

A Study on Knocking Prediction Improvement Using Chemical Reaction Calculation

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ABSTRACT

Compression ratio of newly developed gasoline engines has been increased in order to improve fuel efficiency. But in-cylinder pressure around top dead center (TDC) before spark ignition timing is higher than expectation, because the low temperature oxidization (LTO) generates some heat. The overview of introduced calculation method taking account of the LTO heat of unburned gas, how in-cylinder pressure is revised and some knowledge of knocking prediction using chemical kinetics are shown in this paper.

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INTRODUCTION

Aiming to reduce CO₂ emission affecting the global warming and to use limited oil resources effectively, recent engine research has put emphasis on fuel efficiency. Because engine compression ratio is one of the keys to improve fuel efficiency, some newly developed engines have higher compression ratio over 13. The higher compression ratio induces low temperature oxidization reaction whose partial heat release lifts up the in-cylinder pressure ahead of starting the combustion [1]. Therefore the authors have developed a sub-program which involves a two-zone combustion model introducing chemical reaction calculation to solve a simplified gasoline primary reference fuel (PRF) elementary chemical reaction model in order to simulate the LTO phenomenon accurately. The sub-program is used with our engine performance simulator [2] to approximate real engine drive conditions. This paper shows the calculation system overview, the improved in-cylinder pressure considering the LTO reaction, and some knowledge of knocking prediction comparing to the Livengood- Wu integral method [3].

CALCULATION

Chemical Calculation

Several gasoline PRF reduced elementary reaction models have been developed according to HCCI engine development, and some of them were published [4][5]. Among them, the TSURUSHIMA model [6] was chosen in this study because of its simplified structure. The model consists of only 38 reactions and handles 37 chemical species shown in Table 1. A chemical calculation code embedded in our

2-zone combustion model is originally programed by our hands. This code solves following equation (1) which expresses chemical reaction speed of X_i species by a formula integrating X_i generation and decomposition at each line of the reaction equations.

$$\frac{d[X_i]}{dt} = \sum_j \left(k_{+j} \prod_m [X_m] - k_{-j} \prod_l [X_l] \right) \quad (1)$$

Where, X means number of moles, and X_m is placed in the opposite side of X_i in the chemical reaction equation, and X_l is placed in the same side of X_i. K_{+j} and K_{-j} are rate constants of X_i generation and decomposition respectively. The subscript j means the line number of reaction formulas. In the calculation code, equation (1) was transformed into a recurrence formula like equation (2).

$$[X_i]^n = \frac{[X_i]^{n-1} + \sum_j (k_{+j} \prod_m [X_m]^n) dt}{1 + \sum_j (k_{-j} \prod_{l(l \neq i)} [X_l]^n) dt} \quad (2)$$

Here, dt is the calculation time interval [sec], the subscripts n and n-1 mean the current and the past status every time step by dt respectively.

In Figure 1, from (1), (2), (3) are calculation results at pressure 2MPa and temperature 700K. Their equivalence ratios are Φ=0.8, 1.0 and 1.2. Pressure rises in this calculation because of as burning constant volume. Another chemical reaction calculation was conducted using SENKIN

code of CHEMKIN2 package in order to confirm the precision of our chemical calculation code. But the results are not shown here, because pressure, temperature and chemical species fraction lines are completely identical with those of our code. The circles in [Figure 1](#) indicate the states of chemical equilibrium. The ends of pressure, temperature and chemical species fraction lines are almost close to those circles except the rich combustion. At the rich combustion of equivalence ratio 1.2

shown in (3), the reaction from CO into CO₂ is relatively sluggish, therefore temperature and pressure can't reach the equilibrium states, and the end of the temperature line is lower than the equilibrium state by about 50K. That should be kept in mind when the calculation results are compared to the experimental ones in the next section. The [Figure 1-\(4\)](#) depicts chemical equilibrium status of pressure, temperature and chemical species' mole fractions according to equivalence ratio.

Table 1. Gasoline PRF reduced elementary reaction model used in this work. [6] (cm³-mol-sec-cal units)

