

Study of Low-engine-speed Self-ignition in Gasoline Engine Using Elementary Process Simulation

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ABSTRACT

The mitigation of noise originating in self-ignition in gasoline engines at low speed (“self-ignition noise” below) is an issue in realizing increased commercial appeal. Low-speed self-ignition noise occurs sporadically, producing significant torque fluctuation and engine vibration in each cycle. Synchronizing measurements with the occurrence of the noise and reproducing the phenomenon has therefore represented a challenge, and progress has not been made in its analysis. The research discussed in this paper verified that an elementary process simulation was able to model combustion conditions in which self-ignition noise occurs with sufficient accuracy. Using this simulation, the research studied phenomena occurring at the level of elementary processes when self-ignition occurs, changes in self-ignition characteristics with changes in conditions, and methods of ameliorating self-ignition. The conditions varied in the simulations were air-fuel mixture temperature, compression ratio, excess air ratio, EGR, residual gas and octane number. The results of these studies showed that reducing fuel density by increasing leanness is an effective means of controlling self-ignition when the engine is restarted. In addition, it was shown that it is possible to control self-ignition by reducing the temperature of the air-fuel mixture through reduction of the ratio of residual gas. Further, the simulation can be utilized to predict self-ignition characteristics produced by changes in factors such as the octane number of the fuel and the temperature of the external air in different regions, and to set appropriate specifications, on the desktop.

1. Introduction

Today, issues including the need to combat global warming demand the realization of increased efficiency in internal combustion engines. Methods including increasing the compression ratio, increasing the temperature of the cooling water, and boosted downsizing are available as methods of increasing efficiency in gasoline engines. Because these technologies increase the pressure and temperature of the combustion chamber, they also increase the possibility of abnormal combustion including knocking and pre-ignition due to factors such as high intake air temperature. As Fig. 1 shows, abnormal combustion can be classified into knocking, low-speed self-ignition, low-speed pre-ignition, and runaway pre-ignition. Because low-speed self-ignition results in significant torque fluctuations in each cycle, producing severe engine vibration, conducting stable measurements has represented a challenge to date, and progress has not been made in the analysis of the problem. Previous research^{(1), (2)} has considered changes in conditions and the timing of self-ignition, but has not mentioned the conditions for self-ignition noise.

In addition, very few studies have utilized elementary process simulations in the analysis of low-speed self-ignition. Research on self-ignition at close to idling speed conducted by Nakajima et al.⁽³⁾ elucidated the mechanism of low-speed self-ignition noise. Figure 2 shows the necessary combustion conditions for the occurrence of low-speed self-ignition noise. The engine speed is 750 rpm

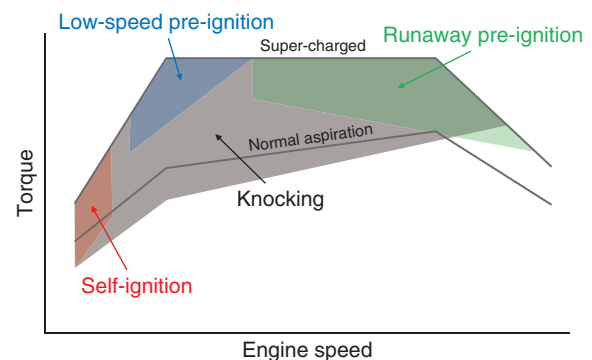


Fig. 1 Classification of abnormal combustion

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and the intake air pressure is atmospheric pressure. The horizontal axes of the graphs show the crank angle, while the vertical axes show mass burnt fraction (MBF), $dP/d\theta$, and in-cylinder pressure. At a crank angle of 0 deg, that is, close to TDC, a low-temperature oxidation reaction commences; at 37 deg ATDC, the remaining approximately 60% of the air-fuel mixture self-ignites, and at close to 40 deg ATDC, the angle at which $dP/d\theta$ is at its maximum, the pistons make contact with their sleeves and self-ignition noise occurs. This paper discusses research based on this mechanism that simulated the occurrence of low-speed self-ignition noise using elementary process simulations to verify the mechanism of occurrence of self-ignition, thus establishing guidelines for the development of countermeasures.

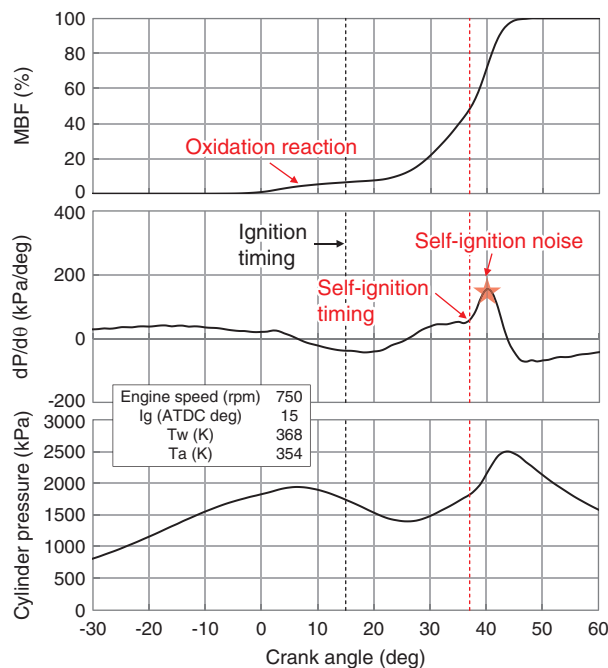


Fig. 2 Combustion generating self-ignition noise

2. Simulation Model of Low-speed Self-ignition

2.1. Application of Elementary Process Simulation

The challenge represented by conducting measurements in the case of low-speed self-ignition makes the use of simulations in conducting various studies a desirable method. Elementary process simulations are a type of simulation making it possible to obtain more detailed data than would be the case in an actual engine test. However, because elementary process simulations are zero-dimension simulations, they are unable to reproduce the propagation of flame by spark ignition. Knocking caused by the self-ignition of the remaining end gas due to the pressure generated by the combustion of the greater part of the air

