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Numerical simulation study on correlation between ion current signal and NO_X emissions in controlled auto-ignition engine

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HIGHLIGHTS

- The relationship between chemical ionization and NO_X generation in CAI combustion was studied.
- The temporal and spatial distributions of electron, ion and NO compositions were simulated with CFD model.
- The feasibility of ion current based NO_X detection is proved by better ion current signal in the experiments.
- The ion current based NO_X detection provides a novel fast feedback control for SCR system.

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ABSTRACT

NO_X is one of the main compositions in the modern engine emissions and the reduction requirements of NO_X have turned to be more stringent. To control NO_X emissions better, the technologies of NO_X sensors are forced to achieve much faster response and higher accuracy. In this paper, the correlation between ion current signals and NO_X emissions is studied by both experiments and simulations in a direct-injection controlled auto-ignition (CAI) engine. The investigation provides the possibility of a novel method of cycle-by-cycle NO_X emissions detection. The simulation results present this positive correlation based on the chemical kinetics theory, and also directly reflect the formation order of the chemical products and the influence of temperature on the rates of main ionization and NO_X generated reactions. Furthermore, the distributions of both ions and NO products are shown with the CFD results, illustrating their in-cylinder space correlation. Combined with the simulation results, the experimental results not only validate the positive correlation between two different fuel types, but also provide the evidences of linear fitting function. Based on the fitting results, the cycle-based NO_X emissions could be estimated.

1. Introduction

As the problems of global environment pollutions have been paid more attention in recent years, the emissions laws are getting more and more stringent. For NO_X is one of the main compositions in the exhausts, the investigation of NO_X reduction technologies has already become popular in the internal combustion engine research field. Controlled auto-ignition (CAI) is a feasible combustion mode for NO_X reduction, due to the lean premixed air–fuel mixture causing low combustion temperature [1,2]. Although the working range of CAI combustion is much narrower than normal spark ignition (SI) combustion [3], which was a big challenge for CAI application in series product engine, the SI-HCCI modes switching technology have provided the possibility for industrialization of CAI combustion [4,5]. In spite of this, the control of the CAI combustion is still difficult as auto-ignition of fuel is mainly influenced by chemical kinetics. In this case, CAI combustion may still cause high NO_X emissions because its cycle-by-cycle variation is sensitively influenced by the combustion parameters and boundary conditions [6,7]. Fig. 1 presents the cycle-by-cycle NO_X emissions under CAI condition measured by the authors in the previous investigation [8]. Even though the average level of NO_X emissions is much lower than that of spark ignition condition, some fluctuated cycles still produced high NO_X. Furthermore, the NO_X produced in such CAI lean combustion cannot be reduced by three-way catalyst (TWC) effectively. In this case, selective catalytic reduction (SCR) would be a solution for such lean combustion condition. For accurate control of urea injection, SCR system normally requires two NO_X sensors – one is placed before the urea injector to measure NO_X and the other one is placed after the SCR

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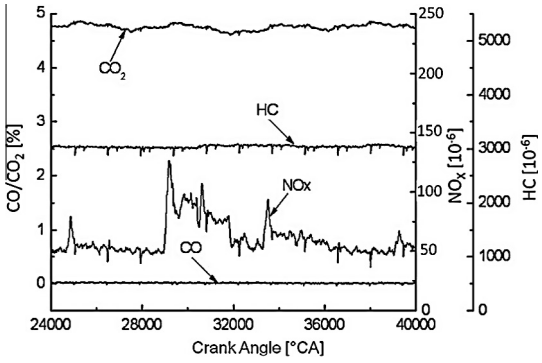

Fig. 1. CAI cycle-by-cycle emissions measurement [8].

for injection correction [9]. Therefore, the NO_X sensor for SCR should not only meet the requirements of high accuracy and fast response, but also have low costs. Most of the current on-vehicle NO_X sensors are working for steady-state conditions with high costs, and the fast response NO_X detection system which has complicated structure with high costs is normally employed only in the lab [10,11]. Although many researches are focused on the NO emissions prediction for model-based control, the prediction model requires necessary assumptions as well and the accuracy of the model mainly depends on both the algorithms and support parameters [12,13]. Compared with the prediction model, the NO_X sensor reflects NO_X emissions more directly and simply. But there is still lack of NO_X sensor adapting to cycle-by-cycle variations for transient state condition.

