A skeletal gasoline flame ionization mechanism for combustion timing prediction on HCCI engines

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Abstract

Ion current sensing technology has the potential to be a low cost and real time combustion phasing solution for HCCI or HCCI-like engine control. Based on a primary reference fuel oxidation mechanism and a C1-C4 hydrocarbon flame ionization mechanism, a skeletal mechanism for gasoline flame ionization process prediction on HCCI engines was developed in this paper. Since the ion concentrations significantly affect the aroused ion current signals, the mechanism is targeted on accurately predicting both the ion production concentrations and other key combustion characteristics. Through the comparison with the results from the detailed gasoline flame ionization mechanism and experimental results, the predicted maximum hydronium (H_3O^+) ion concentration and the concentration variation tendency are validated. Additionally, the auto-ignition delay time (t_{ign}) accurately predicted under HCCI engine conditions. Through coupling with a 3D-CFD engine model, the skeletal mechanism was applied to predict the important information of in-cylinder ion species, which are validated by the experimental ion current amplitudes and phases. The results show that the ion current phase (Ion50) matches well with the positions where the predicted ion concentration reaches its maximum, and the ion current amplitudes are well predicted under the conditions of different equivalence ratios (Φ) and fuel injection ratios (Inj_{ratio}).

Keywords: skeletal mechanism, ion current, flame ionization, HCCI, combustion phase

1. Introduction

As an engine that leads to ultra-low NO_x emissions and high thermal efficiency, the homogeneous charge compression ignition (HCCI) is recognized as a candidate for the next generation combustion engine [1]. However, investigations in global scope suggest that the combustion phase control of HCCI engine is a bottleneck for application of HCCI in production-line engines [2, 3]. Some experimental studies indicated that ion sensing technology is one of the best candidates for the real time combustion phasing control on HCCI engines due to its ruggedness and low cost [4-5]. It is widely reported that a strong linear relationship exists between the CA₅₀ (the crank angle position for 50% burned mass fraction), and the Ion₅₀ (the crank angle position for 50% of the maximal amplitude of ion current signal) [6-8]. However, there are two major issues, which affect the accuracy of ion current signals based combustion phasing. Firstly, the ion current sensor normally provides flame ionization information that is localized near the ion probe. Consequently, determination of absolute ion concentrations is elusive [9]. Secondly, the ion signal is increasingly weaker with leaner air-fuel mixture or lower intake temperature conditions, due to the low ion concentration [7]. In addition, Dong et al [10] found that the low ion production rate leads to a phase delay in the detected ion current signal.

Recently, several technical solutions including ionic sensor location optimization [11], alkali metal based ionization enhancement additives [12] and high frequency AC power source [13], are proposed for improvement of the ion current sensing system. Optimization of any of these proposals will be strongly aided by a chemical kinetic simulation of the in-cylinder flame ionization process. Hence, a flame ionization mechanism designed for large-scale computational fluid dynamics (CFD) analysis is necessary to be developed.

Flame chemi-ionization mechanisms have been studied extensively since early 1950s [14,15]. Based on these previous fundamental studies, several flame ionization mechanisms were recently developed for the CFD analyses.

For example, a simplified methane reaction mechanism with five key flame ionization reactions was constructed by Rao et al. [16]. Dong et al.[17] modeled an HCCI engine with mechanism for gasoline, plus flame ionization mechanism, containing 248 species and 1,233 reactions. Yamashita et al.[18] analyzed the effect of DC electric field on a methane diffusion flame with the assist of an ion mechanism with 11 reactions. The above studies illuminate the importance of the CFD based flame ionization process analysis for better understanding of practical applications.

The goal of this study is to develop a gasoline flame ionization mechanism for investigating the ion current signal based combustion phasing in HCCI engines. First, a skeletal primary reference fuel (PRF) oxidation mechanism (M_{prf}) is developed for the prediction of auto-ignition delay time, heat release process, and key species profiles. Then a flame ionization mechanism (M_{ion}) is generated with the target of reproducing the formation processes of key ion species. Consequently, a final PRF flame ionization mechanism (M_{comb}) is achieved by combining the M_{prf} and M_{ion} . By comparing to the detailed PRF mechanism and the experimental results, the predicted ignition delay time, the concentrations of the key ion species such as H_3O^+ , and its time variation are validated under different test conditions. Finally, the combined mechanism M_{comb} is applied for combustion phase prediction and the predicting results correlate well with the experiments on a gasoline fueled GDI-HCCI test engine.