Table 1 Fuel specifications (RON91)

n-Heptane	0.1823
iso-Octane	0.6642
Toluene	0.1535

Table 2 Engine specifications

Fuel	Gasoline	
Cylinder configuration	In-line 4-cylinder	
Displacement (cm ³)	1799	
Bore (mm)	81.0	
Stroke (mm)	87.3	
Compression ratio	10.5	
Crank offset (mm)	12.0	
Valve diameter (mm)	In.	32
	Ex.	26

fuel mixture as a result of spark ignition is an example of a case in which the application of elementary process simulation represents a challenge. However, because the combustion condition producing self-ignition is self-ignition of the majority of the fuel when the ignition timing is retarded, it is considered that the amount of combusted air-fuel mixture at the time is low, and the effect of factors such as combustion pressure due to spark ignition is limited. It was therefore considered possible to simulate actual tests using elementary process simulation.

2.2. Specifications of Elementary Process Simulation

The research discussed in this paper studied low-speed self-ignition using the type of elementary process simulation applied in simulations such as studies of homogeneous-charge compression ignition (HCCI). The specifications of the simulation were as follows:

- (1) Elementary process simulation
CHEMKIN-PRO (Ver. 2010/06/28)
- (2) Model: Ignition combustion (IC) engine

2.3. Surrogate Fuel

The properties of gasoline can be modeled by varying the ratios of n-heptane, iso-octane, and toluene in a surrogate fuel^{(4), (5)}. The ratio of components was designed based on measurement results to be as close as possible to the fuel used in engine tests. The ratio of components is shown in Table 1.

2.4. Engine Specifications

Table 2 shows the specifications of the engine used in the engine tests and the simulation.

2.5. Comparison of Elementary Process Simulation and Engine Tests

Figure 3 shows the results of engine tests and the elementary process simulation with adjusted parameters. For the tests, the engine speed was 750 rpm, intake pressure was atmospheric pressure, and the intake air

temperature was set at the lowest temperature at which self-ignition noise occurs. In the elementary process simulation also, the intake air temperature was the lowest temperature at which self-ignition occurs. The horizontal axes in Fig. 3 show the crank angle and the vertical axes show MBF, $dP/d\theta$, and in-cylinder pressure. Judging from the mass burnt fraction, a low-temperature oxidation reaction occurred from close to TDC in the engine tests, and the elementary process simulation reproduced this phenomenon. It was considered that in the engine test, after combustion proceeded up to 37 deg ATDC, the remaining approximately 60% of fuel self-ignited, and self-ignition noise occurred at close to 40 deg ATDC, when $dP/d\theta$ was at its maximum. A hot flame also occurred at close to 40 deg ATDC in the elementary process simulation. Therefore, at the lowest intake air temperature at which self-ignition occurs, the low-temperature oxidation reaction commences at almost exactly the same crank angle in the engine tests and in the elementary process simulation. In addition, self-ignition occurs and $dP/d\theta$ reaches its maximum in the engine tests and hot flame is generated in the elementary process simulation at almost exactly the same crank angle. Therefore, if the crank angle at which the hot flame occurs in the elementary process simulation is considered to be the crank angle at which $dP/d\theta$ reaches its maximum in the engine tests, that is, at which self-ignition noise occurs, in the elementary process simulation, the simulation can be considered to reproduce the engine test fairly well, despite its inability to model flame propagation by spark ignition.

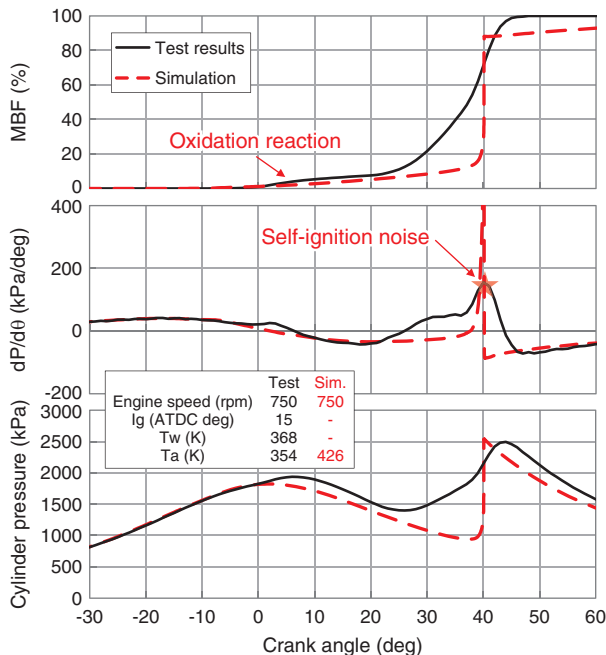


Fig. 3 Results of elementary process simulation

3. Verification of Correlation of Simulation with Engine Test

3.1. Effect of Intake Air Temperature

The correlation between the elementary process simulation with parameters set to make it possible to model combustion in which low-speed self-ignition noise occurs and the engine test was verified by varying parameters. Figure 4 shows the simulation results when the intake air temperature is varied. The horizontal axes show the crank angle with 0 deg as TDC, and the vertical axes show the mole concentration of the three components of the surrogate fuel and oxygen, and the temperature and pressure of the air-fuel mixture. As the compression stroke proceeds and temperature and pressure increase, n-heptane and iso-octane are oxidized, and the amount of oxygen declines. Toluene is not prone to oxidation, and at this stage the toluene is almost completely unoxidized. When the oxidation reaction proceeds further, the volume of fuel and oxygen declines rapidly and temperature and pressure increase rapidly. This crank angle is defined as the crank angle when self-ignition occurs. Because the oxidation reaction takes time when the intake air temperature is low, the engine speed at which self-ignition occurs is lower. Figure 5 compares the engine speeds at which self-ignition occurs in the elementary process simulation and the engine test when the intake air temperature is varied. There is a good

