition (HCCI) Engines," *SAE Paper* 89 2068.