

Effect of Initial Temperature and EGR on Combustion and Performance Characteristics of Homogenous Charge Compression Ignition Engine Fueled with Dimethyl Ether

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Abstract

Homogeneous Charge Compression Ignition (HCCI) combustion is a pioneer method of combustion in which pre-mixed fuel and oxidizer (typically air) are compressed to the point of auto-ignition. HCCI engines can operate with most alternative fuels, especially, dimethyl ether (DME) which has been tested as a possible diesel fuel due to its simultaneously low NO_x and PM emissions. In this paper a single zone detailed chemistry combustion model for determining the time evolution of the homogenous reacting gas mixture in the combustion chamber and performance characteristics of the engine has been developed. The aim of this paper is to analyse the effect of intake temperature and EGR on the characteristics of auto-ignition and operating window of the HCCI combustion considering knock and misfire boundaries.

Keywords: HCCI, DME, Emissions, Performance, EGR

1. Introduction

■ The Homogeneous Charge Compression Ignition (HCCI) engine has been vigorously studied in the last decade because of its high thermal efficiency (potentially 15-20% higher than conventional gasoline engines) and ultra low NO_x and PM emissions compared with SI (gasoline Spark Ignition) and CI (diesel Compression Ignition) engines [1]. The basic idea is to employ a premixed air-fuel mixture that is sufficiently lean or dilute to keep flame temperatures below about 1900 °K to help keep NO_x and particulate production low. Consequently,

the HCCI engine with lean burn characteristics is a very good candidate for future clean and economical passenger vehicle applications. In spite of these great benefits, it has been very difficult to apply HCCI technology to real production engines.

There are major challenges that must be overcome to make the HCCI engine practical. First, the ignition timing and combustion phasing in the HCCI engine cannot be directly controlled because there is no direct trigger, such as spark timing in SI engines or injection timing in CI engines; second, it has low power density because of its lean combustion nature [3]; and finally, the HCCI engine has limited operating range between knock and misfire boundaries. Many studies on dimethyl ether as an alternative fuel or fuel additive have shown that the use of ether may help the simultaneous reduction of both NO_x and particulate matters in premixed charge compression

ignition engines [2]. This is considered to attribute to its high oxygen content and absence of carbon-carbon bonds. Because of its low emission characteristics and little toxicity the works on dimethyl ether as a fuel for HCCI engine is very active recently. Dimethyl ether shows very strong low temperature oxidation, which is common for the most of diesel like fuels. Therefore, the HCCI study of dimethyl ether may also give useful information on the general role of cool flame in HCCI operation of other diesel like fuels [3 and 4].

In this paper a single zone detailed chemistry combustion model has been implemented into the 4-stroke engine fueled with DME. The model utilizes the library of CHEMKINIII code for determining chemical production rates. The system of equations solved in the single zone HCCI combustion model, is based on a fixed mass, variable volume reactor. With considering extended Zeldovich mechanism, the overall mechanism involves 354 chemical reactions and 81 species. As a result, the effect of intake temperature and EGR on the characteristics of auto-ignition, rate of heat release, and performance characteristics of the HCCI engine have been investigated.

2. Modeling technique and kinetic mechanism

A zero dimensional model is selected to study engine Performance and auto ignition characteristics of DME oxidation; because of its simplicity and its ability to predict performance characteristics of HCCI engine [4 and 5]. This model has been developed for the closed cycle with full chemical kinetic considerations both in compression and expansion processes. The following assumptions are considered for this single-zone model:

1. All chemical species are considered to behave as ideal gas.
2. The mixture is considered to be homogenous and there is no spatial-gradient throughout the combustion chamber.
3. The homogenous mixture of fuel and air is formed just before IVC.

For this system the conservation law of energy in differential form is:

$$\delta Q - \delta W = dU \quad (1)$$

The internal energy of a system consisting of the mixture of ideal gases is:

$$U = \sum_{i=1}^{N_s} n_i u_i \quad (2)$$

With differentiating the above equation, we have:

$$dU = \sum_{i=1}^{N_s} (n_i du_i + u_i dn_i) \quad (3)$$

The specific internal energy of each species with the ideal gas assumption is:

$$du_i = c_{v,i} dT \quad (4)$$

Considering the work, heat transfer and mass fraction of each species, the time differential equation form of 1st law of thermodynamics is:

$$\dot{Q} - p \frac{dV}{dt} = \sum_{i=1}^s \bar{u}_i \frac{dn_i}{dt} + n \sum_{i=1}^s \bar{u}_i \frac{d\bar{u}_i}{dt} \quad (5)$$

