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Simulating the Influence of Injection Timing, Premixed Ratio, and Inlet Temperature on Natural Gas / Diesel Dual-Fuel HCCI Combustion in a Diesel Engine

H Ghomashi, P Olley, B Mason and M K Ebrahimi
School of Engineering and Informatics,
University of Bradford, Bradford, BD7 1DP, UK.

Abstract

Dual-fuel HCCI engines allow a relatively small quantity of diesel fuel to be used to ignite a variety of fuels such as natural gas or methane in HCCI mode. The gaseous fuel is mixed with the incoming air, and diesel fuel is sprayed into the cylinder by direct injection. Mathematical modelling is used to investigate the effects of parameters such as premixed ratio (fuel ratio) and pilot fuel injection timing on combustion of a dual-fuel HCCI engines. A CFD package is used with AVL FIRE software to simulate dual-fuel HCCI combustion in detail. The results establish a suitable range of premixed ratio and liquid fuel injection timing for low levels of NO_x , CO and HC emissions along with a reliable and efficient combustion. Dual-fuel HCCI mode can increase NO_x emission with lower premixed ratios in comparison to normal HCCI engines, but it is shown that the NO_x emission reduces above a certain level of the premixed ratio. Due to the requirement of homogenous mixing of liquid fuel with air, the liquid fuel injection is earlier than for diesel engines. It is shown that, with careful control of parameters, dual-fuel HCCI engines have lower emissions in comparison with conventional engines.

Keywords: HCCI engine, dual-fuel, direct injection, premixed ratio, injection timing, natural gas, diesel

1. Introduction

Because of the major contribution that vehicles give to harmful emissions, the trend is to use engines with the lowest practicable emissions. The production of dual-fuel HCCI engines has the potential to help significantly in the reduction of emissions. In a dual-fuel engine a mixture of gas and air is burnt with the assistance of a quantity of liquid fuel, normally diesel.

The combustion in a dual-fuel HCCI engine involves a two stage combustion, the liquid fuel starts the combustion through compression ignition (hence the liquid fuel is also referred to as the ignition fuel, or pilot fuel) and then the natural gas burns rapidly. Dual-fuel HCCI engines have potential efficiency and emissions benefits in comparison with conventional SI and CI engines due to having the efficiency advantages of CI engines (high compression, lean burn and low throttling losses), with the added advantages of having gas as the main fuel and early liquid fuel injection which leads to a more homogenous combustion mixture. Further, dual-fuel HCCI engines have the potential to give lower emissions at low and medium loads in comparison with diesel or gasoline in normal HCCI engines: the HC emission is low due to the lean-burn and the more homogenous mixture of fuels and air in the cylinder; NO_x emission can also be low because the maximum temperature is generally lower than for a single-fuel HCCI engine.

In this work the effects of parameters such as premixed ratio (also known as the fuel ratio) and the injection timing of pilot fuel on the combustion of a dual-fuel HCCI engine are investigated.

Modelling has allowed detailed understanding of HCCI combustion. Kraft [1] investigated the effect of actual non-homogeneity on the performance of a HCCI engine by using a stochastic chemical kinetic model. He used a mechanism with 53 chemical species and 590 chemical reactions. Kusaka et al [2] investigated the combustion of natural gas in HCCI engines by using a multi-dimensional model with a chemical kinetic mechanism including 151 chemical species and 501 fundamental reactions. Kiva and Chemkin software were used for this study. The calculation time was shown to increase considerably in comparison with a zero-dimensional model, but the results of this modelling showed an improvement in accuracy of the maximum temperature and pressure of a cycle as compared with the predictions of a zero-dimensional model. Kong and Reitz [3] studied ignition delay and investigated the effects of turbulence in an engine by using a detailed chemical kinetic model. The results showed that using a two-dimensional model along with a chemical kinetic model gives accurate simulation of many aspects of the combustion of a completely homogenous charge. Flowers et al [4] compared the results obtained from a zero-dimensional and a 3-D model with experimental results. They found that the 3-D model gave significantly better predictions of the start of combustion, maximum pressure, thermal

efficiency and NO_x emissions than the zero-dimensional model.