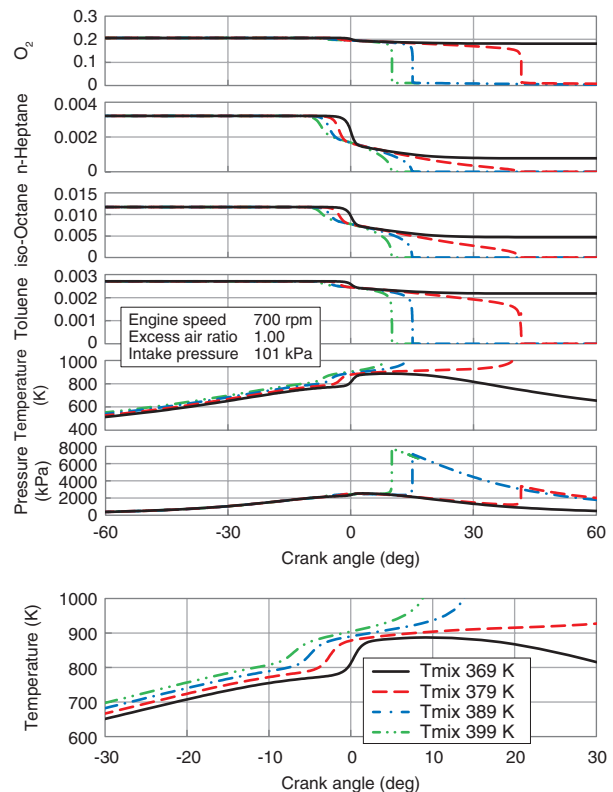


Fig. 4 Results of elementary process simulation

correlation between the engine test and the elementary process simulation.

3.2. Effect of Compression Ratio

Because the compression ratio changes pressure, it is considered to exert a significant effect on self-ignition. Figure 6 shows simulation results when the compression ratio is changed from 9.5 to 12.5. The higher

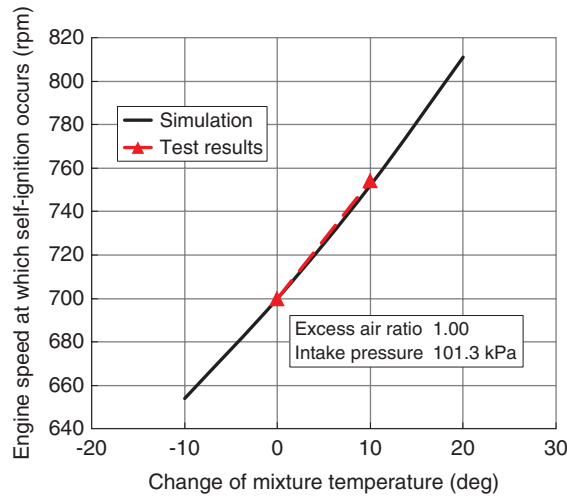


Fig. 5 Relationship between mixture temperature and self-ignition

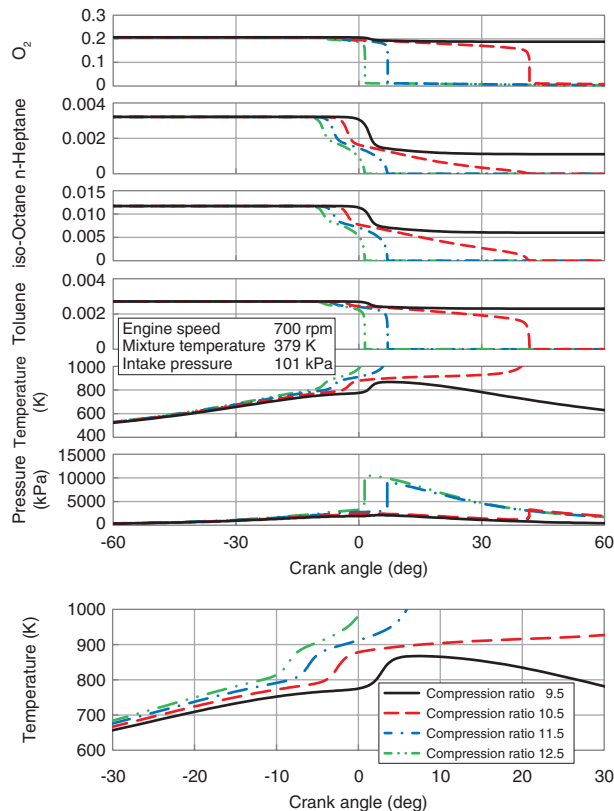


Fig. 6 Elementary process simulation of compression ratio change

the compression ratio, the earlier the commencement of the oxidization reaction and the earlier the occurrence of self-ignition. Figure 7 shows the relationship between the compression ratio and the engine speed at which self-ignition occurs. As when the intake air temperature was varied, there is an almost complete match between engine test results and the results of the elementary process simulation when the compression ratio is varied. This elementary process simulation model, able to reproduce engine test results when temperature and pressure, the important parameters for the elementary process, were varied, was employed to study the effect of operating conditions on self-ignition and countermeasures to apply to self-ignition.