From conservation law of chemical species:

$$\frac{d[X_k]}{dt} = \dot{\omega}_k - \frac{[X_k]}{V} \frac{dV}{dt} \quad (6)$$

The pressure is found from the ideal gas law:

$$p = \left(\sum_{k=1}^s [X_k] \right) \bar{R} T \quad (7)$$

The Eq. (5) can be rewritten to present variation of mixture temperature:

$$\frac{dT}{dt} = \frac{\dot{Q} - \left[\left(\sum_{k=1}^s [X_k] \right) \bar{R} T \right] \frac{dV}{dt} - V \sum_{k=1}^s \bar{u}_k \dot{\omega}_k}{V \sum_{k=1}^s [X_k] \bar{C}_{v,k}} \quad (8)$$

Combination of the above equation results in a system of ordinary differential equations (ODEs). The initial concentration and temperature are specified in the input file which is read by the pre-processor program written in visual FORTRAN. This program also reads a symbolic description of a reaction mechanism and then extracts the needed thermodynamic data for each species involved from the Thermodynamic Database. The unknowns in Eq. (8) are the volume and derivative of volume and the heat transfer. The overall volume change of the charge in the engine cylinder is a function of crank angle based on the so-called slider-crank formula in which V_c , r_c , R and θ show respectively the clearance volume, compression ratio, lever ratio and instantaneous crank angle.

$$V = V_c \left[1 + \frac{r_c - 1}{2} \left(R + 1 - \cos \theta - \sqrt{R^2 - \sin^2 \theta} \right) \right] \quad (9)$$

The rate of change of volume is obtained by analytically differentiating Eq.9:

$$\frac{1}{V_c} \frac{dV}{dt} = \frac{1}{2} (r_c - 1) \left(\sin \theta + \frac{\sin \theta \cos \theta}{\sqrt{R^2 - \sin^2 \theta}} \right) \quad (10)$$

3. Chemical kinetics model

The production rate of each species is calculated according to:

$$\dot{\omega}_i = \sum_{k=1}^{N_r} (v''_{i,k} - v'_{i,k}) (RP)_k \quad (11)$$

The rate of progress variable for the k th reaction is given by the difference of the forward and reverse rates:

$$(RP)_k = K_{f,k} \prod_{i=1}^{Ns} [x]_i^{v_{i,k}} - K_{r,k} \prod_{i=1}^{Ns} [x]_i^{v_{i,k}} \quad (12)$$

For elementary reactions and for third-body reactions we have:

$$(RP)_k = \left(\sum_{i=1}^{Ns} a_{i,k} [x]_i \right) \left(K_{f,k} \prod_{i=1}^{Ns} [x]_i^{v_{i,k}} - K_{r,k} \prod_{i=1}^{Ns} [x]_i^{v_{i,k}} \right) \quad (13)$$

The rate constants for the reactions are generally assumed to have the following Arrhenius temperature dependence:

$$K_k = A_k T^{\beta_k} \exp\left(-\frac{E_k}{R_u T}\right) \quad (14)$$

All the above equations related to chemical kinetics and rate expressions Eqs. (11-14) are derived from CHEMKIN 3.0 instruction manual [6]. The Arrhenius constants for both forward and reverse reaction and thermodynamic properties of each species are derived from a file downloaded from reaction mechanism developer's website. In this study the LLNL mechanism [7] is used to predict DME oxidization process. Extended Zeldovich mechanism has been used to predict NO_x emissions production.

The detailed mechanism of DME oxidation consisting of 354 reactions and 82 species, have been used to predict oxidation process of this fuels. A source program for a variable volume reactor was written to drive the CHEMKIN libraries and calculation of performance characteristics of HCCI engine. The model utilizes CHEMKIN (III) library to determine chemical production rates and Variable-coefficient Ordinary Differential Equation code (dvoid) to solve the problem for resulting stiff system of first order ODEs.