For this study a Deutz F6L912Q diesel engine of known specification is modelled, the engine specification is given later in this work. The modelling method is to combine a 3-D CFD simulation of flows and mixing in a cylinder with detailed analysis of chemical reactions involved in combustion which ultimately produces power and emissions. The behaviour of this engine is investigated by simulation and the simulation results compared with experimental results in Zhang et al [5], for diesel and dual-fuel operation. This preliminary investigation was carried out in order to test the current simulation method against similar diesel and dual-fuel combustions in order to validate and apply the method to the detailed study of dual-fuel HCCI operation.

The major contributions are to establish the effect of liquid fuel injection timing on a dual-fuel HCCI engine's power and emissions, to establish the significant role of inlet air temperature on combustion, and further to show the dependence of combustion duration on the ratio of natural gas and diesel fuels, which affects the performance of all aspects of the engine. It is shown that in a dual-fuel HCCI engine with a *premixed ratio* above a certain value, NO_x emissions decrease. The premixed ratio, r_p , is defined by

$$r_p = \frac{Q_g}{Q_t}, \quad (1)$$

where Q_g is the thermal energy of the mixture due to the gas component (typically natural gas or methane), and Q_t is the total thermal energy of the mixture due to gas and the liquid fuel (typically diesel or gasoline). Hence a value of $r_p = 0$ represents a 'normal' HCCI fuel and a value of $r_p = 1$ represents an all gas fuel.

It is shown that with an increase in the proportion of gas in the fuel, the burning process is more rapid and oxidation becomes more complete. As a result, the amounts of CO and HC emissions decrease remarkably. It is also shown that there is a best liquid fuel injection time for a wide range of conditions, and that the inlet air temperature plays an important role in the vaporization of liquid fuel and the control of combustion.

2. Theoretical and Modelling method

Details of the flow equations and chemical dynamic equations that are used are given in ref. [6]. To simulate a combustion chamber, the first requirement is to give a two dimensional (axis-symmetrical) specification of the piston crown of the engine in the condition of Top Dead Centre (TDC). In this work the selected model is from a Deutz engine for which the shape of the (ω - shaped) piston crown is shown in Figure 1. The shape of the piston is taken from ref. [5]. By using the dimensions of this piston crown, the 2D mesh plan was drawn using GAMBIT software, as shown in Figure 2. To expedite the generation of the mesh, the mesh is a “Map” type and the number of volumes (for two dimensional conditions) is 800. The next step is to save the generated mesh in a NASTRAN format, and finally it can be read by AVL FIRE software.

Figure 1 Specification of the half of piston crown for a Deutz engine; g is a section of the air gap above the piston (all dimensions in mm)

Figure 2 Mesh generated model in GAMBIT software

The model is extended to three dimensions and made moveable using facilities in the AVL Fire software. In this work only 90 degrees of the cylinder is simulated; this is achieved by noting symmetry and using periodic boundary conditions. A sector angle based on the number of the injection holes was determined in this way. With rotational axis symmetry for the combustion chamber all of the fuel injection holes will have identical flow rates and only one section in the geometry for the chamber and injector need be considered. In Figure 3 the generated mesh is shown at the crank angles of 180 degrees after top dead centre (ATDC) and 360 degrees ATDC. Throughout this work the “crank angle” is the ATDC angle. This mesh is continuously moveable between the extreme crank angles. The number of volumes was incrementally reduced between 320 and 360 degrees ATDC in order to maintain the quality of generated meshes. The number of generated volumes between 180 to 320 degrees ATDC was 44730, with 34650 volumes from 320 to 340 degrees ATDC and 29610 volumes between the angles of 340 to 360 degrees ATDC.

Figure 3 3D generated mesh model in crank angles of 180 and 360 degrees ATDC

3. Fuel spray models

AVL FIRE software was used to simulate the injection of droplets from the nozzle as a spray that enters the flow field as a mixture of liquid and gas. The software calculates the spray separation using sub-models. The variation of momentum for the droplets and gas, the drop separation, the evaporation of droplets, the collision of droplets, mutual effects between the droplets and wall and also mutual effects between gas and liquid phases are simulated by a group of models that allow AVL Fire software to deal with the different regimes of the flow. To solve the fuel spray equations, gas and liquid phases should be considered. The gas phase is described by the Navier-Stokes and energy equations; from this velocity, pressure, density and temperature fields are obtained for each time step. There is transfer of mass, momentum and energy between the droplets of liquid fuel and the gas in the cylinder, and the equations of both

phases are thus coupled together.