No	Reaction	A	n	E
! === n-NC7H16, LOW TEMPERATURE REACTION ===				
R1	nC7H16 + O2 = C7H15 + HO2	1.000E+16	0.00	4.600E+04
	REV /	1.000E+12	0.00	0.000E+00/
R2	C7H15 + O2 = C7H15O2	1.000E+12	0.00	0.000E+00
	REV /	2.510E+13	0.00	2.740E+04 /
R3	C7H15O2 = C7H14OOH	1.510E+11	0.00	1.900E+04
	REV /	1.000E+11	0.00	1.100E+04 /
R4	C7H14OOH + O2 = O2C7H14OOH	3.160E+11	0.00	0.000E+00
	REV /	2.510E+13	0.00	2.740E+04 /
R5	O2C7H14OOH => C7KET + OH	8.910E+10	0.00	1.700E+04
R6	C7KET => C5H11CO + CH2O + OH	3.980E+15	0.00	4.300E+04
R7	C5H11CO + O2 => C3H6 + C2H4 + CO + HO2	3.160E+13	0.00	1.000E+04
R8	nC7H16 + OH => C7H15 + H2O	6.000E+14	0.00	3.000E+03
R9	C7H15 + O2 = C7H14 + HO2	3.160E+11	0.00	6.000E+03
	REV /	3.160E+11	0.00	1.950E+04 /
R10	C7H14 + O2 => C5H11 + CH2O + HCO	3.160E+13	0.00	1.000E+04
R11	nC7H16 + HO2 = C7H15 + H2O2	1.000E+13	0.00	1.695E+04
R12	C7H15 => C5H11 + C2H4	2.500E+13	0.00	2.881E+04
R13	C5H11 = C3H7 + C2H4	1.138E+15	-0.42	2.701E+04
! === iso-C8H18, LOW TEMPERATURE REACTION ===				
R14	iC8H18 + O2 = C8H17 + HO2	1.000E+16	0.00	4.600E+04
	REV /	1.000E+12	0.00	0.000E+00 /
R15	C8H17 + O2 = C8H17O2	1.000E+12	0.00	0.000E+00
	REV /	2.510E+13	0.00	2.740E+04 /
R16	C8H17O2 = C8H16OOH	1.510E+11	0.00	2.180E+04
	REV /	1.000E+11	0.00	1.100E+04 /
R17	C8H16OOH + O2 = O2C8H16OOH	3.160E+11	0.00	0.000E+00
	REV /	2.510E+13	0.00	2.740E+04 /
R18	O2C8H16OOH => C8KET + OH	8.910E+10	0.00	1.700E+04
R19	C8KET => C6H13CO + CH2O + OH	3.980E+15	0.00	4.300E+04
R20	C6H13CO + O2 => C3H6 + C3H6 + CO + HO2	3.160E+13	0.00	1.000E+04
R21	iC8H18 + OH => C8H17 + H2O	6.000E+13	0.00	3.000E+03
R22	C8H17 + O2 = C8H16 + HO2	3.160E+11	0.00	6.000E+03
	REV /	3.160E+11	0.00	1.950E+04 /
R23	C8H16 + O2 => C6H13 + CH2O + HCO	3.160E+13	0.00	1.000E+04
R24	iC8H18 + HO2 = C8H17 + H2O2	1.000E+13	0.00	1.695E+04
R25	C8H17 => C6H13 + C2H4	3.617E+17	-1.27	2.970E+04
R26	C6H13 = C3H7 + C3H6	7.204E+13	-0.03	2.790E+04
! === HIGH-TEMPERATURE REACTION ===				
R27	C3H7 + O2 = C3H6 + HO2	3.000E+11	0.00	3.000E+03
R28	C3H6 + C3H6 => C2H4 + C2H4 + C2H4	3.160E+13	0.00	1.000E+04
R29	C2H4 + OH = C2H3 + H2O	1.200E+13	0.00	5.955E+03
R30	C2H3 + O2 = CH2O + HCO	4.000E+12	0.00	-2.500E+02
R31	CH2O + OH = HCO + H2O	2.430E+10	1.20	-4.470E+02
R32	HCO + O2 = CO + HO2	1.350E+13	0.00	4.000E+02
R33	CO + OH = CO2 + H	6.000E+06	1.30	-7.580E+02
R34	H2O2 + OH = HO2 + H2O	1.000E+13	0.00	1.800E+03
R35	H + O2 + M = HO2 + M	2.800E+18	-0.90	0.000E+00
R36	HO2 + HO2 = H2O2 + O2	1.300E+11	0.00	-1.630E+03
R37	H2O2 + M = OH + OH + M	1.200E+17	0.00	4.600E+04
R38	C2H4 + O2 => CH2O + CH2O	3.000E+13	0.00	3.000E+04