2. Mechanism development

2.1 Base gasoline fuel oxidation mechanism

The PRF, blends of iso-octane and n-heptane, is widely used for the research on gasoline-fueled HCCI engines [19]. As noted in the introduction, the goal in this study is to develop a chemical kinetic model for predicting ion production in gasoline HCCI combustion. Concerning the production of ions in hydrocarbon fuel flames, it is widely accepted that the chemi-ion reaction $\text{CH} + \text{O} \leftrightarrow \text{HCO}^+ + \text{e}$ is the primary source of the ions and electros in

flames [14]. To satisfactorily reproduce CH concentrations, auto-ignition delay time (t_{ign}) and heat release rates, different domains of molecules are treated with various degrees of details in this study. In the final combined mechanism M_{comb} , the C0–C2 section that significantly related to CH production is described in detailed form, while the C3–Cn oxidation chemistry is highly simplified. The C3–Cn section, with reactions listed as R1–R34 in the supplementary material, is based on the skeletal PRF oxidation mechanism developed by Andrae et al [20, 21]. In this mechanism, different isomers for large hydrocarbons are described as identical in this section. The reference paper [20] indicates that the mechanism was validated over a wide range of testing conditions of both shock tube and HCCI engine experiments. However, the C0 - C2 section in the Andrae's mechanism is quite brief and then the CH specie profile can be hardly predicted by it. Consequently, it can't be used for the H3O⁺ ion prediction either.

The C0–C2 section involving 32 species and 131 reactions is developed based on the study from Chang et al. [22]. In order to investigate the HCCI heat release process, Chang et al. described the oxidation chemistry of small species with sufficient details. By conducting the sensitivity analysis, the C0–C2 section in this work is compared with the detailed primary reference fuel mechanism (M_{LLNL}) developed by Lawrence Livermore National Laboratory (LLNL) [23]. The M_{LLNL} was successfully used for ion current signal phasing and amplitude analysis by Dibble et al. [12]. Thus, the ion concentrations can be well predicted in the proposed flame ionization mechanism since the CH producing rate is accurately reproduced.

Figure 1. CH specie sensitivity analysis.

Figure 1 shows the CH species sensitivity coefficients of 10 key reactions in the current C0-C2 section and the M_{LLNL} . It is clear that key reactions affecting the CH production are similar in these two mechanisms. Therefore, the constructed C0-C2 section is combined with the aforementioned C3-Cn sub-mechanism, and then the skeletal PRF mechanism M_{prf} is achieved. The mechanism is also analyzed within the Octane number range of 85-90, and the most sensitive reactions are almost unchanged. Taking PRF 90 as the target fuel, the CH species concentrations from the M_{prf} and the M_{LLNL} are compared through a shock tube simulation. The results indicated that the normalized CH species concentration predicted by M_{prf} correlates well with that predicted by M_{LLNL} , as shown in Figure 2. The normalization method is identical with Reference paper 28. The CH specie concentrations are normalized by the peak CH specie concentration of PRF100 at equivalence ratio of 1.

Figure 2. The peak CH species concentrations calculated by the M_{prf} and the M_{LLNL} .

Setting the ignition delay and CH concentration as the targets in the reduction implementation, a further simplification of the M_{prf} is achieved through the method of Directed Relation Graph with Error Propagation (DRGEP) with sensitivity analyses [24]. The reduction starts with the DRGEP method to remove unimportant species and associated reactions from the base mechanism, followed by conducting sensitivity analyses to identify the most important species and reactions. Finally, the mechanism M_{prf} with 55 species and 165 steps is constructed.

