Research Article

Ion Current Simulation Model Design for a Spark-Ignited Engine

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The use of ion current signals generated during the combustion process of mixed gas as a function of initial mixture composition, temperature and pressure to detect cylinder combustion states is the most recent approach in the design, development, and optimisation of automotive engine combustion control. This paper aims to design predictive identification and computationally fast and accurate ion current models for obtaining combustion information in the engine cylinder in real time. To build a more comprehensive ion current calculation model, the effect of the flame ionisation process, the geometry of the spark plugs, and the combustion pressure and temperature are considered in the new building ion current model. The simulation ion current waveform, which has a double-peak structure, is in good agreement with the experiment values; thus, the ion current model has the potential to be used for real-time control and optimisation of engine cylinder combustion.

1. Introduction

In recent years, the energy crisis and its long-term problem, as well as the challenge of CO₂ emissions, have increased concern for the development and design of new energy engines with clean energy, high efficiency, and low emissions. Developing new electronic engine control systems can improve the efficiency of combustion engines, achieve online monitoring of the combustion process, and obtain timely information about the mixture combustion state, allowing for low-carbon and high-efficiency combustion, which has drawn the attention of many researchers and has become an active area of engine combustion diagnostics and optimisation.

The ion current signals produced in the flame combustion process carry rich information about the engine combustion process, and the spark plug as an ion current detecting probe is robust and inexpensive to manufacture; it can be installed in spark-ignition engines to obtain combustion information, such as misfire detection, peak pressure position and in-cylinder pressure, and the total combustion heat release. Given the close relationship between the combustion process and the ions produced, the study discovered that the ion current waveform can reflect the characteristics of flame development, which has been divided into the ignition phase, the front phase, and the postflame phase. By analysing the ion current waveform’s characteristic parameters, a researcher can gain a better understanding of the ion formation process in engines and develop a better control programme for engine performance and emissions [1–5].

In this paper, the new ion current computing model based on the combustion process is developed which considered the spark plug geometry, flame ionisation process, equivalence ratios, and engine model; the pressure model of the entire burning process is used in the simulation calculation, and the ignition energy is considered.

The objectives of this paper are to develop fast and robust tools for analysing the mixture gas combustion process in engine cylinders, which can aid in the design, analysis, and optimisation control of newer engine designs. The ion current comparison between model calculated values and experimental measured results validates the new building model. The ion current model may help in the rapid analysis of engine combustion performance and provide a new technology path for engine combustion performance optimisation control [4–7].
2. Flame Ion Current Theory and Formulation

2.1. The Ion Current in the Front Flame Phase. After the ignition system ignites the air-fuel mixture contained in the cylinder, the flame develops and ions are believed to be formed due to various chemical ionisation processes in the reaction zone of the propagating flame; the ion current is produced in one particular direction after the application of the electric field to ions. The reaction in equation (1) is considered a typical reaction in an internal combustion engine cylinder [8]:

\[ C_2H_6 + 5O_2 \rightarrow 3CO_2 + 4H_2O. \]  

There are various flame ionisation mechanisms proposed for ion generation during the flame burning process [9], as shown in a comprehensive discussion of the feasibility of these mechanisms [7], with the chemi-ionisation reaction in the front flame phase being the dominant initiation ionisation reaction. Equation (2) shows the main elementary reactions that create ions [8] are

\[
CH + O \xrightarrow{k_1} = 5 \times 10^{-14} \text{cm}^3/\text{s} \ CHO^+ + e^-, CH(2\Sigma^+) + O \rightarrow CHO^+ + e^-, \\
CHO^+ + H_2O \xrightarrow{k_2} = 7 \times 10^{-9} \text{cm}^3/\text{s} \ H_3O^+ + CO, H_2O^+ + e \xrightarrow{k_3} = 2.3 \times 10^{-9} \text{cm}^3/\text{s} \ H_2O + H.
\]

2 Scientific Programming

In above set of reactions, it is experimentally found that H^+O is truly the dominant positive ion in hydrocarbon flames [10, 11] and the H^3O^+ ions are produced by proton transfer from CHO^+ to H_2O, which mostly contribute to the formation of the ion current [7–12].

