Chemical Kinetic Analysis on the Effect of the Occurrence of Cool Flame on SI Knock

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ABSTRACT: Zero-dimensional knock simulations have been performed by using the model proposed by Noda et al. [SAE technical paper 2004-01-0618] implemented in CHEMKIN-PRO software. A detailed chemical kinetic mechanism for five-component gasoline surrogate was used with composition corresponding to JIS 2nd-grade gasoline (RON=90.8 and MON=82.9). An interesting effect of the cool flames appearing before the compression by flame propagation on the knocking was observed, which was suggested to play a key role in the recent development of SI engines. Present study implies that the modeling with kinetic mechanisms can be a powerful tool for technology breakthrough of next generation combustion engines.

KEY WORDS: heat engine, spark ignition engine, combustion analysis / Knock Model, Chemical Kinetics [A1]

1. Introduction

The knocking in a spark-ignition (SI) engine is its inherent drawback preventing the improvement of thermal efficiency and a number of researches and developments have been devoted to overcome the problem. The nature of the phenomenon is the autoignition of the unburnt end gas in front of the propagating flame by the chain-branching reactions, and the subsequent development and resonant acceleration of the pressure waves result in the knock vibration. The interaction of the compressible fluid mechanics with the chemical kinetics is also suggested to play an important role. The full elucidation of such a phenomenon by numerical modeling requires the direct Navier-Stokes (DNS) simulation for compressible fluid with a detailed chemical kinetic mechanism for the autoignition of practical fuels. Although such a three-dimensional (3D) simulation is currently impractical for the size of the engine cylinder, the necessary technological elements are under steady development, for example for the fast solver for the chemical kinetics and transport of huge number of chemical species. This means that, even though the fully coupled 3D-DNS calculation with detailed chemical kinetics is impossible, the each element by its alone is in practical level for the qualitative understanding and seed search for the technological development.

In this study, in order to evaluate the potential of the detailed chemical kinetic mechanism for the five-component gasoline surrogate developed in the CSTI-SIP "Innovative Combustion Technology" project, zero-dimensional simulations for the SI knock have been performed. The knock-limit ignition timings were calculated by modeling the compression of end gas by reciprocating piston and flame propagations and the effect of the occurrence of cool flame was analyzed.

2. Simulation Methods and Conditions

The zero-dimensional chemical kinetics simulations in this study were performed with CHEMKIN-PRO software version 15151. The knock modeling for an SI engine was done by the "SI Engine Zonal Simulator" code implemented in version 15141 and later. The model is based on that reported by Noda et al., in which detailed chemical kinetics is solved for the end-gas condition calculated assuming the constant-speed reciprocating engine cylinder with a 'burnt' zone in which the combustion equilibrium is assumed and its mass fraction varies with a given function of the crank rotation angle. The end gas is assumed to be adiabatic from the burnt zone but the pressure equilibrium is

| Table 1 Specification and operating conditions of the modelled SI engine |
| Engine speed | varied; 600, 900, or 1200 rpm |
| Compression ratio | varied from 12 to 22 |
| Bore and Stroke | 8.5 cm and 10.82 cm |
| Connection rod/crank radius ratio | 3.3 |
| IVC (= start of calculation) | ~120.2° ATDC |
| Intake temperature and pressure | 353 K (80°C) and 101.325 kPa (1 atm) |
| Woschni correlation parameters | $a = 0.1$, $b = 0.8$, $T_{\text{wall}} = 434$ K, $C_1 = 2.28$, and $C_2 = 0.00324$ |

Note: In SI unit (m s$^{-1}$ K$^{-1}$). Note that it should be 0.324 (cm s$^{-1}$ K$^{-1}$) in cgs based unit used in CHEMKIN.
established between two zones. Parameters and operating condition of the simulated SI engine are summarized in Table 1.