2.2 Ionization mechanism

The hydrocarbon flame ionization mechanism was investigated in several studies in the last twenty years [7]. Those

studies indicated that the generation of positive ions from neutral particles is based on the reaction path $\text{CH} + \text{O} \rightarrow \text{CHO}^+ + \text{e}$ [16], followed with the reaction of $\text{CHO}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{CO}$. In subsequent studies, the reactions of formation of positive ions of $\text{C}_2\text{H}_3\text{O}^+$, CH_3^+ and C_3H_3^+ are recorded in hydrocarbon flames along with H_3O^+ and CHO^+ [25]. By comparing the concentration and the mobility of these ions, the hydronium ion (H_3O^+) was identified as the major source for arousing the ion current signal when an external electric field is exerted on a hydrocarbon flame [26]. Consequently, the accurate description of the H_3O^+ is of importance for the current study.

The flame ionization mechanism proposed by Prager et al. (M_{Prager}) [27] was taken as the base mechanism to describe the ion production process in this study. The M_{Prager} which is composed of 11 ionic species and 67 reactions has already been validated by the experimental data achieved in a diffusion flame, and it was successfully used to analyze ionization processes in a zero-dimensional HCCI model as well [28]. For reducing this base ionization mechanism, its interaction with the developed PRF oxidation mechanism M_{prf} is analyzed.

Figure 3. Schematic CH specie reaction path analysis.

A reaction path analysis is conducted to be shown in Figure 3. The main reaction path of CH radical at engine-like temperature and equivalence ratio conditions in a closed homogeneous reactor is presented. Compared to the CH oxidation reaction path, it can be seen that only a small percentage of the CH radical is converted into CHO^+ along

the ionization path. Such a result indicates that the ionization process has a minor effect on the combustion process, and normally it is neglected when the thermodynamic features of the flame are the major concern. Thus, a further reduction of M_{Prager} , can be conducted alone without affecting the combustion phenomena. Based on the H_3O^+ species sensitivity analysis, a skeletal mechanism M_{ion} with 7 species and 24 reactions is achieved.

Besides the positive ions of CHO^+ , H_3O^+ , $\text{C}_2\text{H}_3\text{O}^+$, CH_5O^+ , the negative ions, O_2^- and O^- , are considered with electrons in the M_{ion} since these negative ions can potentially affect the ion current signal measurements through the am-bipolar diffusion effect [27], and the consideration of this feature would be helpful for the future studies.

Finally, the fuel oxidation mechanism M_{prf} and the ionization mechanism M_{ion} are combined directly and no modifications of the reaction constants are made. The final flame ionization mechanism M_{comb} with 62 species and 189 reactions is obtained.

3. Mechanism validation

3.1. Auto-ignition delay time (t_{ign})

Figure 4. Validation of the skeletal PRF mechanism for ignition delay time predictions (PRF 100).

The validations under engine conditions presented in this section are carried out by a closed homogenous reactor model in commercial software Chemkin-Pro. The further validation based on the HCCI engine testing results will be discussed later. Figure 4a shows the validation of t_{ign} for iso-octane, the simulation under different equivalence ratios at the pressure of 40 bar is compared to the shock tube experimental data from Fieweger et al. [19]. Figure 4b is the comparison between shock tube experiments and simulation of iso-octane with stoichiometric fuel-air mixture at initial pressures of 13, 16, 34, 40, 45 bar. The above tested conditions can cover most boundary conditions in practical HCCI engines. It can be seen that the calculated t_{ign} with the newly developed mechanism in this study is in a good agreement with the experiments. The comparison is also made under PRF equals 85 and 90, which reveals similar conclusion.

3.2 Hydronium ion concentration

As mentioned in section 2.2, the hydronium (H_3O^+) ion was the major source for generating an ion current signal, and the signal amplitude and phase can be strongly affected by the H_3O^+ ion production. Due to the lack of H_3O^+ ion concentration data directly from a hydrocarbon flame with the engine-like boundary conditions, the calculated H_3O^+ ion concentration in the current work is compared to that from the detailed primary reference fuel mechanism M_{LLNL} , which was successfully applied to predict the ion current signal variations by Dibble et al [28]. Figure 5 shows the comparison of H_3O^+ ion concentrations predicted by these two mechanisms in the closed homogenous reactor model. The model is the same as section 3.1 with the fuel of PRF 90. From the results, the predicted concentration values by the M_{comb} correlates well with those of M_{LLNL} .