The ionisation reaction rates (k_1, k_2, and k_3) are shown in Equation (2), which are given in reference [12]. As the ion species produced in the above reactions reached a steady-state concentration, the ion concentrations can be expressed as follows:

\[
[CHO^+] = \frac{k_1[CH][O]}{k_2[H_2O]}, \\
[H_3O^+] = \frac{k_2[CHO^+][H_2O]}{k_2[e^-]} \times \frac{k_3[CH][O]}{k_3[e^-]_{\max}}.
\]  

Based on the Saha equation, the local thermal equilibrium concentration is the function of temperature, as shown in the following equation:

\[
\frac{n_i n_e}{n_{i-1}} = 2 \left( \frac{2\pi m_i kT}{\hbar^2} \right)^{3/2} B_i \frac{B_i}{B_0} \exp \left[ \frac{-E_i}{kT} \right].
\]  

In Equation (4), T is the absolute temperature, \( \hbar \) is Planck’s constant, \( k \) is Boltzmann’s constant, the \( n_i \) and \( n_{i-1} \) are the number density of the ionised state \( i \) and \( i-1 \), respectively, \( n_e \) is the electron number density, \( m_e \) is the electron mass, \( E_i \) is the ionisation energy of the state \( I \), and \( B_0 \) is the internal partition function.

The electron drift velocity is a function of the mobility of electrons \( \mu \) and the electrical field \( X \), which is expressed as [10]

\[
\nu_d = \mu X.
\]

In classical physics, the particles mean free path length \( \lambda \), the possibility of interaction between particles (which can be defined by their cross sections \( S \)), and the ion number density that passes through a volume can be expressed as follows:

\[
\lambda = \frac{1}{n_{tot} S},
\]

\[
n_{tot} = \sum x_i n_i,
\]

where \( x_i \) is the species fraction and \( n_i \) is the number density of species, \( i \).

The combustion temperature is the major contributor to the electron drift velocity in the combustion reaction, and the effect of the electrical field is relatively small [10]; the electron drift velocity expression is shown in the following equation:

\[
\mu = \frac{e\lambda}{m_e v_T},
\]

\[
v_T = \sqrt{\frac{8kT}{\pi m_e}}.
\]

In the above equation, \( v_T \) is the mean random velocity of the electrons and \( m_e \) is the electron mass.

Since the combustion gas volume in the engine cylinder is cylindrical, the formula of the ion current can be expressed as follows:

\[
I_1 = U \frac{\pi r^2 \rho^2}{Sd} \left( \frac{\pi^3 x_i}{8m_e kT} \right)^{1/2} A,
\]

\[
A = \sqrt{\left( \frac{2(2\pi m_i kT)^{3/2}/\hbar^2} \right) B_i/B_0 \exp \left[ -E_i/kT \right]} \left( \frac{n_{tot}}{n_{tot}} \right).
\]

In Equation (11), \( T \) is the combustion temperature, \( n_{tot} \) is the number density of total species, and \( x_i \) is the species fraction, where \( n_{tot} = P/kT \) [6, 10].

2.2. The Ion Current in the Postflame Phase. The thermal NO formation mechanism is the so-called extended Zeldovich mechanism [10, 11], and the thermal NO formation
mechanisms consist of three elementary reactions in Equation (12) which were used for the estimation of the formation rate of NO from molecular nitrogen in near stoichiometric air-fuel mixtures.

\[
\begin{align*}
O_2 + N_2 & \rightarrow NO + N, \\
N + O_2 & \rightarrow NO + O, \\
N + HO & \rightarrow NO + H.
\end{align*}
\]

(12)