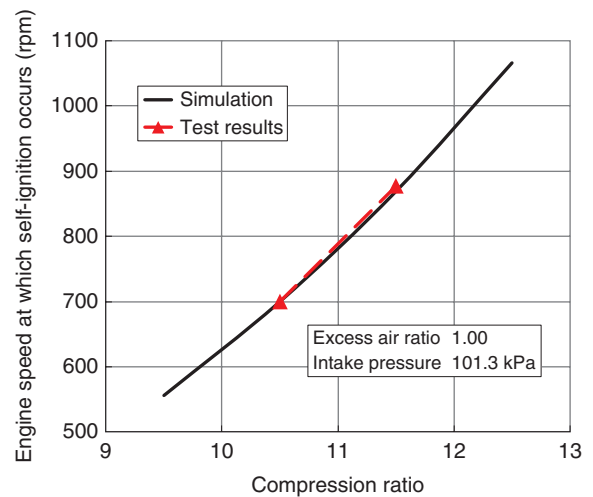


Fig. 7 Relationship between compression ratio and self-ignition

4. Mechanism of Low-speed Self-ignition

4.1. Effect of Excess Air Ratio

The excess air ratio is considered to have a significant effect on self-ignition characteristics. The richness or leanness of the mixture has been shown to have an effect in engine tests conducted under a limited range of conditions, but because it is challenging to conduct the tests, the mechanism of these effects has not been clarified. Figure 8 shows the relationship between the excess air ratio in engine tests and the intake air pressure under which self-ignition occurs and the torque produced under those conditions. While the intake air pressure at which self-ignition occurs is higher for both rich and lean conditions than for the theoretical air-fuel ratio, because rich mixtures produce a greater amount of torque for the same amount of intake air, the rich mixture produces a greater amount of torque. It is believed that the improvement in the self-ignition characteristic on the rich side is due to a significant cooling effect resulting from the latent heat of vaporization,

but the detailed causes of the decline on the lean side are unknown. A detailed study was therefore conducted using the elementary process simulation. Figure 9 shows the simulation results for the theoretical air-fuel ratio, $\lambda = 1.20$ and $\lambda = 0.83$. Factors such as the latent heat of vaporization and residual gas components were not considered. Table 3 shows the temperature of the air-fuel mixture before and after TDC.

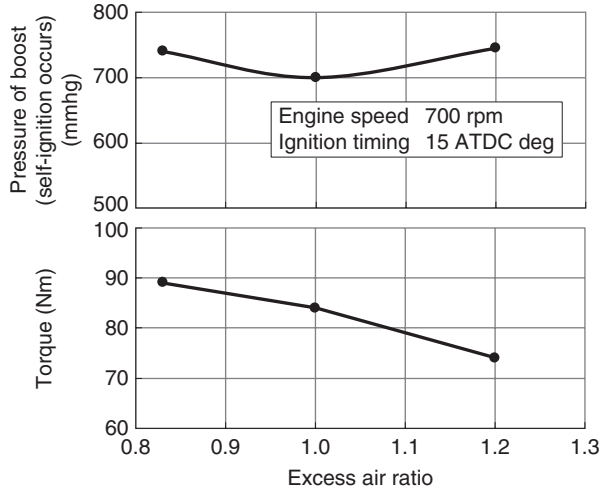


Fig. 8 Relationship between excess air ratio and pressure boost of self-ignition

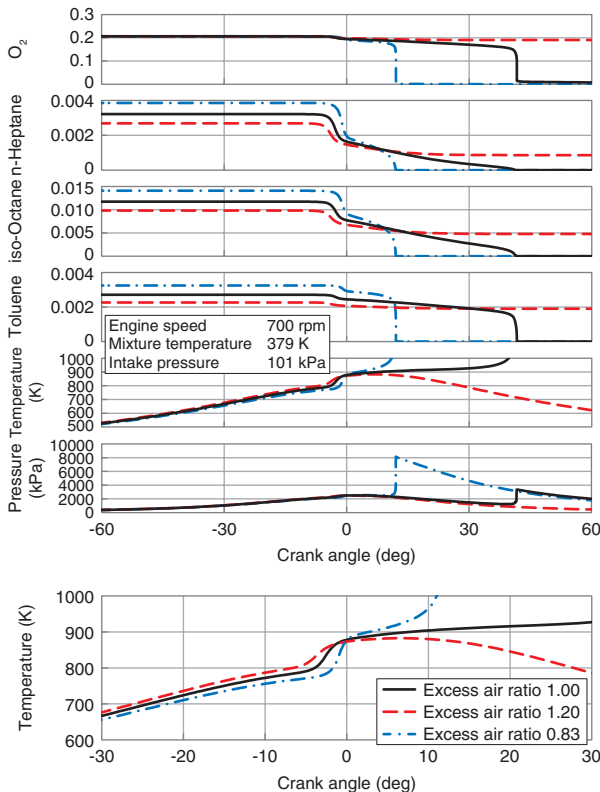


Fig. 9 Simulation results of change in excess air ratio

Table 3 Comparison of cylinder temperature

Excess air ratio		0.83	1.00	1.20
Mixture temperature (K)	BTDC 10 deg	753	772	788
	ATDC 10 deg	1000	905	880

Table 4 Conditions of simulation

Excess air ratio		0.83	1.00	1.20
Same intake pressure	Intake pressure (kPa)	101	101	101
Same torque		84.4	84.4	101

(1) Temperature during compression

Because hydrocarbons are polyatomic molecules, their ratio of specific heat is low. Therefore, because the ratio of specific heat is higher at $\lambda = 1.20$, when the ratio of fuel is lower, the temperature during compression is also higher at this air-fuel ratio.

(2) Temperature following commencement of oxidization reaction

When the oxidization reaction begins, the situation is reversed, with the temperature becoming higher at $\lambda = 0.83$, when the ratio of fuel is higher, than at $\lambda = 1.20$.

In this case, it is the rich mixture, $\lambda = 0.83$, which is most prone to self-ignition. Figure 10 shows changes in the engine speed at which self-ignition occurs when the air-fuel ratio is varied. The black line shows results when the excess air ratio is varied for the same intake air pressure, and the red line shows results when the excess air ratio is varied for the same torque. Table 4 shows the conditions employed. Increasing the leanness of the mixture is effective in controlling self-ignition at the same intake air pressure, but promotes self-ignition at the same torque. This is believed to be because the effect of increasing the leanness of the mixture in controlling the oxidization reaction is overwhelmed by the effect of the increased pressure in promoting the oxidization reaction. The results of the simulation that did not consider the cooling effect