Figure 5. The peak H_3O^+ ion concentrations calculated by the M_{comb} and the M_{LLNL} .

4. Ion current signal and combustion phase prediction in HCCI engines

4.1. Engine testing and ion sensing system

A GDI-HCCI engine was applied for the experimental study in this section. The schematic diagram of the test engine and the ion sensing system is shown in Figure 6a. The engine specifications can be seen in Table 1.

Table 1. Engine specifications

Type	2-Cylinder in-line, DI
Displaced volume	800 cc
Bore $\times$ Stroke	95 mm $\times$ 114 mm
Connecting Rod	178.98 mm
Compression ratio	13.5
Engine speed	1200 rpm
Fuel type	Gasoline (95 Octane)
Injector	High pressure swirl injector
Injection pressure	10 MPa
Nozzle hole number	6
Hole diameter	0.179 mm
Head bottom	Flat

Figure 6. Test engine structure and the fuel injection strategy.

Through the adjusting of variable valve timing (VVT system), different residual gas amounts can be achieved during the negative valve overlap (NVO) interval. Then the fresh intake air-fuel mixture is heated to achieve HCCI combustion. Furthermore, by applying a two-stage fuel injection strategy as shown in Figure 6b, the fuel injected during the NVO interval will be reformed by the active thermo-atmosphere derived from residual exhaust gas recompression. Such a fuel-reforming process enables a lower air-fuel mixture temperature to trigger an HCCI combustion [29]. Consequently, a boarder HCCI operating range can be achieved as well. Here, the parameter Inj_{ratio} is defined as the ratio between the fuel amount Inj_1 injected during the NVO interval to the fuel amount Inj_2 injected during the compression stroke. In the ion sensing system, a spark plug is used as the ion current sensor, and a 200V DC power source is exerted to supply the electric field. The details of this system can be seen in [11, 18, 30].

4.2 Numerical combustion model

The CFD model used in this study is developed from KIVA-3V code [31]. The chemistry solver is coupled with the KIVA-3V code for analyzing detailed combustion and flame ionization processes. A cross section of computational mesh based on the geometry of the test engine is demonstrated in Figure 7.

Figure 7. The cross section of the engine computaional model.

There are 20,136 total cells at compression top dead center (TDC). The location of the ion probe in the model is the physical location of the spark plug ion sensor used in experiments. The reported ion concentrations represented the average within a 2 mm radius of the spark plug ion sensor probe position. Under condition of 1200 rev/min engine speed and 80 °C coolant temperature conditions, the numerical in-cylinder pressure and heat release rate under both high and low equivalence ratios are compared to the experimental values for the modeling validation. To stabilize the HCCI combustion, the fuel amount Inj_I , which injected during NVO interval, is set at 3.6mg. As shown in Figure 8, the numerical results agree well with the measured data. The predicted pressure rise rates and heat release rates are a bit higher than the experimental results. However, the start of combustion (SOC) and the location of CA50, which are crucial for this study, are well predicted. Further validation of the numerical pressure and heat release values can be seen in the following sections by comparing with the experiments.

Figure 8. Numerical and experimental in-cylinder pressure and heat release rate.

Figure 9. The distribution of the H_3O^+ ion and the heat release

Through the 3D-CFD model, the ion producing process is analyzed. By keeping the equivalence ratio $\Phi=0.7$, and the coolant temperature at 80°C , the predicted H_3O^+ ion concentration and released heat distribution at combustion phase CA10 and CA50 are shown in Figure 9a and 9b, respectively. The cut-plane is the middle cross section of the combustion chamber. It can be seen that the H_3O^+ generation is closely related to the zone with heat release at both CA10 and CA50 positions. It indicates that the ion current signal can be a good combustion phase indicator on HCCI engines.