4. Heat transfer model

The dominant heat transfer mechanism in the HCCI engine is forced convection from the bulk gas to combustion chamber walls. The radiation effect is very small because of low-soot, low temperature combustion of the premixed lean mixture in a typical HCCI engine. Among the existing heat transfer models suggested for IC engines, the Woschni model is used in this analysis because of its simplicity and wide acceptance [8]. The empirical constants of Woschni equation in this study have been derived from reference 8.

$$h = 129.8 B^{-0.2} P^{0.8} T^{-0.55} [2.28 S_p + f(p)]^{0.8} \quad (15)$$

$$f(p) = 3.34 \times 10^{-4} \frac{V_d T_r}{P_r V_r} (p - p_{mot}) \quad (16)$$

The motored pressure is derived from the following differential equation:

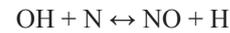
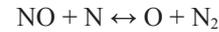
$$\frac{dp_{mot}}{dt} = \frac{(\gamma_{mot} - 1)}{V} \frac{dq_{ht,mot}}{dt} - \gamma_{mot} \frac{P_{mot}}{V} \frac{dV}{dt} \quad (17)$$

Finally, the cylinder pressure derived from ideal gas law.

$$P = \rho RT \quad (18)$$

5. NO_x formation model

The most widely accepted mechanism for modeling of NO_x formation is suggested by Zeldovich (Heywood 1988). The principal source of NO formation is the oxidation of the nitrogen present in atmospheric air. The nitric oxide formation chain reactions are initiated by atomic oxygen, which forms from the dissociation of oxygen molecules at the high temperatures reached during the combustion process [3]. In order to model NO_x formation for the HCCI combustion extended Zeldovich mechanism has been used. Extended Zeldovich Mechanism is as follows:



6. Validation of the model

Figure shows the comparison of zero dimensional thermo-kinetic model with experimental results conducted on the single-cylinder four-stroke engine by Yao and Zheng for mixture temperature of 348 K and mixture equivalence ratio of 0.215 at IVC [3].

The predicted pressure values by single zone HCCI model are rather larger than the actual measurements and the maximum pressure occurs earlier. The difference is related to the zero dimensional model which can not capture in cylinder temperature and mixture variations that caused all chemical species in the cylinder to reacts instantaneously. However the calculated ignition timing agrees well with the measured result as shown in Fig. 1.

TABLE 1. Specification of the considered diesel engine

Bore	215 mm
Stroke	275 mm
Compression ratio	13.5:1
Intake valve close	40 °ABDC
Exhaust valve open	55 °BBDC
Speed (rpm)	1000
Maximum dp/dtheta	20 bar/CA

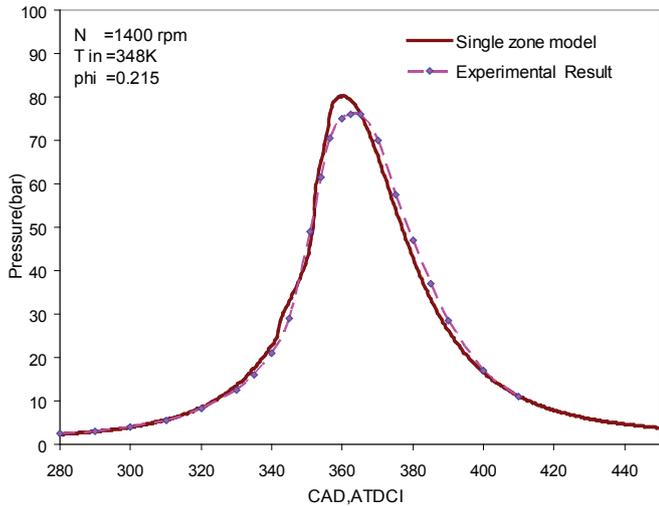


Fig. 1. Comparison of pressure profiles of experiment with single zone model

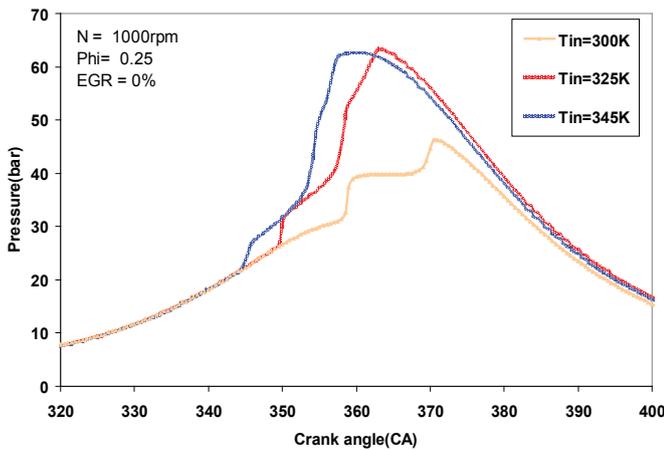


Fig. 2. Effect of initial temperature of the mixture on pressure trajectory where PHI = 0.25