The spray momentum equation is written as follow:

$$m_d \frac{d u_{id}}{d t} = F_{idr} + F_{ig} + F_{ib} , \quad (2)$$

where u_{id} is the particle velocity, m_d is the particle mass, F_{ig} is the force on the particle due to gravity, F_{ib} is the buoyancy force due to the mass of the displaced gas. F_{idr} is the drag force, given by

$$F_{idr} = D_p \cdot u_{irel} , \quad (3)$$

where u_{irel} is the relative velocity of the drop and D_p is the drag function, given by

$$D_p = \frac{1}{2} \rho_g A_d C_D |u_{irel}| , \quad (4)$$

where C_D is the drag coefficient, A_d is the cross sectional area of a drop, and ρ_g is the fluid density of the gas phase. The relationship for the acceleration of a particle is as follows. It is obtained by summing all forces and dividing by the mass of the particle:

$$\frac{d u_{id}}{d t} = \frac{3}{4} C_D \frac{\rho_g}{\rho_d} \frac{1}{D_d} |u_{ig} - u_{id}| (u_{ig} - u_{id}) + \left(1 + \frac{\rho_g}{\rho_d} \right) g_i , \quad (5)$$

where u_{ig} is the velocity of the gas, ρ_d is the density of the droplet, and g_i is gravity.

Time-integration of the above equation gives the particle velocity and integration of velocity gives the position vector of the particle, according to

$$\frac{d x_{id}}{d t} = u_{id} . \quad (6)$$

In this work, multi- component methods are applied to simulate evaporation of the fuel. This extended method is the Abramzon-Sirignano method. In this method the mass change rate of the drop (while the temperature is higher than the boiling point) is obtained from the following equation:

$$\frac{d m_d}{d t} = \frac{Q_C + Q_R}{V} , \quad (7)$$

where V is the evaporation heat of the particle and Q_C and Q_R are the convection and

radiation heat transfer respectively. When the temperature of particles are lower than the boiling point, the mass rate is obtained from

$$\frac{d m_d}{d t} = \pi \rho_d \beta_g D_d Sh^* \ln \left(\frac{1 - Y_{V,\infty}}{1 - Y_V} \right) . \quad (8)$$

In the above relation Y_V is the mass fraction of vapour, D_d is droplet diameter, and β_g is the diffusion coefficient. Sh^* is the Sherwood number (or mass transfer Nusselt number) and is obtained from the following relation:

$$Sh^* = 2 + \frac{Sh_0 - 2}{F_M}; Sh_0 = 2 + 0.552 Re^{\frac{1}{2}} Sc^{\frac{1}{3}} , \quad (9)$$

where Re is the Reynolds number and Sc is the Schmidt number.

In Multi-Component form, the mass transfer of each particle into the drop is done separately. Hence the general mass rate for each drop is [6]:

$$\dot{m} = \sum_{i=1}^n \dot{m}_i \quad (10)$$

In the above relation n is the number of particles in the drop.

4. Combustion models

The existing combustion models in the software provide the facility to investigate and simulate the combustion process in a cylinder at different conditions of premixed, partial premixed and non-premixed combustions as shown in Figure 4. In this work, the ECFM-3Z model of ICE is used for the simulation of combustion.

This combustion model can describe the diffusion and the premixed non-homogeneous turbulent combustion based on the flame surface density transfer equation. Fuels with different chemical species can be defined using this model. The reaction rate for each part of the fuel is calculated separately and the combustion products are determined based on the chemical and temperature state of each volume, for each volume in turn.

Figure 4 The zones in calculation cells in ECFM-3Z [7]

In order to define the diffusion and premixed combustion processes, each calculation volume is divided by three regions: 1) a region with pure fuel, 2) a region with pure air and residual gas (if available) and 3) a region with a mixture of air and fuel and residual gases. In the ICE module ECFM-3Z, the transfer equation is solved for the average amounts of chemical species for each calculation cell [7].

5 Comparison with experimental results

The specification of the Deutz diesel engine is shown in Table 1. Experimental results for this engine are given by Zhang et.al. [5] for two conditions: with only diesel fuel and also with dual fuel. The initial conditions for the results from the experimental works are given in Table 2.