By using the parameters shown in Table 1, heat loss to the cylinder wall was estimated by using the following correlations proposed by Woschni, \(^{(1)}\) where \(Nu\) and \(Re\) are Nusselt and Reynolds numbers, \(\overline{u}\) is the average cylinder gas velocity, \(S_p\) is the mean piston speed, \(T_0, V_0, \) and \(V_d\) are initial temperature and volume and displacement volume and \(p, p_i,\) and \(p_a\) are pressure, initial pressure and the motored cylinder pressure.

\[
Nu = a Re^b
\]

\[
\overline{u} = C_1 \overline{S}_p + C_2 \frac{V_d T_0}{p_a^{\beta/\alpha}} (p - p_m)
\]

Time evolution of the mass fraction, \(x_b\), of the burned gas is approximated by the Wiebe function \(^{(4)}\) shown in Eqs. (3) and (4) with two parameters, \(\alpha\) and \(\beta\). Here, \(t\) is the dimensionless time expressed by Eq. (5) in which the crank rotation angle, ignition timing, and combustion duration are represented by \(\theta, \theta_{\text{ign}}\) and \(\Delta\theta\), respectively. The time at the maximum mass burning rate, \(t_{pk}\), is given by Eq. (6).

\[
x_b(t) = 1 - \exp(-\alpha t^\beta)
\]

\[
\frac{dx_b}{dt} = \alpha \beta t^{\beta-1} \exp(-\alpha t^\beta)
\]

\[
t = \frac{\theta - \theta_{\text{ign}}}{\Delta\theta}
\]

\[
t_{pk} = \left(\frac{\beta - 1}{\alpha \beta^2}\right)^{1/\beta}
\]

The Wiebe parameters assumed at engine rotation speeds 600, 900 and 1500 rpm are summarized in Table 2 and the corresponding change of the mass burning rates as a function of crank rotation angle are drawn in Fig. 1. The effective width of heat release in crank angle is assumed to be nearly constant (\(\approx 15\) degree) if the ignition timing is advanced at high rotation speed, as observed in the experiments.

Two types of the five-component mixtures have been designed as common gasoline surrogate for the CSTI-SIP project “Innovative Combustion Technology”. One of the surrogate mixtures designated as “SSR”, corresponding to JIS 2nd grade and “high-octane” (JIS 1st grade).

3. Pressure and Temperature Profiles around Knock

**Limit at engine speed 600 rpm**

Figure 2 shows the calculated pressure and temperature traces at engine speed 600 rpm. The compression ratio (CR) was increased from upper to lower traces; \(a\) 14.5, \(b\) 15.0, \(c\) 15.5, \(d\) 16.0, \(e\) 16.5 and \(f\) 17.0. At each compression ratio, the evolution of pressure is shown to the left) and end-gas temperature is shown to the right. The ignition timing, \(\theta_{\text{ign}}\) was scanned from 4.5 degree BTDC to 0.5 degree ATDC with 0.5 degree interval. No autoignition of end gas was observed at CR = 14.5. At CR = 15.0, the temperature traces show the autoignition of end gas at \(\theta_{\text{ign}} = -4.5\), -4.0 and -3.5 although the observed pressure spikes are small and scarcely visible at \(\theta_{\text{ign}} = -3.5\). This is because the mass fraction of the unburnt end gas was very small, that is, almost burned out, when the autoignition occurred. If we define the minimum pressure spike noticed as “knock” at the level

Table 3 Composition and octane numbers of the SIP common gasoline surrogate mixtures

| Constituent          | SSR \(^{a}\) | SSSH \(^{a}\) |
|----------------------|-------------|--------------|
| isoctane (C\(_2\)H\(_8\)) | 29.0        | 31.0         |
| n-heptane (C\(_7\)H\(_14\)) | 21.5        | 10.0         |
| methylecyclohexane (C\(_6\)H\(_12\)) | 5.0        | 5.0         |
| diisobutylene (C\(_8\)H\(_16\)) | 14.0        | 14.0         |
| toluene (C\(_7\)H\(_8\)) | 30.5        | 40.0         |
| MON                | 90.8        | 100.2        |
| MON                | 82.9        | 88.8         |

\(^{a}\) “SSR” and “SSSH” stand for the SIP common surrogate mixture corresponding to “regular” (JIS 2nd grade) and “high-octane” (JIS 1st grade).