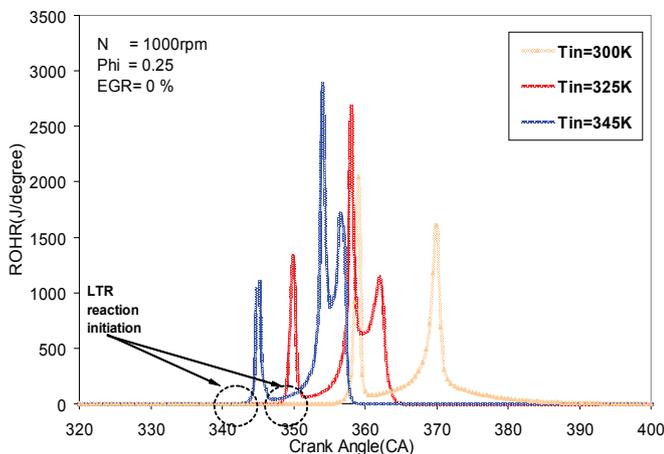


Fig. 3. Effect of initial temperature of the mixture on rate of heat release where PHI = 0.25

It is also worthwhile to mention that the first inflection in the calculated pressure (the first step pressure rise) is due to strong low temperature kinetics reaction in the DME HCCI combustion which has been reported in a similar analysis by Yao and Zheng by the use of zero-dimensional thermodynamic model coupled with SENKIN detailed chemical kinetic code [3].

The specification of the RK215 industrial diesel engine which is considered for calculating the results of the single zone HCCI model is summarized in table 1 For considering knock phenomenon, maximum permissible rate of pressure rise per crank angle (tp/dt) has been assumed up to 20 bar per crank angle [9].

7. Results and discussion

Figs. 2 and 3 show the effect of initial temperature of the mixture on cylinder pressure and rate of heat release (ROHR) for initial pressure of 100 kPa and equivalence ratio of 0.25. In all cases temperature and the amount of EGR in intake valve close condition has been considered as the initial condition. It can be clearly seen that increasing initial temperature significantly advances the beginning of HR by LTR and consequently advances the start of auto ignition which enhances maximum pressure of the cylinder and ROHR. Also three stage heat release (HR) is the results of higher initial temperature which corresponds to hot flame combustion [4]. Furthermore, some researchers have shown that in HCCI combustion of gasoline and its surrogate fuels, a three-stage auto ignition is achieved [10].

Heat release curve of DME-air oxidation is a result of two stage auto ignition: low temperature reaction (LTR) and high temperature reaction (HTR). LTR appears in the range 750-800 K and HTR above 1000 K. In LTR region the, concentration of CH_2O , CO , and H_2O_2 is increased so DME is called to have strong LTR reaction. It has been shown that temperature is dominant for the LTR reactions. Between LTR and HTR regimes CO , CH_2O , and H_2O_2 increase gradually, and the DME oxidation rate decreases. This region (850-1000 K) is called negative-temperature coefficient region (NTCR).

When the temperature increases above 1000 K, HTR is dominant .In this region DME, CH_2O and H_2O_2 concentration decreases and CO mole fraction increase at the same time [3]. Table 2 shows the effect of four different initial temperature of the mixture on performance characteristics of HCCI engine.

It can be concluded that increasing initial temperature significantly increases the rate of heat release and maximum temperature of the cylinder. In higher initial temperature lower IMEP and power density are achievable since the start of ignition by LTR reactions takes place earlier in compression stroke.

Although, increasing the initial temperature from 300 to 325 K, the rate of pressure rise is increased significantly and NO_x emission production correspondingly promoted greatly [9]. When the initial temperature is lower than 300 K, the maximum in cylinder temperature is less than 1200 K and complete oxidation of CO to CO_2 can't be performed which results in incomplete combustion [3].