The NO formation rate is much slower than the combustion rate, and most of the NO formation takes place in the postflame regions. The concentration [NO] is defined as follows:

\[
\frac{d[NO]}{dt} = 6 \times 10^{16}T^{-1/2} \exp\left(-\frac{69090}{T}\right) (O_2)_{eq}^{1/2} (N_2)_{eq}.
\]

(13)

The eq subscript stands for equilibrated conditions and the unit is moles/cm^3 sec. In the equation, the temperature and the amount of O_2 are strongly dependent on the rate of NO formation in the postflame phase. This finding suggests that thermal ionisation is the source of the ion current in the postflame region, and NO+ dominating the ion current in the postflame region is consistent with much of the theory and experimental work in the thermal ionisation process [10, 11]. The ionisation ratio of NO is obtained from Saha’s equation shown in Equation (4), and the electron drift velocity shown in Equation (5) can be calculated from basic gas kinetic theory. The result of the derivation, where the ion current is a function of temperature, has the following form:

\[
I_2 = A\phi \frac{n_{tot}}{N_{tot}} T^{1/4} \exp\left(-\frac{E_i}{2kT}\right).
\]

(14)

In the above formula, \(E_i\) is the ionisation energy of species \(s\), \(n_{tot}\) is the total number density, and \(\phi\) is the species fraction of species \(s\). The symbol \(A\) is a constant which is shown in Equation (11).

So, because the total ion current includes the ion current produced by the chemical ionisation reaction as well as the ion current produced by the thermal ionisation reaction, the total ion current equation is as follows:

\[
I_{tot} = I_1 + I_2.
\]

(15)

2.3. Ion Current Measuring Circuit. The ion current in the combustion chamber is measured using a modified version of the spark plug inserted into the engine cylinder. The ion current measurement circuit is shown in Figure 1 [13, 14].

During the experiment, after the spark ignition is successful, the ion current generated during the combustion process is measured and the data are collected, and the combustion pressure data generated during the combustion process are collected using the ion current measurement circuit. The collection of the ion current data and combustion pressure data adopts the ADVANTECH 1710L data acquisition card, which holds an acquisition accuracy of ±2.48% [13, 14].

2.4. Engine Calculation Model. The engine geometry is taken into account in the calculation, and the relationship between the rotation of crank and engine cylinder volume is as follows:

\[
V(\theta) = V_c + \frac{\pi R^2}{4} \left(1 + a - a \cos(\theta) - \sqrt{1 - \left(a \sin(\theta)^2\right)}\right).
\]

(16)

An analytic model for the combustion pressure is given in closed form, which is based on connection with components that are simple and convenient to measure and tune, and the model’s advantage is that no ordinary differential equations must be numerically solved. The expression of the analytic model for the combustion pressure is

\[
p(\theta) = \begin{cases} 
T_{c}(\theta) & \text{for } \theta_{ivc} < \theta < \theta_{soc} \\
(1 - x_b) p_c(\theta) + x_b p_e(\theta) & \text{for } \theta_{soc} < \theta < \theta_{evo}
\end{cases}
\]

(17)

The expression of the model is further decomposed as follows [4–6]:

\[
p_c(\theta) = \frac{V_{ivc}}{V(\theta)} k_s,
\]

\[
T_c(\theta) = T_{ivc} \frac{V_{ivc}}{V(\theta)} k_s^{-1},
\]

\[
p_e(\theta) = p_3 \frac{V(\theta)}{V(\theta)} k_s
\]

\[
x_b(\theta) = 1 - e^{-b(\theta - \theta_{soc}/\Delta \theta)^{m+1}}
\]

\[
p_3 = \frac{T_3}{T_2}
\]

\[
T_3 = T_2 + \Delta T_{comb}
\]

\[
\Delta T_{comb} = \frac{\eta Q_{LHV}}{c_v} \left(\frac{1}{1 + A/E X_b}\right)
\]

\[
p_2 = \frac{p_c(\theta)}{p_c(\theta)}
\]

\[
T_2 = T_c(\theta)
\]

\[
\theta_e = \Delta \theta_d + \frac{1}{2} \Delta \theta_b
\]