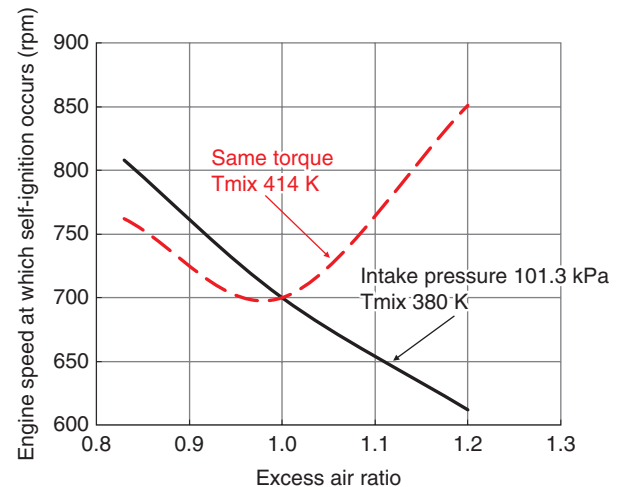


Fig. 10 Relationship between excess air ratio and self-ignition

of the latent heat of vaporization also showed that the rich mixture was more prone to self-ignition, and this is believed to be due to the fact that the ratio of fuel is higher and the temperature increase due to the oxidization reaction is greater.

4.2. Effect of EGR

Countermeasures against self-ignition utilizing the excess air ratio are acceptable as temporary measures, but constant application could result in increased emissions. Control of self-ignition by means of EGR was therefore studied as an alternative measure. In addition to possessing an identical effect to the other method in terms of diluting the fuel, EGR presented a greater advantage in having a low ratio of specific heat due to the high amounts of the three-atom molecules CO_2 and H_2O . Figure 11 shows results for the elementary process simulation. The temperature of the EGR is the same as that of the air-fuel mixture. Table 5 shows the temperature of the air-fuel mixture close to TDC when the fuel is diluted by increasing the leanness of the mixture and by EGR. The temperature of the mixture during compression is lower when EGR is employed than when the leanness of the mixture is increased. Figure 12 shows the relationship between the EGR rate and the engine speed at which self-ignition occurs. The black line shows results when the EGR rate is varied for the same intake air pressure, and the red line shows results when the EGR rate

Table 5 Comparison of cylinder temperatures

Excess air ratio	1.00	1.00	1.20
EGR ratio	0.0	0.167	0.0
Mixture temperature (K)	BTDC 10 deg	772	778
	ATDC 10 deg	905	853

Table 6 Conditions of simulation

EGR ratio	0	0.1	0.2
Same intake pressure	Intake pressure (kPa)	101	101
Same torque		81.1	90.1

Table 7 Fuel specifications

RON	87	91	95	100
n-Heptane	0.2247	0.1823	0.1602	0.1256
iso-Octane	0.6215	0.6642	0.5781	0.5183
Toluene	0.1538	0.1535	0.2617	0.3561
C/H ratio (weight)	5.6717	5.6724	5.9951	6.3145

is varied for the same torque. Table 6 shows the conditions used in the simulation. At the same torque, the effect of improvement in self-ignition due to EGR is minimal. It is believed that this is due to the fact that the intake air pressure increases in the percentage corresponding to the ratio of EGR, promoting the oxidization reaction and canceling the effect.

4.3. Effect of Octane Number

The phenomenon of self-ignition of the air-fuel mixture is known to be affected by the chemical structure of the fuel^{(6), (7)}. It was therefore considered that the octane number could provide an indicator for the self-ignition characteristics of the fuel. When changing the octane number of the surrogate fuel, it is necessary to change both the octane number and the C/H ratio to the correct figure. Table 7 shows the ratios of components in RON and the

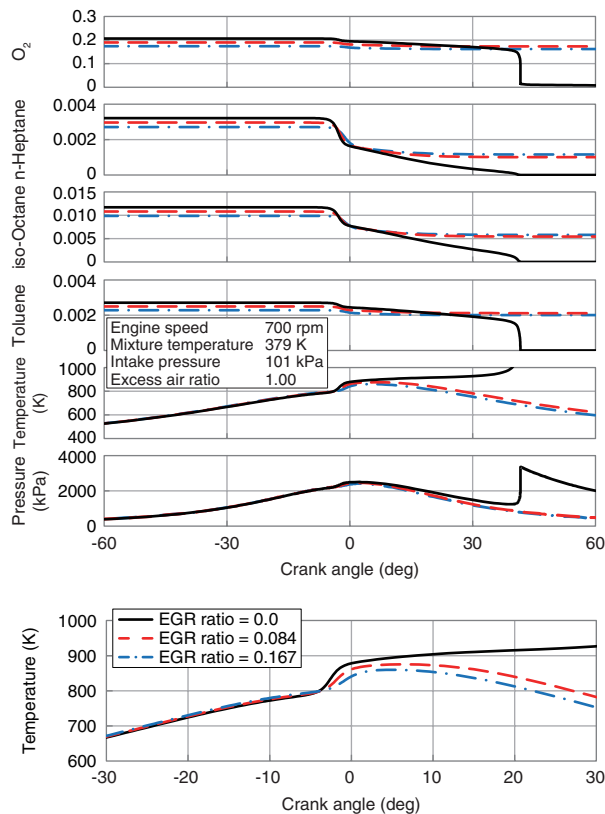


Fig. 11 Simulation results of EGR

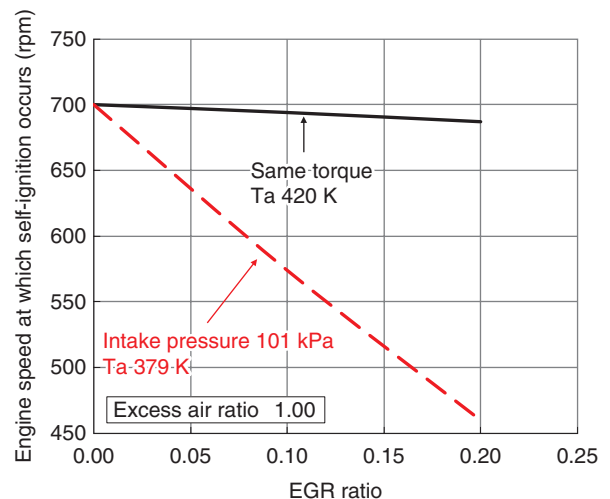


Fig. 12 Relationship between EGR ratio and self-ignition

surrogate fuels. Figure 13 shows the results of simulations conducted to study the differences between these fuels. There is a close relationship between the octane number and self-ignition characteristics, and this is mainly due to differences in the ratio of toluene, which remains almost entirely unoxidized in the low-temperature oxidation reaction. Figure 14 shows the relationship between RON and the engine speed at which self-ignition occurs. This shows that as in the case of knocking, RON provides an