The feasibilities of using ion current (IC) signal detecting in-cylinder combustion have been already proved. The results of IC signal characteristics researches proved the close relationship between IC signal and combustion [14–16]. Especially the timing parameters of IC signal can reflect combustion phases accurately [17]. After that, other researchers have reached successes in knock/misfiring detection and combustion feedback control based on the IC signal [18–21]. Due to this close relationship between NO_X emissions and combustion intensity, Naeim Henein started to study the correlation between thermo IC signal and NO_X emissions in diesel engine since 2008 [22] and Kenichiro Ogata also began to investigate this correlation in HCCI engine in recent years [23]. These previous researches on the correlation of IC signal and NO_X emissions have provided the possibility of a novel fast on-vehicle NO_X detection method with low costs, but most of the studies are still focused on the thermo IC signal under steady-state condition, there is very few researches on cycle-by-cycle investigations of chemical IC signal especially combined with the chemical mechanism.

In this paper, the correlation between chemical IC signal and NO_X emissions in CAI combustion mode is studied. The results of CFD simulations combined with the reaction mechanism explain the correlation based on chemical kinetics theory and directly reflect the in-cylinder composition distribution during the combustion process.

2. CAI engine test bench and simulation model

The engine is modified with the compression ratio of 11.5 and 800 cc displacement. The detailed specifications of the test engine can be found in reference 20. The IC signals are measured by spark plug based on the DC ion current detection system which does not require any modification to the engine [16].

The chemical kinetics based 0-D simulation model is set according to the test engine parameters and the 3-D model is shown in Fig. 2. The fuel type of simulation is ethanol. Both of the models have been verified with the combustion pressure and the in-cylinder ion current. Fig. 3 shows the verification results. The ion current is calculated from the electron concentrations with Eq. (1) [24].

As the state of 0-D model is ideally homogeneous and only able to reflect the global mean electron concentration, the IC of 0-D results is weaker than that of the experimental and CFD results. The ideal state and the simplified mechanism of theoretical ionization processes cause rapid combustion and reaction rate. Even in CFD simulation, the reactions are still ideally influenced by the temperature. Furthermore, the real ion current shape is also influenced by the shape of electrical field which is different from the probe point in CFD simulation. Therefore, all these reasons lead to shorter IC duration in simulation than in experiments. But the simulation results of the pressure, peak of IC and phases still match well with experimental data, and thus the models are verified.

$$I = en_{ion}\pi r^2 E\frac{e\bar{\lambda}}{m_{ion}v_{ion}} \quad (1)$$

e – unity charge
E – electrical field Strength
n_{ion} – number density of ions/electron
$\bar{\lambda}$ – migration rate
r – electrodes radius
m_{ion} – unit mass of ion/electron
v_{ion} – ion/electron thermo motion velocity

3. Simulation results analysis

The chemical ionization and NO generated reactions are shown in Table 1 [25,26]. According to Arrhenius Equation, when temperature coefficient $b = 0$, temperature is positively related to reaction rate; when temperature coefficient $b < 0$, temperature is negatively related to reaction rate. Fig. 4 shows the influence of temperature coefficient b on Arrhenius Equation [27]. In this case, the rates of reaction 1 and 7 have a positive correlation with combustion temperature. CHO^+, e^- and NO can be all enhanced by increased temperature and then the increased CHO^+ concentration causes more H_3O^+. Even though CHO^+ converts into H_3O^+ very soon in reaction 2, the quantity of e^- is mainly reduced by reaction 3 and 4 which happen much slower. Therefore, H_3O^+ and electron are considered

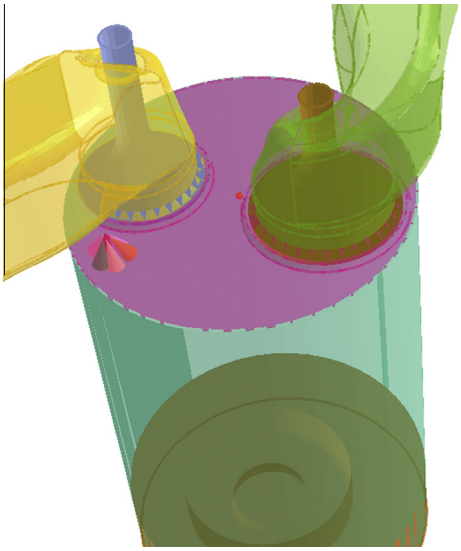

Fig. 2. 3-D model for CFD simulation.