Fig. 1 Mass burning rate profiles assumed for the engine speeds of 600, 900, and 1500 rpm

![Fig. 1 Mass burning rate profiles assumed for the engine speeds of 600, 900, and 1500 rpm](image-url)

\(\theta_{\text{ign}} = \frac{\Delta\theta}{\beta (\beta - 1/\alpha)}\)

Table 2 Parameters for the Wiebe function

| engine speed [rpm] | \(\alpha\) | \(\beta\) | \(\Delta\theta\) [degree CA] | \(\theta_{\text{ign}}\) |
|--------------------|----------|--------|--------------------------|-----------------|
| 600                | 7.0      | 5.00   | 45.6                     | varied          |
| 900                | 7.0      | 5.35   | 48.0                     | varied          |
| 1500               | 7.0      | 5.75   | 51.0                     | varied          |
of $\theta_{\text{ign}} = -4.5$, approximately at least 10% unburnt end gas is necessary for "knock". Below, in this study, this criterion is assumed for the knock limit. According to this, the knock limit ignition timing is 4.0 BTDC for CR = 15 case shown in Fig. 1-b).

For CR = 15.5 shown in Fig. 1-c), at six ignition timings, BTDC 4.5, 4.0, 3.5, 3.0, 2.5, and 2.0 show the end-gas autoignition, among which four cases, BTDC 4.5, 4.0, 3.5, and 3.0 are considered to as "knocking" since more than 10% unburnt gas is remaining when the autoignition occurred. The criterion also seems to be appropriate judging from the pressure traces. In this case, the knock limit ignition timing is 2.5 BTDC. It is interesting to see the unexpected behavior observed when the CR was further increased to 16.0. The number of cases where the autoignition is observed decreased to 4 (4.5, 4.0, 3.5 and 3.0 BTDC) compared to 6 at CR = 15.5. The knock limit was determined to be 3.5 BTDC, that is, the knock limit advanced when the CR was increased from 15.5 to 16.0. By increasing CR to 16.5, although the knock limit retarded to 3.0 BTDC, this is still advanced compared to the case of CR = 15.5 (2.5 BTDC). By further increase of CR to 17.0, the knock limit largely retarded to 1.5 BTDC.

4. Knock Limit at 600 rpm

The knock limits defined as above are plotted on the torque curves as a function of ignition timing in Fig. 3. For compression ratio CR = 14.5 or smaller, no knock was observed until minimum advance for best torque (MBT) at around –6.0 degree. For the case of CR = 15.0, the torque (38.84 N m) at the knock limit $\theta_{\text{ign}}$ (~4 degree) is nearly equal to the MBT torque (38.85) at CR = 14.5. When CR was increased to 15.5, as described above, knock limit $\theta_{\text{ign}}$ retards to ~2.5 degree and maximum torque decreased down to 38.79. However, interestingly, when CR was increased
to 16.0, the knock limit advances to −3.5 degree and maximum torque increased to 38.906 which is larger than the case of CR = 14.5. At CR = 16.5, knock limit retards again to −3.0 degree but the maximum torque slightly increased to 38.912. This is the maximum knock-limit torque at this engine speed. Finally at CR = 17.0, the knock limit retards significantly to −1.5 and torque also decreases to 38.78. This interesting phenomenon of advanced knock limit at increased CR may suggest that the optimal operating condition exists above the CR ratio usually considered to be the upper limit, and the possible improvement of the thermal efficiency of SI engine.