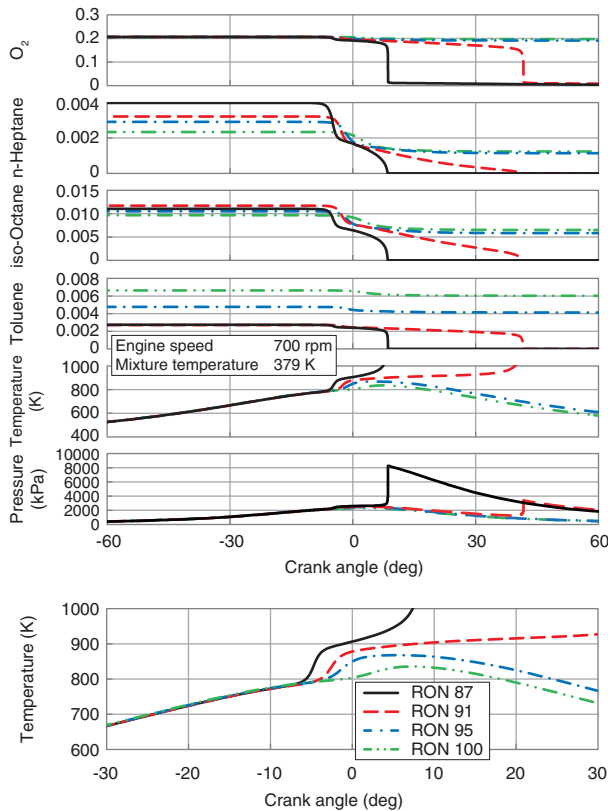


Fig. 13 Simulation of octane number

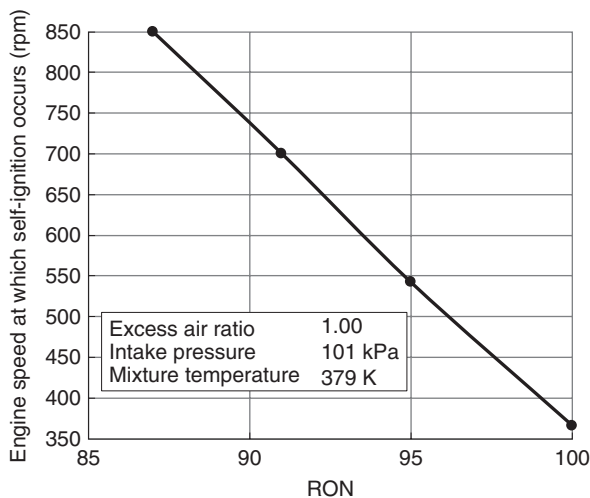


Fig. 14 Relationship between RON and self-ignition

indicator of the likelihood of self-ignition of the fuel.

From Figs. 4, 6, 9, 11, and 13, no matter which parameters are varied, the oxidation reaction will proceed even during the expansion stroke when the temperature of the air-fuel mixture exceeds 900 K, and hot flame is generated suddenly when it exceeds 950 K.

5. Countermeasures against Low-speed Self-ignition

5.1. Reduction of Residual Gas

When it was cooled to the same temperature as the air-fuel mixture, EGR displayed little effect in mitigating self-ignition. It was therefore considered that the negative effect of residual gas, a factor in increasing the temperature of the air-fuel mixture, would be high. An engine test was conducted using a cam profile that reduced valve overlap, as shown in Fig. 15. Figure 16 shows the relationship between intake air temperature and the ignition timing