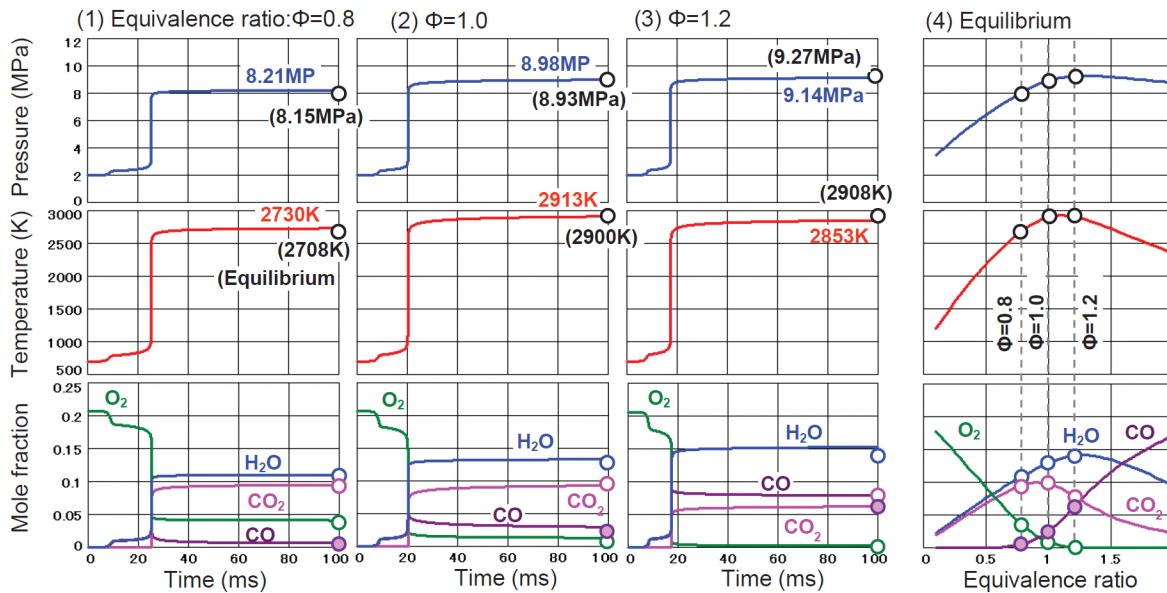


Fig.1. Temperature, pressure and mole fraction before and after self-ignition at constant volume.

Combustion Subprogram

The two zone model handles an unburned zone and a burned zone, and it works operations of cutting a portion of gas from the unburned zone and moving it to the burned zone according to a time-series mass combustion rate which is defined as input data like a diagram in Figure 2. The unburned gas moved to the burned zone is affected by the ambient high temperature of the burned gas, and then abruptly reacts with heat release. The burned zone is also calculated by the chemical reaction, not by the chemical equilibrium, for the sake of unification.

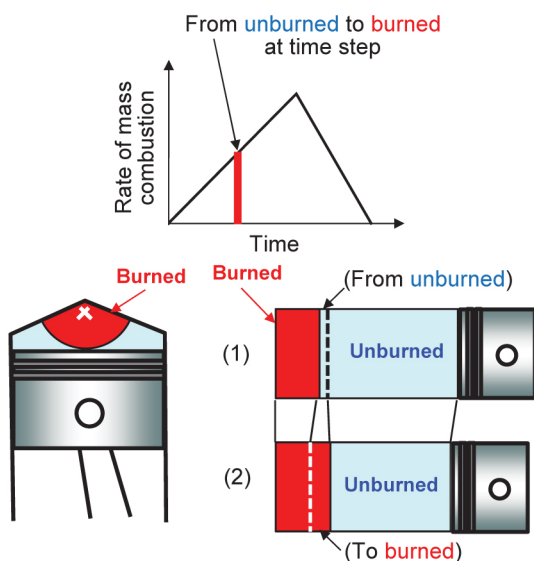


Fig.2. Calculation procedure of two zone combustion model.

The actual calculation procedure after this operation has following steps. At first, the burned gas volume V_{b2} at the next time step is assumed, and the internal energy is calculated by equation (3). Then the temperature T_{u2} is figured out from the internal energy and the chemical species' number of moles by using the function $F(\cdot)$ expressed as (4). The pressure P_{b2} is easily calculated by equation (5)

called the ideal gas law. On the other hand, the unburned gas volume V_{u2} can be obtained by the subtracting burned gas volume V_{b2} from the cylinder volume V_{cy1} at equation (6), and pressure P_{u2} is estimated via the same process as the burned gas through equations (7),(8),(9). If the pressure P_{b2} and P_{u2} are not the same, the assumption of the V_{b2} is amended, and the series of the calculation should be repeated again until the deviation between P_{b2} and P_{u2} is admissible.

$$U_{b2} = U_{b1} - P_1(V_{b2} - V_{b1}) + \Delta Q_{chem_b} + \Delta Q_{loss_b} \quad (3)$$

$$T_{b2} = F(X_{b2,i(i=1,ns)}, U_{b2}) \quad (4)$$

$$P_{b2} = \frac{m_{b2} R_g T_{b2}}{V_{b2}} \quad (5)$$

$$V_{u2} = V_{cyl2} - V_{b2} \quad (6)$$

$$U_{u2} = U_{u1} - P_1(V_{u2} - V_{u1}) + \Delta Q_{chem_u} + \Delta Q_{loss_u} \quad (7)$$

$$T_{u2} = F(X_{u2,i(i=1,ns)}, U_{u2}) \quad (8)$$

$$P_{u2} = \frac{m_{u2} R_g T_{u2}}{V_{u2}} \quad (9)$$

Where, the subscript u and b express unburned and burned states respectively, 1 and 2 express the previous and current states respectively. And m is a total number of moles. R_g is the gas constant. ΔQ_{chem} is heat during a time step generated by changing the chemical composition, and ΔQ_{loss} is heat loss from the cylinder