The possible cause of this phenomenon can be seen in Fig. 2, especially the temperature traces shown to the right. With increasing compression ratio, the temperature traces show the heat release by cool flames, although it is not very clear in the pressure traces shown to the left. Even in the case of CR = 14.5, where no autoignition was observed, the temperature traces when compared with the pressure traces indicate the cool flame heat releases at the late stage of the compression by flame propagation. At increased compression ratio, the cool flames are followed by the thermal ignition (i.e., knock), and knock limit largely retarded at CR = 15.5. However, at around CR = 15.5 to 16.0, cool flames start to appear earlier at around 10 degree ATDC, just after the top dead center (TDC). Then, apparent advancement of knock limit was observed at CR = 16.0. It should be noted that there is no chemical kinetic reason to think that the cool flame inherently inhibits the autoignition. The cool flame is essentially the preliminary stage of the thermal ignition. However, as shown by the temperature profile at CR = 16 in Fig. 4, when the cool flame occurs before the end-gas compression by flame propagation, the higher pressure of end gas suppresses the compression work applied from the burnt region, and results in the lower temperature of end gas compared to the case of CR = 15.5 in Fig. 4. This seems to be the major reason for this phenomenon. However, though expected to be minor, partial oxidation by cool flame may also slightly decreases the heating value of the end gas, and more detailed analysis will be needed for better understanding of this phenomenon.

For the practical application and observation in SI engines, in which the direct measurement of temperature is difficult, it may be interesting to investigate how this phenomenon appears in the pressure traces. The calculated pressure profiles are expanded and shown in Fig. 5 at fixed ignition timing (3.5 BTDC). The pressure traces at around 30 ATDC shown in Fig. 5-b indicates that the autoignition intensity is reduced when CR is increased from 15.5 to 16.0. The pressure traces around TDC in Fig. 5-a) indicates the occurrence of cool flame at CR = 16.0 and larger.

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**Fig. 3** Torque as a function of ignition timing at compression ratio varied from 14 to 17 at 600 rpm. At each compression ratio, knock limit is indicated by a circle, ○, while the first knocking condition is marked by a cross, ×.

**Fig. 4** Temperature profiles around knock limit at 600 rpm and ignition timing of 3.5 BTDC.

**Fig. 5** Pressure profiles around knock limit at 600 rpm and ignition timing of 3.5 BTDC.
This phenomenon invokes the recent development of high-compression ratio SI engine reported by Yamakawa et al.,\(^\text{5}\) in which the reported knock-limit torque does not significantly drop from CR = 13 to 15. Since they reported this at engine speed of 1500 rpm, the present investigation was extended to higher engine rotation speed below.

5. Knock Limits at Higher Engine Speed of 900 rpm

It may be the case that, though the zero-dimensional calculation does not quantitatively reproduce the experimental observation, it may qualitatively tell an essence of the phenomena, that is, similar thing may be observed at different condition than real. As described above, the effect of the engine speed was first investigated in this study. It is known that the heat-release (burning) period as measured in the crank angle in SI engine does not significantly depend on the engine speed because of the

![Fig. 6 Torque as a function of ignition timings at compression ratio varied from 15 to 19 at 900 rpm. □: Knock limits, ×: first knocking conditions](image_url)

![Fig. 7 Pressure and temperature traces of stoichiometric S5R/air at engine speed 900 rpm at compression ratios a) 16.0, b) 16.5, c) 17.0, d) 17.5, e) 18.0, and f) 18.5](image_url)
enhanced flame speed at stronger turbulence caused by the higher engine speed. The parameters for the Wiebe function were set accordingly, that is, the heat release profile is nearly the same if the ignition timing is advanced for the high rotation speed as shown in Fig. 1. Similarly to Fig. 3, the knock limits calculated at engine speed of 900 rpm are marked on the torque-ignition timing curves in Fig. 6. Detailed pressure and temperature traces are also shown in Fig. 7.

