Diesel Ignition Model Considering Charge Heterogeneity and Global Reaction Rates

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ABSTRACT

A model has been developed to compute the ignition delay (ID) in direct injection diesel engines under actual running conditions. The model takes into consideration the heterogeneity of the charge, and the global rates of the autoignition reactions. The region where ignition starts in the fuel spray is divided into elements which successively mix, form an ignitable mixture, and start the formation of chain carriers. Autoignition is considered to occur when the cumulative concentration of the chain carriers reach a critical value. Data on autoignition of fuels in constant volume vessels is utilized to compute a Global Autoignition Function $\beta(T,P)$, which varies with temperature and pressure. The model indicates that autoignition occurs when the normalized cumulative concentration of the chain carriers, $\psi(t)$ reach unity. The computed values of the ID were found to be in good agreement with experimental data obtained in an actual engine running under different ambient temperatures.

INTRODUCTION

The ignition delay (ID) affects many aspects of the diesel engine operation including its fuel economy, the emission of species such as hydrocarbons, nitrogen oxides, and smoke particulates. Furthermore, the rate of pressure rise and the peak cylinder gas pressure are directly related to the mass of the premixed charge which depends to a great extent on the length of the ID period. Peak engine power may be limited by the peak cylinder gas pressure, engine noise and vibration which are caused by the high rates of pressure rise.

Correlations for ID are needed for diesel engine cycle simulations and for the design of combustion chambers for high power-density engines that can run on regular as well as alternate fuels. Many ID correlations are based on investigations conducted in constant volume vessels under steady state conditions of air pressure, temperature and charge motion [1-4]. These investigations are desirable because they deal with a limited number of controlled variables, consume less time and are less expensive to run than experiments conducted in actual engines [5-8]. However, there has always been discrepancies between ID data obtained in engines and in constant volume vessels.

The goal of this paper is to develop a method to compute ID in engines from global reaction rates calculated from data obtained in constant vessels, taking into consideration the heterogeneity of the charge. The computed results are compared with experimental data obtained in a research engine running at different ambient temperatures ranging between 25°C and -5°C.

COMBUSTIBLE MIXTURE FORMATION DURING ID

Investigations in direct injection diesel engines indicate that the fuel spray is composed of a core, rich in relatively large and dense droplets, and an envelop containing smaller size droplets interacting with the entrained air. The shear layer at the spray periphery, caused by the high velocity gradient between the liquid and compressed air, has been found to produce flow circulation resulting in vortices [9]. The vortices were found, by using a double-pulse laser sheet, to be the result of instabilities which grow in the downstream direction of the spray. At the same time, air is induced into the spray periphery by streams moving toward the spray axis. The interaction between the air motion and spray droplets produce the stripe-shaped structure in the periphery. Similar observations have been made by using a double-pulse holographic interferometry technique [10]. The microscopic images at the spray periphery indicated the presence of stripes of high fuel-vapor concentrations, from which the vapor diffuses to areas of less fuel concentration.

Autoignition under such conditions is demonstrated by high speed photography of diesel combustion under engine conditions. The first visible flame was observed in a hump at the periphery of the spray [11]. If the hump is assumed to be a large scale vortex, autoignition starts at the same location as the large scale vortex. The model developed in this paper incorporates these experimental observations.
DIESEL IGNITION MODEL

The model considers the following:

1. A small volume of the charge in the spray envelop, in the form of a vortex, ignites first and starts the combustion process.

2. The mixture in the vortex is heterogeneous, but ensemble has an auto-ignitable equivalence ratio.

3. The mass of the auto-ignitable charge is composed of small elements, which successfully intermix and form an auto-ignitable mixture and start the effective chemical reaction to form chain carriers.

4. Autoignition starts in the vortex when the cumulative concentration of the chain carriers reach a critical concentration.