2.4.1. Intake Valve Close to Start of the Compression Process. Using a polytropic compression model, pressure and temperature are calculated during the compression stroke from IVC to SOC and displayed as a function of the crank angle and the coefficient \(k_s \approx 1.3\).

\[
p_c(\theta) = \frac{V_{ivc}}{V(\theta)} k_s
\]

\[
T_c(\theta) = T_{ivc} \frac{V_{ivc}}{V(\theta)} k_s^{-1}
\]

(19)
After to finish the compression stroke, the polytropic expansion stroke to begin, Equation (19) is performed to simulate the expansion stroke [4, 6, 8, 11, 12, 15].

2.4.2. Starting Combustion Process. After successful ignition, the combustion temperature rises in the cylinder due to the burning mixture, and the cylinder temperature is closely related to the LHV (low heating value) of the fuel, specific the burning mixture, and the cylinder temperature is closely related to the LHV (low heating value) of the fuel, specific heat, A/F, and effective combustion efficiency.

\[ T_3 = T_2 + \Delta T_{\text{comb}} \]
\[ \Delta T_{\text{comb}} = \frac{\eta_c Q_{LHV}}{c_v} \frac{1}{1 + A/F} x_b. \]  

(20)

The burned fraction of the combustible mixture in the cylinder is described by the Wiebe function combustion model, which is as follows:

\[ x_b(\theta) = 1 - e^{-a (\theta - \theta_{\text{soc}}) / \Delta \theta} \]  

(21)

Where \( \theta \) is the angle degree of crankshaft rotation, \( \theta_{\text{soc}} \) is the degree at the starting of combustion, \( \Delta \theta \) is the duration degree of combustion, \( a \) and \( m \) are adjustable parameters of the Wiebe function which fitted to the values \( b = 5 \) and \( m = 2 \) to resemble actual mass fraction burned curves [4, 6, 11, 14–17].

2.4.3. Starting Expansion Process. After successful ignition, the combustion temperature rises in the cylinder due to the burning mixture.

During the expansion stroke (from SOC to EVO) process, the pressure and temperature are calculated using the polytropic expansion model, and the expression coefficient \( k_v = 1.35 \). The parameters of \( V_3 \), \( p_3 \), and \( T_3 \) in the following equation are related to the three-state in the ideal Otto cycle and described as follows [4, 6, 11, 16]:

\[ T_v(\theta) = T_3 \left( \frac{V_3}{V(\theta)} \right)^{k_v - 1} \]

\[ p_v(\theta) = p_3 \left( \frac{V(\theta)}{V_3} \right)^{k_v}, \]
\[ p_3 = \frac{T_3}{T_2}, \]
\[ p_2 = p_c(\theta), \]
\[ T_2 = T_v(\theta). \]  

(22)

Using the inverting the pressure ratio analysis (Matkunas, 1986, 1984, and 1983), the \( p_3 \) can be measured experimentally [17–20].

3. Simulation and Experimental Analysis

Based on the new building model, the ion current is calculated using the previously listed calculation formula, and the calculation parameters are shown in Table 1, 2, and 3.

The contribution of the major ionisation reaction and the species of charged ions to ion current generation are calculated. The parameters of several ion sources that dominate the ion current are as follows: the number of moles of \( \text{H}_2 \text{O} \) is 0.125 and its ionisation energy \( E_i = 12.6 \text{ eV} \), the ionisation energy of \( \text{NO} \) is \( E_i = 9.27 \text{ eV} \), the ionisation energy of \( \text{CHO} \) is \( E_i = 9.88 \text{ eV} \), the number of moles of \( \text{N}_2 \) is 0.75 and its ionisation energy \( E_i = 15.5 \text{ eV} \), and the ionisation energy of NO is \( E_i = 9.27 \text{ eV} \).

