A Computational Study about Effects of Operating parameters and EGR compositions on Autoignition Reactivity for DME HCCI Combustion

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ABSTRACT

This study was computationally explored how the fuel autoignition reactivity was affected by operating parameters such as fuel, pressure, intake temperatures, engine speed and EGR compositions for HCCI combustion. This is done for DME and CHEMKIN-PRO was used as a solver. At first, influence of the operating parameters and EGR compositions were showed. And then, in order to clarify the mechanism of them on autoignition reactivity, data-sets of kinetic were analyzed to investigate the elementary reaction path for heat release at transient tempeatures by using contribution matrix.

Key Words : Operating parameters, EGR, Di-methyl Ether, Autoignition Reactivity, HCCI

HCCI combustion offers both high-efficiency and very low NOx and particulate emissions [1] [2]. However, it has not been reached at production stage since combustion phasing is very difficult to control as conventional engine s [3]. This means to control of autoignition reactivity [4].

HCCI combustion is controlled by chemical re action depending on thermal properties such as intake gas temperature, intake gas pressure, eq uivalence ratio and residual gas composition as called exhaust gas recirculation (EGR). Therefo re, the fundamental understaning of how these parameters influence on autoignition is very important for its further development.

The objective of this study is to investigate th e influence of engine operating parameters and and EGR compositions on autoignition reactivit y for DME fueled HCCI engine. Then, in order to investigate the mechanism of those paramet ers, contribution matrix has been used. Contrib ution matrix is a method to extract important reaction paths from a reaction mechanism [5].

In this study, DME which has negative temper ature coefficient was used as a fuel. Therefore, it has two-stage heat release as called LTHR (low temperature heat release) and HTHR (hig h temperature heat release). Curran's DME mo del was used in this study, which has 78 elem ents and 351 elementary reactions [6].

Calculations were carried out using a single-zo ne model of CHEMKIN-PRO as a solver. The single zone model treated the in-cylinder charg e as a 0-dimensional and thermodynamic prope rties while all gases were assumed to be ideal gases.

Calculation was performed only in one compres sion and expansion as shown in Fig.1. Combus tion analysis period was modeled according to the specifications of the engine in Table 1.

Definition of combustion duration was defined by method from Ando et al. [5] as shown in F ig.2.

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Table 1 Engine specifications

Process	Only 1 Compression & Expansion
Bore x Stroke	83 mm x 92 mm
Displacement	498 cc
Connecting Rod length	145.8 mm
Crank Radius	43.74 mm
Intake Valve Close, IVC	ATDC -136°
Exhaust Valve Close, EVO	ATDC 125.4°
Compression ratio	19.5

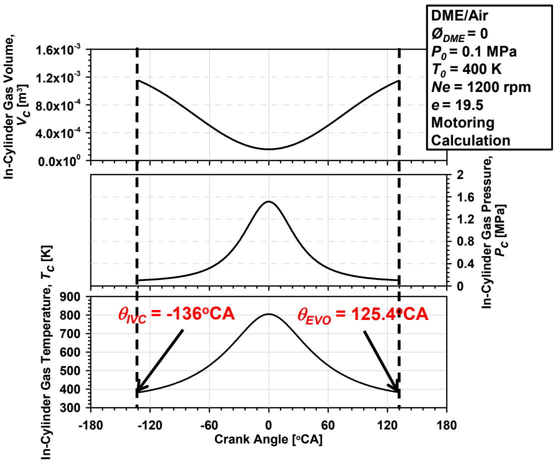


Fig. 1 Combustion analysis period..

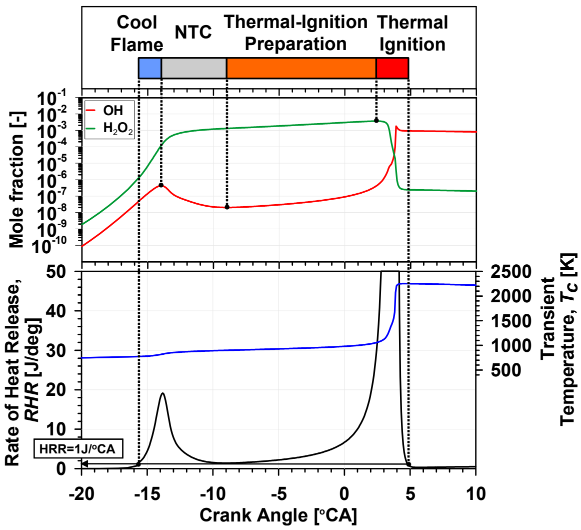


Fig. 2 Definition of key combustion timings.