Model	F6L912Q
Bore ×Stroke	100×120mm
Number of Cylinders	6
Displacement	5.65 litres
Compression Ratio	17
Inlet valve opening	32 BTDC
Inlet valve closing	60 ATDC
Exhaust valve opening	70 BBDC
Exhaust valve closing	32 ATDC
Injector nozzles	4
Injector nozzle diameter	0.285mm
Maximum power	88kW @ 2800rpm

Table 1 Specification of the Deutz engine

Fuel	Speed (RPM)	Air Intake Temp. (K)	Diesel Fuel (g/cycle)	Natural Gas (g/cycle)	Start of Injection (degrees BTDC)
Diesel only	1604	365	0.048	0	7
Dual-fuel	1602	365	0.006	0.042	10

Table 2 Conditions for the experimental results

Experimental results have been extracted for the average pressure in cylinder, apparent heat release rate, and also for the emission of NO_x . It should be noted that the experimental heat release rate is an estimated or *apparent* heat release rate – calculated from the heat release required to give the measured pressure conditions [8]. The simulation was run with matching conditions to the dual-fuel and diesel only settings. Figure 5 shows the comparison for pressure and apparent heat release rate with diesel fuel only, and Figure 6 shows the same comparison for the dual-fuel condition. The agreement for the diesel engine is seen to be very good in terms of both peak values and the point at which they occur. For the dual-fuel engine the peak values are seen to be in close agreement, but the simulated pressure peak is

approximately 2 degrees behind the experimental result, with a greater delay for the apparent heat release rate. Experimental results for NO_x output are also available in ref. [5] as being 4.08 g/kwh in diesel mode and 3.24 g/kwh in dual-fuel mode. For the same conditions the current simulation gave 4.43 g/kwh and 3.47 g/kwh, respectively, which represents an error of less than 9% in both cases. Overall the comparisons, for the simulation of a very complex situation, may be considered good.

Figure 5 Comparison of the pressure and heat release rate curves of the baseline Deutz diesel engine by simulation and experimental means.

6. Effects of varying liquid fuel injection timing

The homogeneity of the fuel-air mixture can be controlled by varying the fuel injection timing, and as a result the power, efficiency and emissions of the engine can be controlled. With early injection of fuel, there is more time to form a homogenous mixture of fuel and air. However the injected fuel will not evaporate easily due to the lower temperature of the chamber at the beginning of the compression stroke, which causes a fuel layer to be formed on the cylinder wall and as a result the fuel consumption and emissions will be increased. The fuel

injection angle should be made more 'narrow' to prevent collision of fuel with the cylinder wall as the fuel injection timing is advanced [9]. Figure 7 shows recommended values of injection angle for different fuel injection.

Figure 6 Comparison of the pressure and heat release rate curves of the dual-fuel engine by simulation and experimental means.

Figure 7 : The variation of injection angle versus fuel injection timing

To obtain the optimum condition for fuel injection timing, the injection timing was varied from 30 up to 110° BTDC and results are compared with a conventional diesel engine. Figure 8 illustrates the variation of IMEP for different fuel injection timing, with an inlet temperature of 380 K and an engine speed of 1600 RPM. Results are shown for premixed ratios, r_p of 0 and 0.55 with the total fuel energy being kept constant for comparison; $r_p = 0.55$ was chosen after tests at a range of premixed ratios, as shown later in this work.

Figure 8 The variation of IMEP in inlet temperature of 380 K and 1600 RPM for different fuel injection timing

Figure 8 shows the variation of IMEP with injection timing for $r_p = 0$ and $r_p = 0.55$; the results for 'conventional' diesel engine injection are also shown (injection shortly before TDC). Early fuel injection encourages a homogenous mixture in the combustion chamber before the combustion, but as shown in Figure 8, very early fuel injection timing causes a decrease of IMEP and thus power. This is partly caused by an earlier start of combustion causing an increase in negative work [10]. Another issue is the lower temperature of the air while the liquid fuel injects, leading to poor evaporation and the formation of a liquid fuel layer on cylinder walls. Later fuel injection suffers from inhomogeneous mixing.

Figure 9 shows the variation of cylinder pressure at $r_p = 0$ with an inlet temperature of 380K and an engine speed of 1600 RPM, for different liquid fuel injection timings. Earlier fuel injection is seen to give earlier (and usually higher) peak pressures. However, fuel injection at 110 degrees BTDC gives a significantly lower peak caused by the low temperature formation of a liquid fuel layer on the cylinder wall.