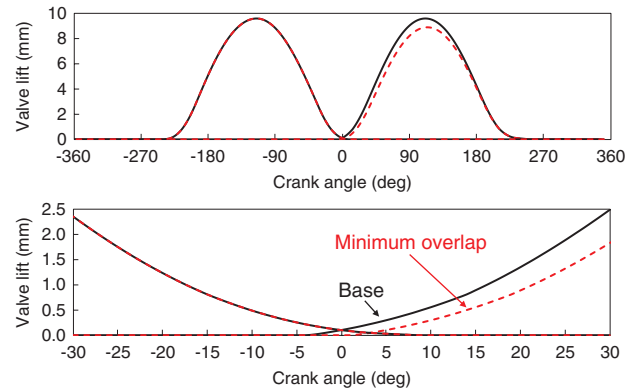


Fig. 15 Profile of reduced overlap cam

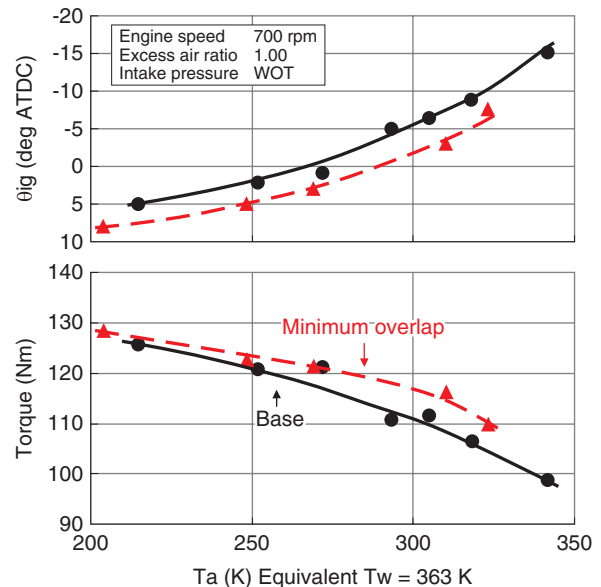


Fig. 16 Effect of residual gas reduction

immediately before the occurrence of self-ignition or knocking and the torque produced under these conditions. The self-ignition characteristic is improved across the entire temperature range, representing a maximum improvement of 8% when converted to torque. In order to conduct a detailed analysis of these test results, a simulation was conducted with the temperature difference between the residual gas and the air-fuel mixture set at 700 K, corresponding to wide-open throttle. Figure 17 shows the results of this simulation. When the amount of residual gas increases, the temperature of the air-fuel mixture increases, and the oxidization reaction commences earlier. Figure 18 shows the relationship between the ratio of residual gas and the engine speed at which self-ignition occurs. The black line shows results obtained for an assumed temperature difference of zero between the residual gas and the air-fuel mixture, and the red line shows results for an assumed temperature difference of 700 K. The residual gas has a greater effect in promoting self-ignition due to the increase in the temperature of the air-fuel mixture than the effect of EGR in controlling self-ignition. Based on these results, it was considered that the factor behind the control of self-ignition when the valve overlap was reduced was the reduction of the temperature of the air-fuel mixture by the reduction of the amount of residual gas. In addition, it was conjectured that there was almost no promotion of self-ignition by increase in the density of the fuel.

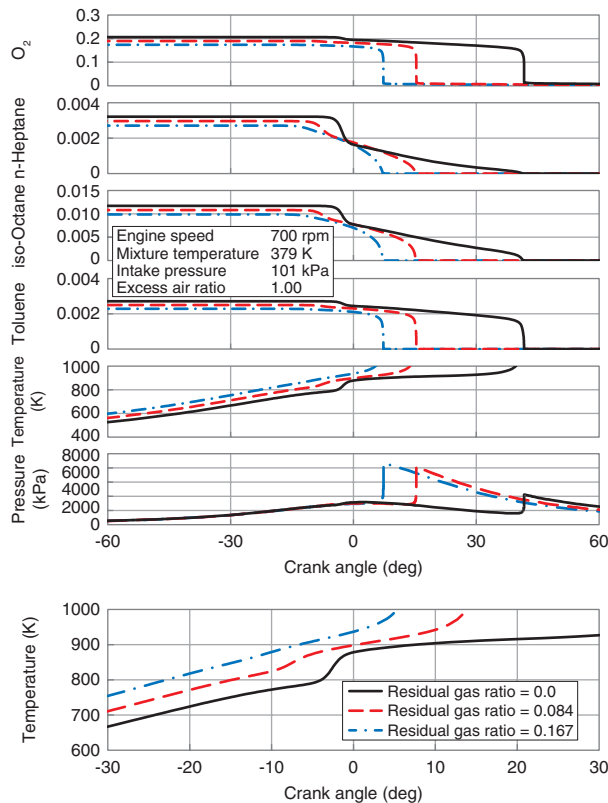


Fig. 17 Simulation of residual gas ratio change

5.2. Controlling Self-ignition when the Engine is Restarted

Self-ignition when the engine is restarted represents an important issue, for example in engines employing idle-stop mechanisms, which are becoming more widespread. The conditions prevailing when the engine is restarted are

- (1) High in-cylinder temperature
- (2) Intake air pressure: Atmospheric pressure
- (3) Low friction

A reduction in torque to a degree that did not have a major effect on the increase in engine speed would therefore be allowable as a measure to attempt to prevent self-ignition. Increasing the leanness of the excess air ratio, which had been effective in controlling self-ignition at the same intake air pressure, was therefore considered as an improvement measure. For the basic simulation conditions, intake air temperature was adjusted with consideration of changes in charging efficiency to make it possible to obtain results corresponding to those obtained from engine tests. Figure 19 shows a comparison of results for 250 rpm, corresponding to engine restart, and for 700 rpm, corresponding to idling. At 250 rpm, corresponding to engine restart, the crank angle at which the oxidization reaction commences is retarded, but self-ignition occurs because the engine speed is low and the time for the compression stroke is extended. The temperature and pressure at which self-ignition occurs differ, but the states of oxidization of the three components of the surrogate fuel are almost identical. Figure 20 shows results for the simulation when the excess air ratio is made leaner. Because the engine speed for restart is set, these simulation results show the air-fuel temperature at which self-ignition occurs. At the appropriate leanness for engine restart, the air-fuel mixture temperature at which self-ignition occurs increases, and self-ignition is controlled.

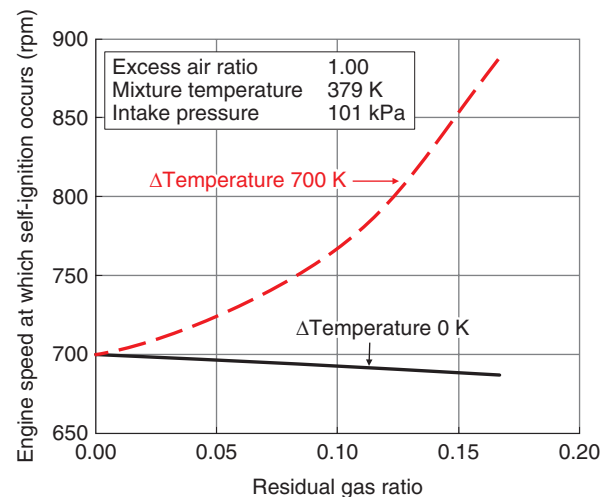


Fig. 18 Relationship between residual gas ratio and self-ignition

5.3. Prediction by Application of Simulation Results

By combining various simulation results, it is possible to simulate factors such as how self-ignition characteristics change in response to such changes as the country of sale and the type of gasoline used. For example, combining simulation results for the effect of the compression ratio and the effect of RON makes it possible to estimate the compression ratio to be employed in order to achieve the same self-ignition characteristic to an RON of 91 and