To gain better understanding of the mechanism of autoignition reactivity affected by the operating parameters, contribution matrix has been done to investigate the contribution of each elementary reaction for heat release. This matrix is constructed by contribution ratios heat release at transient temperature. Eq.1 shows the definition of contribution ratio.

$$CHR_{j,Tt} = \frac{HR_{j,Tt}}{\sum_{j=1}^{N} abs(HR_{j,Tt})} \qquad (1)$$

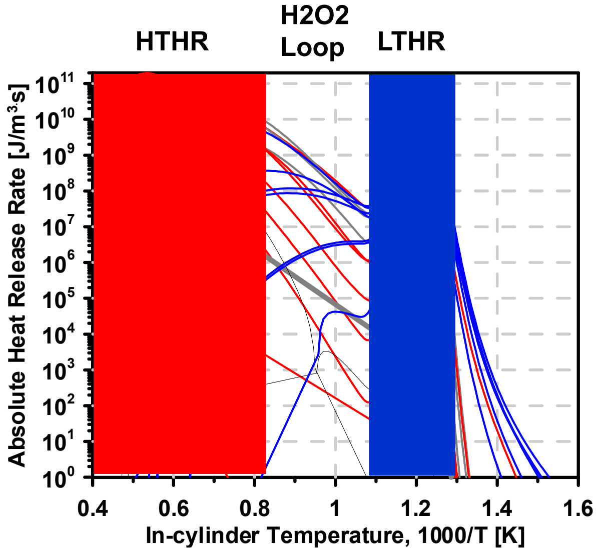
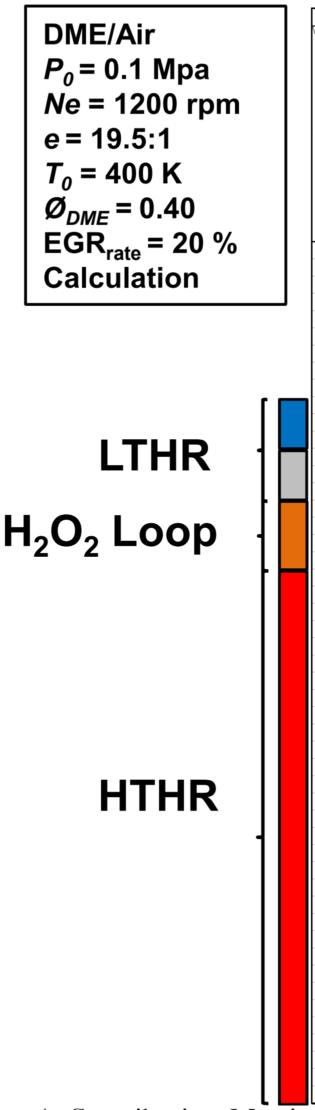


Fig. 3 Absolute Values of Heat Release Rates by Major Elementary reactions plotted against temperature. (Phi = 0.5, EGRrate = 50%, Ne = 1200rpm, Po = 0.1MPa, To = 400K).