Figure 9 The variation of pressure at $r_p = 0$, at an inlet temperature of 380K and engine speed of 1600 RPM for different fuel injection timing.

Figure 10 shows the exhaust and emissions versus the liquid fuel injection timing. Combustion with 'conventional' diesel injection (shortly before TDC) is also shown. It is seen that the emission of CO increases sharply as fuel injection is performed earlier. The reason for this increase is that with earlier fuel injection timing during the compression stroke, suitable conditions to form a homogenous mixture are available, which causes more rapid combustion and a reduction of time for oxidation of the intermediate products to CO_2 [11]. In Figure 10 the NO_x emissions are seen to decrease markedly with earlier liquid fuel injection. The cause of this was identified to be a reduction in average temperature in the cylinder with earlier injection; the main cause of NO_x is thermal NO_x , which markedly reduces with average temperature. Strongly related to this is the general trend for an increase in HC emission with earlier fuel

injection, again caused by lower average cylinder temperatures and the resulting increase of unburned hydrocarbon.

Figure 10 The variation of emissions with inlet temperature of 380 K and 1600 RPM engine speed for different fuel injection timings

Considering all results together, the optimum time for fuel injection is approximately 70 degrees before TDC (crank angle of 290 degrees). In this condition CO emission is high but MEP is maximum, and the NO_x and HC emissions, which are hard to decrease, are relatively low. In particular, with a premixed ratio r_p of 0.55, NO_x and HC emissions are significantly lower than for a conventional diesel engine, and CO emission is approximately equal.

7. Effects of varying premixed ratio

The direct effects of varying the premixed ratio, r_p are now shown. For these simulations a liquid fuel injection angle of 70 degrees before TDC is used, as indicated by the previous section. Figure 11 shows the effects of premixed ratio, and inlet air temperature on cylinder pressure during the cycle.

In Figure 11 the points of peak pressure move closer to being just after TDC as the premixed ratio is increased. For both 320 K and 360 K the curves close together at higher values of r_p , but this is much more pronounced at the higher temperature where a high rate of liquid fuel evaporation is encouraged. Evaporation of liquid fuel, and subsequent mixing, becomes a limiting factor at the lower temperature where the point of peak pressure advances with increasing r_p due to the faster combustion of the gaseous fuel. The lower temperature curves show a misfire at $r_p = 0$ where insufficient evaporation occurred for a satisfactory combustion. It can be seen, by comparing any pair of curves at a certain value of r_p , that the point of peak pressure varies considerably with the inlet temperature; thus inlet air temperature is indicated as a useful means of controlling combustion in dual-fuel HCCI engines.

In terms of emissions, a strong point of HCCI engines is the significant decrease of NO_x emissions due to a lower temperature in the combustion chamber, compared with conventional engines. However with dual-fuel a mixture of natural gas in the diesel fuel causes a faster combustion which can give an increase in the average temperature in the cylinder. The formation of most NO_x occurs at temperatures above 1800 K and as a result the amount of this emission will increase in dual-fuel condition [11].

Figure 11 The effects on cylinder pressure of varying premixed ratio for two inlet air temperatures.

Figure 12 shows the amount of NO_x in ppm (mass) predicted for different inlet air temperatures and premixed ratio. In this figure it can be seen that the NO_x emissions tend to

increase with r_p up to a certain point, and then decrease. The value of r_p which gives the peak value varies with air inlet temperature. At the three highest temperatures of 340K, 360K and 380K the peak is at an r_p value of 0.44 or 0.33, whereas at 320K the peak is significantly higher at 0.65 (although the absolute amounts involved are much lower at 320K). The reason that peak NO_x emissions occurs at higher r_p values at low inlet temperatures is suggested by the steady rise of cylinder pressure with r_p that is shown in Figure 11 (and the associated rise in peak cylinder temperature). The reduction in NO_x output above a certain value of r_p is an important result that assists in designing low NO_x emission dual-fuel HCCI engines. The reason for the decrease appears to be that as thermal NO_x is created by the reaction of nitrogen and oxygen, an increase in r_p decreases the amount of these gases in the cylinder due to replacement by gaseous fuel, and causes the reduction of NO_x emissions. At an inlet temperature of 320K, the increase of NO_x output is not too damaging: the highest is 16 ppm at $r_p = 0.65$ which equates to 0.1 g/KWh, which is well within the Euro VI standard (approved for 2013) of 0.4 g/KWh.