RATE OF FORMATION OF CHAIN CARRIERS

The detailed elementary reactions for the autoignition of single heavy hydrocarbon fuels, suitable for diesel engines, are not known. Meanwhile, diesel fuels are distillates containing several heavy hydrocarbons of different compositions and molecular structures. This makes it almost impossible to develop detailed kinetic models for actual fuels in diesel engines. However, investigations on the autoignition of fuels (knock) in gasoline engines indicated that the increase in the concentration of a chain carrier such as OH to a critical value can be utilized to predict the onset of knock. In the present model, autoignition is considered to occur when a critical concentration of the chain carriers is reached. The critical concentration is the same if the fuel is injected in a constant volume vessel or an engine. Accordingly, the global rate of the reactions for the formation of the critical chain carriers concentration can be determined from data obtained in constant volume vessels. The two major differences between engines and constant volume vessels are:

a. The gas motion in engines is in the form of swirl and tumble, which might not be duplicated in constant volume vessels. We feel that the gas motion affects only the physical part of the ID, which is known to be negligible in automotive diesel engines.

b. The gas temperature and pressure remain almost constant in constant volume vessels during the ID period. This is not the case in engines, where both temperature and pressure vary during ID period, depending on the injection timing and the length of ID.

In the current model, the variation in both the temperature and pressure will be accounted for by developing a Global Autoignition Reaction Function \( \beta(T, P) \).

GLOBAL AUTOIGNITION REACTION FUNCTION \( \beta(T, P) \)

The autoignition reactions in the engine are considered to take place in \( n \) elements over \( n \) successive short time intervals. During each interval the temperature and pressure are assumed to remain constant. Figure 1 illustrates the time intervals \( t_i \) and elements \( m_i \).

![Figure 1. Pressure-Time diagram for successive elements during ID period.](image)

The change in the concentration of the chain carriers \( [C] \) for each element during any time interval can be given by

\[
\frac{d[C]}{dt} = \beta(T, P)
\]

(1)

Where \( \beta(T, P) \) is computed from data obtained in constant volume vessels for the fuel. In this paper, the fuel is \( n \)-dodecane. The data is at the same temperature and pressure as in the engine, of each time interval. Since in constant volume vessels autoignition occurs when the concentration of the chain carriers reach the critical value \( [C_c] \) after an ID period \( \tau \), \( \beta(T, P) \) may be given by

\[
\beta(T, P) = \frac{[C_c]}{\tau}
\]

(2)

\( \tau \) is calculated from the correlation developed by Igura et al [12] for \( n \)-dodecane. The correlation is,

\[
\tau = A P B C \exp(D/T)
\]

(3)

Where \( P \) is pressure in atm., \( T \) is the absolute temperature (K) and \( \Phi \) is the oxygen concentration in air. The constants for \( n \)-dodecane are \( A = 0.845, B = -1.31, C = 2.02 \) and \( D = 4350 \). Figure 2 illustrates the method of computing \( \beta(T, P) \) from ID data in vessels. In the engine, \( \beta(T, P) \) varies with time according to the variations in temperature and pressure, as illustrated in figure 3.

A general form for the concentration of the chain carriers
in the m th element at the start of autoignition can be given by

$$\frac{[C_{lg}]}{m} = \sum_{i=m}^{n} \beta_i t_i$$  \hspace{1cm} (4)

The concentration of the chain carriers from all the n elements can be given by

$$[C_{lg}]_1 + [C_{lg}]_2 + [C_{lg}]_3 + \cdots + [C_{lg}]_n$$

$$= \beta_1 t_1 + 2\beta_2 t_2 + 3\beta_3 t_3 + \cdots + n\beta_n t_n$$  \hspace{1cm} (5)

If all time intervals are equal to t, equation (5) takes the form

$$\sum_{i=1}^{n} [C_{lg}]_i = \beta_1 t + 2\beta_2 t + 3\beta_3 t + \cdots + n\beta_n t$$  \hspace{1cm} (6)

Since the critical concentration of the chain carriers should be the same in both the engine and vessel, autoignition should take place in the engine according to equation (7)

$$\sum_{i=1}^{n} \left( \frac{[C_{lg}]}{[C_c]} \right) = \frac{t}{\tau_1} + \frac{t}{\tau_2} + \frac{t}{\tau_3} + \cdots + \frac{t}{\tau_n} = 1$$  \hspace{1cm} (7)