	LTHR										H_2O_2 Loop				HTHR							
Reactions	287	280	295	296	293	274	297	294	190	40	46	32	50	51	7	25	26	8	49	42	10	188
T [K]	ch3och2o2<=>ch3och2+o2	ch3och3+o2<=>ch3och2+ho2	o2ch2och2o2h<=>ch2och2o2h+o2	o2ch2och2o2h<=>ho2ch2ocho+oh	ch3och2o2<=>ch2och2o2h	ch3och3+oh<=>ch3och2+h2o	ho2ch2ocho<=>och2ocho+oh	ch2och2o2h=>oh+2ch2o	ch3o2+M<=>ch3+o2+M	ch3o(+M)<=>ch2o+h(+M)	hco+o2<=>co+ho2	ch2o+oh<=>hco+h2o	h2o2+o2<=>2ho2	2oh(+M)<=>h2o2(+M)	co+oh<=>co2+h	h2o+M<=>h+oh+M	h+o2(+M)<=>ho2(+M)	h+o2<=>o+oh	ho2+oh<=>h2o+o2	ho2+o<=>oh+o2	o+h2o<=>2oh	h2o2+oh<=>h2o+ho2
400	0.0	-100.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
440	0.4	-0.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
481	1.9	-2.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
522	32.2	-43.5	0.8	0.2	-0.2	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
564	39.5	-51.5	3.6	1.8	-1.2	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
612	35.5	-37.4	9.8	8.4	-3.3	5.0	-0.1	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
656	30.8	-18.5	14.9	15.3	-5.4	10.8	-2.3	1.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0
699	28.2	-4.2	15.0	16.0	-6.2	15.8	-8.6	2.6	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.4	0.0	0.0	0.0	0.0	0.0
745	28.2	-0.1	12.8	13.8	-6.6	17.9	-11.0	4.8	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.8	0.0	0.0	0.0	0.0	0.0
773	28.6	0.0	11.3	12.2	-7.0	18.5	-10.8	6.5	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.7	0.0	0.0	0.0	0.0	0.0
778	28.6	0.0	10.9	11.9	-7.0	18.5	-10.7	6.8	0.8	0.0	0.1	0.1	0.0	0.0	0.0	0.0	1.8	0.0	0.0	0.0	0.0	0.0
808	24.3	0.0	8.2	9.3	-7.0	16.3	-9.8	8.5	1.4	-0.1	2.4	2.0	0.4	0.0	0.0	0.0	3.2	0.0	0.9	0.0	0.0	0.0
896	10.8	0.0	1.5	1.8	-3.8	8.0	-1.9	6.7	2.6	-3.2	11.0	5.1	5.5	-0.4	0.0	0.0	11.7	-0.1	0.6	0.0	0.0	0.2
927	9.6	0.0	0.9	1.0	-3.3	8.5	-1.1	6.0	4.9	-4.1	14.6	6.1	4.8	-3.5	0.0	0.0	8.8	-0.1	0.3	0.0	0.0	0.3
931	9.3	0.0	0.8	1.0	-3.2	8.5	-1.0	5.9	5.1	-4.2	14.7	6.1	4.7	-3.8	0.0	0.0	8.8	-0.1	0.3	0.0	0.0	0.3
987	4.7	0.0	0.2	0.3	-1.6	8.2	-0.3	3.1	4.7	-5.6	16.2	7.1	5.6	-7.7	0.0	0.0	9.7	-0.1	0.4	0.0	0.0	0.6
1030	2.4	0.0	0.1	0.1	-0.8	8.0	-0.1	1.7	3.5	-5.6	17.3	8.3	6.2	-10.5	0.1	0.0	9.4	-0.2	0.6	0.0	0.0	0.8
1077	1.1	0.0	0.0	0.0	-0.4	7.6	0.0	0.8	2.2	-5.1	18.0	9.7	6.8	-13.0	0.1	0.0	8.7	-0.2	0.8	0.0	0.0	1.2
1130	0.5	0.0	0.0	0.0	-0.2	7.1	0.0	0.3	1.3	-4.5	18.1	10.8	7.2	-14.6	0.1	0.0	8.0	-0.3	1.2	0.0	0.0	1.6
1213	0.1	0.0	0.0	0.0	0.0	6.0	0.0	0.1	0.5	-3.6	17.3	12.0	7.6	-15.6	0.2	0.0	7.9	-0.4	1.9	0.0	0.0	2.0
1249	0.1	0.0	0.0	0.0	0.0	5.4	0.0	0.1	0.3	-3.3	16.7	12.3	7.7	-15.5	0.3	0.0	8.3	-0.6	2.3	0.1	0.0	2.0
1294	0.0	0.0	0.0	0.0	0.0	4.7	0.0	0.0	0.2	-3.0	15.7	12.4	7.7	-15.1	0.4	0.0	9.0	-0.8	2.8	0.1	0.0	1.9
1338	0.0	0.0	0.0	0.0	0.0	3.9	0.0	0.0	0.1	-2.7	14.6	12.3	7.5	-14.3	0.6	0.0	10.1	-1.1	3.3	0.2	0.0	1.7
1385	0.0	0.0	0.0	0.0	0.0	2.8	0.0	0.0	0.1	-2.4	13.1	11.9	7.3	-13.0	0.8	0.0	11.8	-1.5	4.0	0.3	0.0	1.4