The change of the engine speed from 600 to 900 rpm corresponds to shortening of compression/expansion time scale by a factor of 2/3. The rate of the reaction that produce cool flame is, of course, the function of real time, not that of crank rotation angle. On the other hand, the reciprocating piston movement is a function of crank angle and also the flame propagation is supposed to be nearly a function of crank angle due to the turbulence enhancement of the flame speed. This means that the both cool flame and thermal ignition do not occur at the same crank angle under the same condition when only the engine speed is increased from 600 to 900 rpm. For this reason, the autoignition condition is expected to shift up to higher pressure and higher temperature region. When Fig. 7 (900 rpm) is compared with Fig. 2 (600 rpm), the difference does not seem to be significant except that the range of the compression ratio and ignition timing is different. However, the difference is unambiguous for the knock limits shown in Figs. 6 and 3. As can be seen in Fig. 6, the knock-limit ignition timing retards monotonically above CR = 16. The inverse advance of knock limit observed in the case of 600 rpm did not appear but a trace signature was seen between CR = 17.5 and 18 where knock limit stopped to retard. However, no merit in torque was observed compared to the lower compression ratios. This is quite different from the case of 600 rpm shown in Fig. 3. Similarly to Fig. 5, the expanded pressure traces at constant ignition timing, 7.5 BTDC, are shown in Fig. 8. Due to the 2/3 shortening of reaction time, the occurrence of cool flame delayed compared to the case of 600 rpm. This is 'too late' to improve the knock limit.

6. Knock Limit at 1500 rpm

The calculations were further extended to the engine speed of 1500 rpm. The calculated knock limits are shown in Fig. 9 and the expanded pressure traces at ignition timing of 12 BTDC are shown in Fig. 10. For this case, the absolute time for compression/expansion is shortened by 2/5 (40%) compared to the case of 600 rpm. The significant shortening of reaction time delays the autoignition (in crank angle) and the MBT can be reached up to CR = 16. The knock-limit best torque is observed at CR = 18 where small torque gain due to cool flame is observed. These CR are too large compared to the real SI engines but seems to be reasonable considering the shortening of the reaction time. One clear difference of the present calculation from the real SI engine seems to be much stronger turbulence at high engine speed which cannot be considered in the zero-dimensional calculations. The constant intake-air temperature and pressure and cylinder wall temperature assumed in this study may not apply to the practical experiments, either.

7. Concluding Remarks: Relations with the Current IC Engine Technology

The fact that the occurrence of cool flame advances the knock...
limit at certain condition is similar to the fact reported by Yamakawa et al.\cite{5} during the development of MAZDA's high compression-ratio engines (Skyactive-G) as described above. However, the present zero-dimensional calculations do not agree quantitatively with the observation in real engine, that is, the phenomenon is only observed at low engine speed 600 rpm in calculations while it is reported to occur at 1500 rpm. However, the present study suggests that such a zero-dimensional calculation with detailed chemistry can be a powerful tool for the initial development of new technology.

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References

(1) CHEMKIN-PRO 15151, ANSYS Reaction Design: San Diego, 2016.
(2) Noda, T., K. Hasegawa, M. Kubo, and T. Itoh, "Development of Transient Knock Prediction Technique by Using a Zero-Dimensional Knocking Simulation with Chemical Kinetics," SAE Technical Paper 2004-01-0618 (2004).
(3) Heywood, J.B., Internal Combustion Engine Fundamentals, McGraw-Hill, New York (1988).
(4) Oppenheim, A. K., Combustion in Piston Engines: Technology, Evolution, Diagnoses and Control, Springer-Verlag, Berlin (2004), p. 141; Oppenheim, A. K., Dynamics of Combustion Systems, 2nd Edition, Springer-Verlag, Berlin (2008), p. 55. According to Oppenheim, proper name of the founder of "Wiebe function" is I. I. Vibe (1902–1969) at Ural Polytechnic Institute.
(5) Yamakawa, M., Youso, T., Fujikawa, T., Nishimoto, T., Wada, Y., Sato, K., and Yokohata, H., "Combustion Technology Development for a High Compression Ratio SI Engine," SAE Int. J. Fuels Lubr., Vol. 5, No. 1, pp. 98-105 (2012).

Fig. 10 Pressure profiles around knock limit at 1500 rpm and ignition timing of 12.0° BTDC