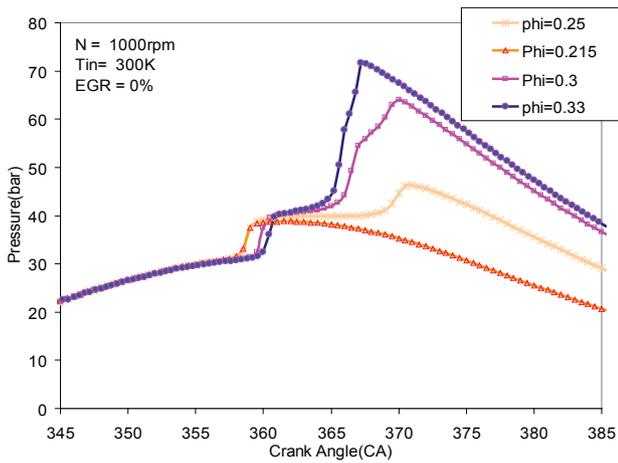


Fig. 4. Effect of different equivalence ratios on pressure trajectory where $T_{in}=300K$

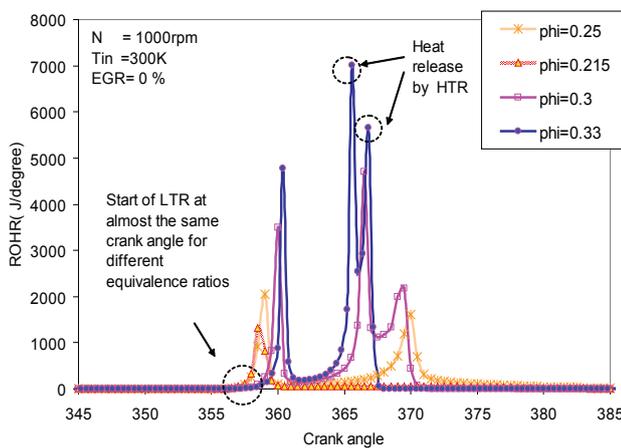


Fig. 5. Effect of different equivalence ratios on the rate of heat release where $T_{in} = 300 K$

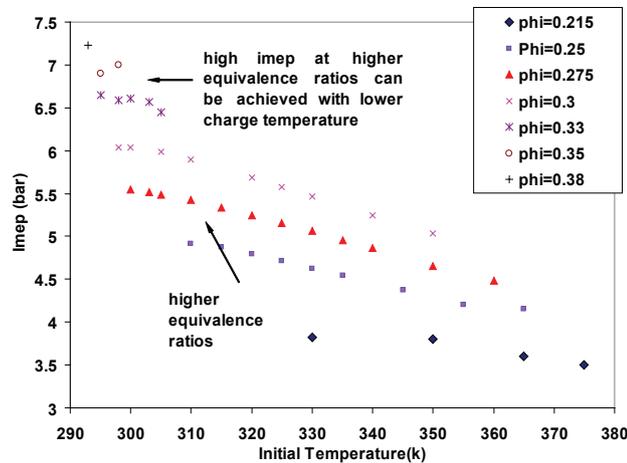


Fig. 6. Effect of various initial equivalence ratios and initial temperature of the mixture on IMEP

Figs. 4 and 5 show the cylinder pressure and heat release rate with different equivalence ratio for initial temperature of 300 °K and initial pressure of 100 kPa. It can be seen that increasing equivalence ratio has no significant effect on ignition timing, but the ROHR becomes too high and the HR duration decreases which can cause serious engine mechanical stresses. Results show that, at equivalence ratios more than 0.3, where $T_{in} = 300 K$, engine tends to knock.

Table 3 shows the effects of various equivalence ratios on performance characteristics of HCCI engine where initial temperature is 300K for all cases. In higher equivalence ratios, maximum pressure of the cylinder, maximum available work, IMEP and maximum $dp/d\theta$ are increased. Also the maximum temperature is enhanced which individually increases the NO_x emission production effectively.

In higher equivalence ratios (e.g. 0.38) in the same initial temperature of 300 K, the rate of pressure rise would reach as high as 30 bar per crank angle which is an indication of knock phenomenon in this situation. Consequently, this point can not be considered as an operating point for the engine.

Also in equivalence ratios less than 0.25, the rate of pressure rise would be less than 5 bar per crank angle and the maximum in cylinder temperature wouldn't be enough for CO oxidation and incomplete combustion occurs and consequently thermal efficiency would be decreased [11].