Figure 12 Variation of NO_x emissions versus different premixed ratios and inlet air temperatures.

Figures 13 and 14 show a significant decrease in both HC and CO emissions when the proportion of natural gas is increased in the mixture. The increase of gaseous fuel causes more rapid burning and complete oxidation of the fuel, especially at high air inlet temperature. The

rapid combustion leads to the reduction on CO, and the increase in average temperatures in the cylinder allows enough time for completion of combustion.

Considering all results together, a premixed ratio in the range 0.55 to 0.76 appears to give all benefits of fast reliable combustion, with low CO and HC emissions, and has the benefit of the reduced NO_x output above a value of approximately $r_p = 0.55$.

Figure 13 Variation of HC emission at different inlet temperatures and premixed ratios

Figure 14 Variation of CO emission versus different premixed ratios and inlet air temperatures.

Figure 15 Variation of IMEP for different air inlet temperatures and different premixed ratios

Figure 15 shows the indicated mean effective pressure (IMEP) versus different temperatures and premixed ratios. With a low inlet air temperature of 320K, IMEP is seen to vary considerably as r_p increases. As the air inlet temperature increases this variation is much less and the shape of curve becomes a relatively flat line. The reason for this trend of changes is that the diesel fuel evaporates less at low temperatures. Hence, with a decrease of the air inlet temperature, the evaporation of liquid fuel decreases and causes slower combustion and a decrease in produced power.

8. Discussion

The findings show that the mixture of natural gas and diesel fuel has a great influence on an engine's power and emissions. The combustion in dual-fuel HCCI engines can be controlled by changing the inlet temperature, the premixed ratio and the liquid fuel injection timing. The results are summarized as follows:

Inlet air temperature has a significant effect on the start of combustion so that inlet

temperature can be used to help control the start of auto ignition, although the effects on emissions must be considered. Maximum mean temperature in the cylinder and NO_x emissions grow due to increasing inlet temperature, but CO and HC emissions decrease.

Early liquid fuel injection can give a homogenous mixture in the chamber before combustion, and up to a certain point it improves power and overall emissions, particularly NO_x emissions. Beyond a certain point, approximately 70 degrees BTDC in this work, the power and efficiency reduce caused by temperatures being too low to evaporate fuel efficiently before combustion, and combustion occurring too early before TDC. If the average temperature in the cylinder is decreased, CO and HC emissions tend to increase with earlier liquid fuel injection, but are generally below those of a conventional diesel engine when using $r_p = 0.55$.

Combustion duration depends highly on the premixed ratio, r_p . More natural gas in the mixture leads to a decrease in the duration of combustion, which tends to give an effective combustion. Gaseous fuels can relatively easily form a homogenous mixture. Hence an increase of r_p gives a more rapid burning process and oxidation of the fuels becomes more complete. As a result, the emissions of CO and HC emissions decrease remarkably with r_p . Increasing the ratio of natural gas to diesel fuel causes an increase of the average temperature in the cylinder which increases NO_x emissions in comparison with the single-fuel, however beyond a premixed ratio of approximately 0.55, NO_x emissions decrease.

9. Conclusions

Major findings in this work are as follow:

- NO_x emissions initially increase as the premixed ratio increases, but with an increase of premixed ratio beyond a certain amount (around 0.44 in this work), NO_x emissions decrease significantly for a wide range of air inlet temperatures.
- An increase in the amount of gaseous fuel in the mixture causes the emissions of CO and HC to decrease remarkably (by typically a factor of 10 as r_p is increased from zero to around 0.65). More gaseous fuel in the mixture leads to a decrease in the duration of combustion and causes more effective combustion. The decrease appears to be caused

by gas mixing more rapidly with air than does liquid fuel.

- An early liquid fuel injection helps achieve a relatively homogenous mixture in the chamber before combustion, and thus enables efficient HCCI combustion; too early reduces efficiency and increases emissions due to the formation of a liquid layer on the cylinder walls. 70 degrees before TDC was found to be appropriate for liquid fuel injection over a wide range of conditions.

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