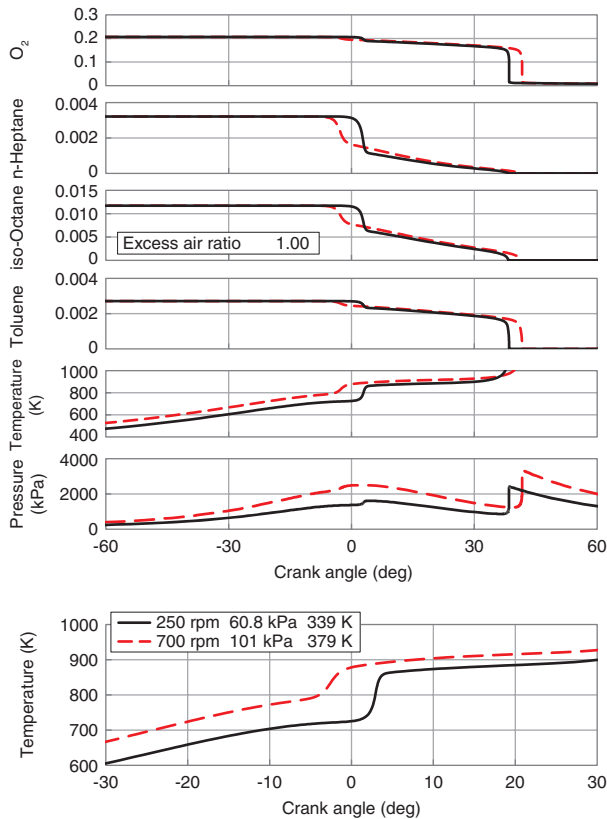


Fig. 19 Simulation at engine restart

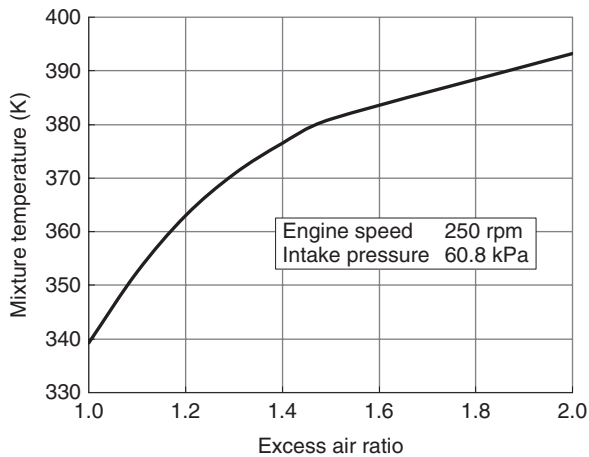


Fig. 20 Relationship between excess air ratio and self-ignition

a compression ratio of 10.5 when the RON is changed, as shown in Fig. 21. This is merely one example. The simulations will be effective in such procedures as conducting desktop studies of changes in specifications in relation to changes in use conditions in different regions.

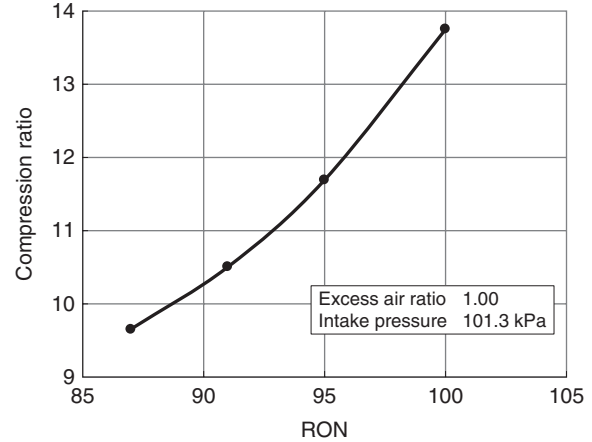


Fig. 21 Simulation of relationship between RON and compression ratio

6. Conclusion

An elementary process simulation model capable of modeling combustion conditions in which low-speed self-ignition noise occurs has been formulated and employed in analyses, producing the following findings.

- (1) Simulation of combustion producing low-speed self-ignition noise

Using CHEMKIN-PRO, it was possible to simulate measurement results for the timing of the commencement of low-temperature oxidation reactions and self-ignition and the changes in self-ignition characteristics with changes in parameters. This model was employed in conducting a variety of studies of low-speed self-ignition for which actual measurements would represent a challenge.

- (2) Mechanism of self-ignition

The self-ignition that occurs close to 40 deg ATDC and is the cause of low-speed self-ignition noise results from the following mechanism: A low-temperature oxidation reaction commences due to the increase in temperature and pressure during compression; there is a further increase in temperature, and when the temperature of the air-fuel mixture exceeds 900 K, the oxidation reaction proceeds irreversibly, and at a temperature in excess of 950 K, the reaction proceeds in a burst and a hot flame is produced. The reduction of the temperature and pressure of the air-fuel mixture can be considered as a general orientation for the control of self-ignition. For the same amount of air, the reduction

of the concentration of fuel in the mixture by the excess air ratio or EGR can be indicated. In addition, because the readily oxidizable straight-chain components of the fuel, as typified by n-heptane, are reduced in volume when the RON increases, the tendency towards self-ignition declines. RON can be considered a good indicator of the tendency of a fuel to self-ignite.

(3) Method of control of self-ignition

Reduction of the ratio of residual gas can be employed as a method of reducing the temperature of the air-fuel mixture. The elementary process simulation showed that the effect of this reduction in temperature exceeds the increase in the temperature of the mixture during the low-temperature oxidization reaction due to the increase in the concentration of the fuel. In addition, at engine restart, because the intake air pressure is basically atmospheric pressure, it is acceptable to reduce torque by using excess air, and the increased leanness of the mixture is effective in controlling self-ignition.

(4) Usefulness of simulation in studying specifications

Combining the results of various simulations makes it possible to simulate the ways in which self-ignition characteristics will change in response to factors such as different areas of sale and changes in the gasoline employed, making the simulation useful in studying changes in specifications.

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