TABLE 2. Effect of initial temperature on performance characteristics

T_0	P max	Max $dp/d\theta$	Theta Pmax	T max	Start of LTR	Imep	Isfc	NO_x	Ipower
K	bar	bar/CA	ATDC	K	ATDC	bar	g/kWh	ppm	kW
300	64.1	5.3	11	1660	-3	6.04	225	0.02	50.3
310	70.8	6.9	4	1730	-7	5.9	223	0.11	49.1
320	71.2	15	1	1760	-10	5.69	224	0.5	47.4
325	70	18	0	1780	-17	5.58	225	0.9	46.5

TABLE 3. Effects of various equivalence ratios on performance characteristics of HCCI engine, $T_{in} = 300\text{ }^\circ\text{K}$

PHI	P max	Max dp/dtheta	Theta P max	T max	Start of LTR	Imep	Isfc	NO _x	Ipower
	bar	bar/CA	ATDC	K	ATDC	bar	g/kWh	ppm	kW
0.275	55.2	6	13	1550	-2	5.55	245	4e-3	46.2
0.3	64.1	12	10	1660	-2	6.04	225	0.02	51
0.33	71.6	17.8	8	1760	-2	6.61	226	0.1	55.1
0.35	75.4	30	7	1820	2-	7	226	1.2	58.3

Figs. 6 and 7 show the effect of various initial equivalence ratios and initial temperature of the mixture on Imep and Isfc respectively. It can be concluded that higher Imep is achievable at higher equivalence ratios and lower temperature of the mixture and the operating regime between knock and misfire at higher load situation would be narrower which shows the instability of combustion in those regions.

In low loads, the fuel consumption will suffer due to the poor combustion efficiency and improper combustion phasing. It can be concluded that in full load operation of DME HCCI engine, with considering knock and incomplete combustion boundaries, maximum indicated power of 55-60 KW can be achieved which is virtually 30 percent of the very power which is attainable in diesel mode operation. But the emissions level specially those of NO_x, Soot and particulated matter in this operation mode is remarkably lower than those of Diesel mode operation.

Another parameter that can affect the combustion phasing is amount of EGR. In addition to the thermal effect, the inert gases contained in the EGR can be used to control the ROHR due to their impact on chemical reaction rate, which can reduce the ROHR, and thus lower peak cylinder pressure [12]. It has been well confirmed that hot EGR enhances combustion in four-stroke HCCI mainly due to high temperature of the resulting intake mixture, rather than the existence of "active radicals" [13].

Figs. 8 and 9 show the variation of cylinder pressure and heat release rate with three EGR amounts. These figures show that increasing amount of EGR leads to extension of heat release rate duration and therefore operating window in which more initial temperature can be used, for a constant equivalence ratio, to achieve controlled auto-ignition [14 and 15].

Increasing the EGR amount causes the decrease of oxygen in the mixture that can lower the ROHR. The rate of low temperature chain branching reaction then becomes lower due to decrease in oxygen amount [16]. It can be concluded that the amount of EGR does not have any significant effect on first stage of HR by LTR, but the maximum ROHR is decreased nearly 60% in this case. Also the start of HTR is retarded showing the effect of EGR on extension of heat release duration, which proportionally reduces the mechanical stresses in the combustion chamber. Table 4 shows the effect of EGR amount on performance Characteristics of the engine for PHI = 0.33 and $T_{in} = 300\text{ }^\circ\text{K}$.

At lower equivalence ratios, e.g. 0.25 and low intake temperatures, the exothermic oxidation reaction of OH and CO can't be completed and lower indicated power and IMEP are achieved. So, equivalence ratio of 0.33 has been chosen for investigation of the effect of EGR amount on performance and auto ignition characteristics at an initial temperature of 315 K.

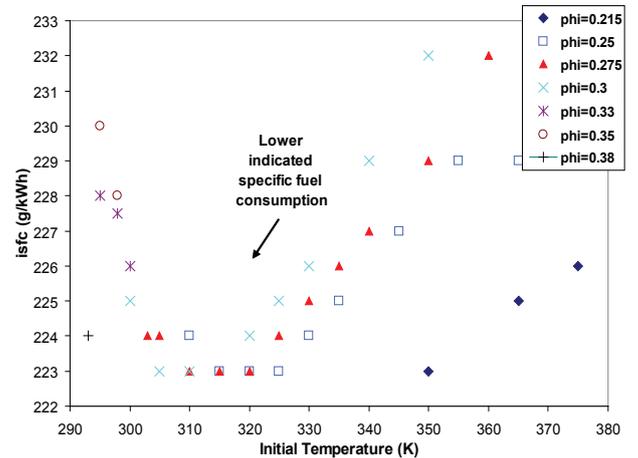


Fig. 7. Effect of various initial equivalence ratios and initial temperature of the mixture on ISFC