4.3 The prediction of ion current signal amplitudes

Based on the CFD model, the calculated H_3O^+ ion concentrations were compared with the experimental results. Figure 10a shows the variation of the peak cylinder pressure, the ion current signal amplitudes and the predicted H_3O^+ ion concentrations for 3 typical equivalence ratios (Φ). The in-cylinder peak pressure values and signal amplitudes are collected from 60 consecutive cycles under each Φ condition. It shows that the predicted ion concentration captures the trend of the experimental data well. In addition, the effect of two-stage injection on the

signal amplitudes is investigated. Figure 10b shows the ion concentrations and the ion current signal amplitudes at 3 injection ratios (Inj_{ratio}). When the Inj_{ratio} increases from 0.2 to 0.6, the fuel reforming process is enhanced and the heat was released faster [31]. Consequently, the peak cylinder pressures, the signal amplitudes and the predicted ion concentration become higher.

Figure 10. Comparison of the ion current signal amplitudes and the predicted peak ion concentrations

Figure 11 demonstrates the predicted ion concentration variations of both $Inj_{ratio} = 0.2$ and $Inj_{ratio} = 0.6$ cases. In the former case, more fuel is injected during the compression stroke. Comparing to the $Inj_{ratio} = 0.6$ case, it can be seen that the ion concentration is more heterogeneous at the position of CA10. However, the ion concentration at CA50 position is lower in the $Inj_{ratio} = 0.2$ case. Such predictions are in good agreement with the signal amplitude variations on the test engines. Therefore, the developed mechanism can be potentially used for analyzing the observability of ion current signal and optimizing the ion sensing system.

Figure 11. In-cylinder H_3O^+ ion distribution under different Inj_{ratio} conditions

4.4 The prediction of ion current signal phases

The comparison between the combustion phase CA50, the ion current phase Ion50, and the position with maximum H_3O^+ ion concentration P_{ion_max} are conducted in this section. When the equivalence ratio increases from 0.6 to 0.8, the variations of CA50, Ion50 and P_{ion_max} are shown in Figure 12a. The CA50 and the Ion50 are collected from 60 consecutive cycles under each Φ condition. From the results, the position of P_{ion_max} is correlative well with the Ion50. Moreover, a linear relationship does exist between the Ion50 and CA50. The relation between CA50, Ion50 and P_{ion_max} under different injection ratio (Inj_{ratio}) conditions are shown in Figure 12b. When the Inj_{ratio} increases from 0.2 to 0.6, the CA50 significantly advanced due to the faster heat release rate. Under such a condition, the linear relation between Ion50 and CA50 still exists. Besides, the variation of Ion50 is well captured by the P_{ion_max} . The above two terms of comparisons indicate that the developed mechanism M_{comb} can be used for the prediction of the ion current signal phases on HCCI engines.

Figure 12. Phase comparison between the CA50, Ion50 and the P_{ion_max}

5. Conclusions

In this study a skeletal gasoline flame ionization mechanism with 62 species and 189 reactions is developed for predicting the ion current signal on HCCI engines. There are some new and insightful results obtained:

- 1) A PRF oxidation mechanism M_{prf} that can accurately reproduce the ignition delay time under different engine operating conditions is developed. Especially, the CH radical, which is crucial for arousing the positive ions (and electrons) in the gasoline ionization process, can be predicted as well.
- 2) Through reaction path and sensitivity analysis, a hydrocarbon flame ionization mechanism M_{ion} is developed and combined with the fuel oxidation mechanism M_{prf} . Therefore, the concentration of the key positive ion H_3O^+ can be predicted for PRF gasoline surrogates in HCCI conditions. The calculated results are in good agreement with the detailed primary reference fuel mechanism M_{LLNL} , which previously successfully used for ion current signal prediction in gasoline HCCI engines.

- 3) Through coupling with the engine CFD model, the developed mechanism in this paper M_{comb} is used for predicting the ion current signal on a GDI-HCCI engine. The results show that the variations of the signal amplitude can be captured by the calculated peak H_3O^+ ion concentration. The phases of the signal are in good correlation with $P_{\text{ion_max}}$, the position where the peak H_3O^+ ion concentration appears. The developed mechanism M_{comb} demonstrates the ability of predicting the ion current signal behaviors in HCCI engines.

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