Equation (7) represents the normalized cumulative concentration of the chain carriers. Equation (7) becomes,

$$\Psi_n(t) = \frac{t}{\tau_1} + \frac{t}{\tau_2} + \cdots + \frac{(n-1)t}{\tau_{n-1}} + \frac{t}{\tau_n} = 1$$  \hspace{1cm} (8)

**CUMULATIVE CHAIN CARRIERS FUNCTION $\Psi_n(t)$**

The general form of equation (8) is,

$$\Psi_n(t) = \sum_{i=1}^{n} \left( \frac{i \times t}{\tau_i} \right) = 1$$  \hspace{1cm} (9)

$\Psi_n(t)$ is the normalized cumulative chain carriers function. Where $\tau_i$ is calculated from equation (3).

**EXPERIMENTAL WORK**

Experiments were conducted on a single-cylinder, air-cooled, four-stroke-cycle direct-injection diesel engine. The specifications of this engines are, bore = 95 mm, stroke = 95 mm and C.R. = 17:1. The engine was installed in a cold room and the tests covered a range of temperatures between -5°C and 25°C. The instrumentation included a flush mounted piezo-quartz water-cooled pressure transducer a needle lift detector, air flow-meter, and thermocouples to measure intake air and exhaust gas temperatures. A 24 channel high response data acquisition system was used to retrieve the data. The ID was determined from the needle lift and the inflection point of $dP/d\theta$. Figure 4 shows a sample of the data for n-dodecane. Figure 5 shows the variation of the ID with the change in ambient temperature. Figure 6 is a map showing iso-ID lines calculated from equation (3) for the constant volume vessel. The path of the charge temperature and pressure during the ID period in the engine is superimposed on the figure for four different ambient temperatures. The charge temperatures during the ID period are calculated from the equation of state.
COMPARISON BETWEEN PREDICTED AND MEASURED RESULTS

The ID predicted from the present model is determined by plotting $\psi(t)$ versus the time elapsed from the start of injection, for four different ambient temperatures, as shown in figure 7. The time at which $\psi(t)$ reached unity is shown in the figure and is considered to be the end of ID. A comparison between the computed ID and the measured values is given in figure 8. The ID computed from equation (3) are also shown on the same figure. The temperatures and pressures used in equation (3) are the mean values during ID period. It is clear that correlations obtained in constant volume vessels over predict the ID under engine conditions.

Figure 4. Determination of ID time from experimental engine data.

Figure 5. Experimental data for ignition delay at different ambient temperatures.

Figure 6. Experimental pressure-temperature path during ID period in an engine at different inlet temperatures, superimposed on iso-ID lines of a constant volume vessel.

Figure 7. Normalized cumulative chain carriers function $\psi(t)$ calculated for different ambient temperatures.

Figure 8. Comparison between the model and measured ID results.
CONCLUSIONS

1. A model has been developed to determine ID in diesel engines, taking into consideration the heterogeneity of the charge and the variation in both the charge temperature and pressure during the ID period.

2. The model is based on the fact that autoignition takes place when the chain carriers reach a critical concentration. Due to the heterogeneity of the charge, many elements contribute to the formation of the critical concentration of the chain carriers. The accumulation of chain carriers enhances the increase of the chain carriers concentrations. The contribution of each element is calculated from a Global Autoignition Reaction Function $\beta(T,P)$.

3. The Global Autoignition Reaction Function $\beta(T,P)$ is computed from ID data obtained for the same fuel in constant volume vessels.

4. The start of autoignition is determined when the normalized cumulative concentration of the chain carriers function $\psi(t)$ reaches unity.

$$\psi(t) = \sum_{i=1}^{n} \left( \frac{i \times t}{\tau_i} \right) = 1$$

5. The computed ID periods showed a fairly good agreement with those measured in direct injection diesel engines at different ambient temperatures ranging from -5°C to 25°C.

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REFERENCE