Figure 2 shows the calculated ion current results, the experiment measured ion current and the pressure change over the crank angle. Following a successful ignition, ion current signals are produced in the front flame during the chemi-ionisation process. The first peak of the ion current signal increases rapidly as the combustion reaction progresses; then, some of the generated ions are recombined quickly, and to produce more stabler new molecules, other ions have longer residential to the post-flame phase.

As shown in Figure 2, the calculated results and the experiment measured ion current signals have a double-peak structure, with the ion current decreasing after the first peak produced by the chemi-ionisation reaction until the second peak produced by the thermal ionisation.

Based on the chemi-ionisation theory and the derivation from formula (2) to (15), the first peak of the ion current
produced is mainly due to the concentration of the H\(^3\)O\(^+\) ion increase with combustion temperature. CHO\(^+\) ions are produced firstly in the chemi-ionisation reaction; then, some protons transfer from CHO\(^+\) to H\(_2\)O, and H\(^3\)O\(^+\) is produced. The concentration of H\(^3\)O\(^+\) ions will reach the maximum value at the first peak of ion current waveform timing along with the combustion going on, so the first peak of the ion current is mostly constituted of H\(^3\)O\(^+\). Then, some CHO\(^+\) are recombined quickly, and the ion current decreases. The pressure and temperature of the mixture combustion in the cylinder increase as the combustion reaction progresses; under high pressure and high-temperature conditions, NO\(^-\), ions are the dominant ions generated by thermal ionisation reactions. When the ambient temperature is approximately 2000 K, the ionisation energy of the NO molecule is low: 9.26405 eV [21, 22]. At high temperatures, it easily ionises to NO\(^+\), resulting in an increase in the rate of NO\(^+\) production. As a result, the amplitude of the thermal ion current reaches its maximum, and the second peak of the ion current appears in the postflame combustion phase.

Figure 2 shows the change in cylinder pressure and ion current as the crank angle changes. The ion current waveform exhibits a double-peak structure as the combustion pressure changes; the ion current reaches the first peak before the TDC (top dead center), but the pressure reaches the peak after the TDC, and the second peak position of the ion current is consistent with that of the pressure peak position. Based on the ideal \(PV = nRT\), the cylinder temperature and pressure are closely related, and the ion current signals produced ionisation reaction that depends on combustion temperature and pressure, revealing that the ion current characteristic curve in the combustion reaction essentially reflects the intrinsic characteristics of the cylinder pressure and temperature during the combustion process.

Compared to the calculated and experimentally measured curve of the ion current in Figure 2, the calculated ion current follows the experimental ion current very closely; however, the peak and its width values of the calculated ion current are smaller than the experimental values, and the first peak timing are later than the experimental peak timing. The main cause of the above error is that the calculated model of the ion current primarily considers the predominant ionisation reaction mechanism and the predominant charged ions, resulting in calculated values of the ion current that are smaller and later than experimentally measured values.

### 4. Conclusion

This study developed the most recent model for predictive identification and computationally fast and accurate ion current for obtaining the combustion information in the engine cylinder in real time. The effect of the chemical ionisation and the thermal ionisation mechanisms, engine cylinder and spark plug geometry, and temperature and pressure of the entire combustion process are all considered in the model calculation formula to build a more comprehensive ion current calculation model. Because the
dominant function of the ionisation reaction mechanism and charged ion sources are emphatically considered in the calculations, the predicted peak value and the width of the ion current are smaller than the experimentally measured values. This model will be provided with a fast analytical method for considering the ion current as a function of the combustion flame ionisation reaction process, combustion pressure, and temperature; based on this model, a fast, robust tool for computing the ion current of the combustion process in the cylinder can greatly aid in the design, development, analysis, and control of new engine operating regimes.

**Data Availability**

The dataset can be accessed from the corresponding author upon request.

**Conflicts of Interest**

The authors declare that they have no conflicts of interest.

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