1399	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.0	0.1	-2.4	12.5	11.6	7.3	-12.5	1.0	0.0	12.5	-1.7	4.2	0.4	0.0	1.3
1432	0.0	0.0	0.0	0.0	0.0	1.6	0.0	0.0	0.0	-2.2	11.0	10.8	7.0	-11.3	1.3	0.0	14.2	-2.2	4.9	0.6	-0.1	1.1
1472	0.0	0.0	0.0	0.0	0.0	0.6	0.0	0.0	0.0	-2.0	8.6	8.8	6.5	-9.5	1.9	0.1	16.7	-3.1	6.0	1.1	-0.2	0.9
1514	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	-1.9	5.7	5.9	5.5	-7.5	2.8	0.1	19.1	-4.1	7.1	1.8	-0.4	0.7
1542	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.9	4.4	4.6	4.8	-6.4	3.4	0.1	19.7	-4.7	7.7	2.1	-0.5	0.5
1576	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.7	3.6	4.0	4.2	-5.4	4.1	0.2	19.6	-5.3	8.5	2.4	-0.8	0.4
1614	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.5	3.2	3.9	3.7	-4.6	4.9	0.2	19.1	-5.8	9.8	2.8	-1.0	0.4
1661	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-1.1	2.7	3.8	3.0	-3.6	6.5	0.4	18.6	-6.6	12.0	3.4	-1.6	0.3
1717	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.7	1.9	3.3	2.0	-2.3	10.1	0.7	19.4	-7.6	15.7	4.4	-2.8	0.3
1758	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.4	1.1	2.1	1.3	-1.3	15.2	1.3	21.6	-8.3	19.1	5.2	-4.4	0.3
1799	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.3	0.6	0.8	-0.5	21.0	2.3	24.5	-8.4	22.0	5.7	-5.9	0.3
1844	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.6	-0.2	22.8	3.1	25.1	-8.2	23.2	5.5	-6.4	0.3
1889	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.5	0.0	22.7	3.7	24.8	-8.2	23.9	5.2	-6.6	0.4
1931	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	0.2	22.4	4.2	24.4	-8.2	24.5	4.9	-6.7	0.4
1970	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.3	0.4	21.9	4.7	24.2	-8.1	25.3	4.6	-6.8	0.5
2022	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.3	0.6	21.2	5.2	23.9	-7.8	26.7	4.1	-7.0	0.5
2074	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.1	0.2	0.9	19.9	5.4	23.9	-7.2	29.2	3.3	-7.0	0.7
2106	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-0.1	0.0	0.1	0.1	1.4	18.2	5.1	24.5	-6.1	32.6	2.4	-6.6	0.9
2141	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	-17.2	-2.0	-33.3	18.9	3.3	1.2	0.0	5.6	-13.4
2186	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	-12.1	-1.5	-35.9	19.0	2.5	8.1	0.4	4.6	-10.5
2229	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	-7.6	-1.1	-38.9	18.8	1.6	13.6	0.8	3.7	-8.0
2270	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	-3.7	-0.8	-42.2	18.3	0.8	18.1	1.2	2.9	-5.9
2324	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	1.2	-0.5	-45.2	16.8	-0.4	22.4	1.6	1.7	-3.2
2369	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	4.6	-0.3	-44.6	14.6	-1.3	23.9	1.8	0.7	-1.1
2402	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	6.7	-0.1	-43.9	13.2	-1.8	24.7	2.0	0.2	0.2
2407	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	6.9	0.0	-43.4	13.2	-1.8	24.9	2.0	0.1	0.4

Fig. 4. Contribution Matrix to Heat release.

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