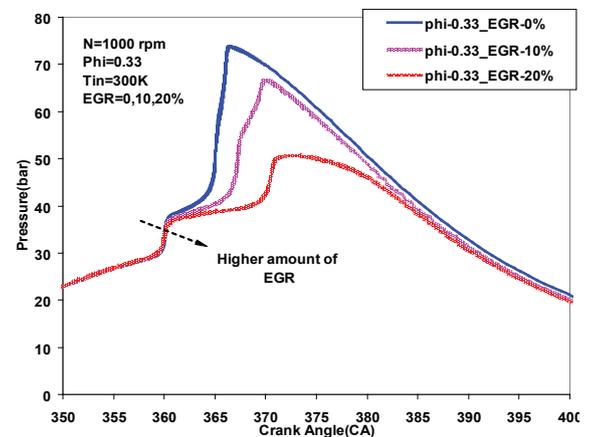


Fig. 8. Effect of various EGR amount on in cylinder pressure trajectory, $T_{in} = 300\text{ K}$, PHI = 0.33

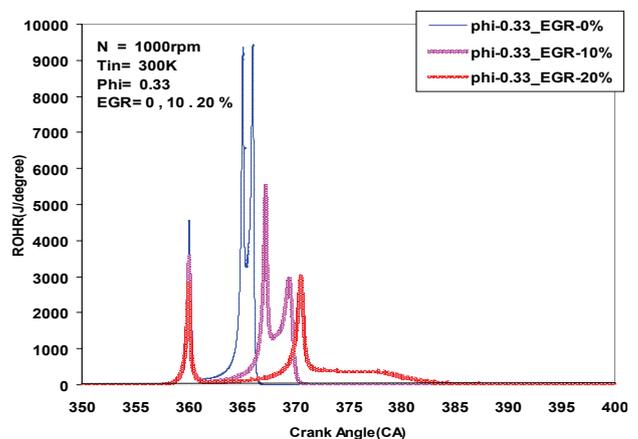


Fig. 9. Effect of various EGR amount on ROHR where $T_{in} = 300\text{ K}$ and PHI = 0.33

TABLE 4. Effect of EGR amount on performance characteristics where $T_{in} = 300 \text{ }^\circ\text{K}$ and $\text{PHI} = 0.33$

PHI = 0.33	Pmax	Max dp/dtheta	Theta Pamx	T max	Start of LTR	Start of HTR	Imep	Isfc	NOx	Ipower
% EGR	bar	bar/CA	ATDC	K	ATDC	ATDC	Bar	g/kWh	ppm	kW
0	71.6	24	8	1765	-2	4	6.2	226	0.35	50.1
10%	65	14.5	10	1685	-2	5	5.5	228	0.04	43.2
20%	52	10	14	1465	-2	7	4.8	232	7e-4	38.7

8. Conclusions

The result is summarized as follows:

- The first step pressure rise in the DME HCCI combustion is due to strong low temperature kinetics reaction which can also be finding in HCCI operation of other diesel surrogate fuels.

- Higher initial temperature advances the beginning of the first stage of heat release significantly by low temperature reactions and consequently advances the start of auto ignition which proportionally increases the rate of pressure rise within the cylinder.

- At high equivalence ratios, higher IMEP can be achieved with lower mixture temperature at IVC. In the middle range of IMEP, wide range of intake mixture temperature, considering knock and misfire boundaries, can be applied.

- Results show that increasing equivalence ratio has less effect on the onset of the first peak in the ROHR and the timing of the LTR occurs almost at the same crank angle at different DME concentrations, while the time interval between the stages of HR is substantially decreased and the heat release rates can become too high causing serious engine mechanical stresses.

- While EGR can't delay the initiation of cool flame by LTR (the first stage of auto ignition), it significantly delays the bulk combustion by high temperature reactions.

- Increasing the amount of EGR can increase the operating regime between knock and misfire in middle load range (less than 0.35) remarkably.

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Abbreviations

<i>ABDC</i>	:	After Bottom Dead Center,
<i>BBDC</i>	:	Before Bottom Dead Center
<i>HCCI</i>	:	Homogenous Charge Compression Ignition
<i>DME</i>	:	Di-Methyl Ether
<i>EGR</i>	:	Exhaust Gas Recirculation

<i>ROHR</i>	:	Rate of Heat Release
<i>HTR</i>	:	High Temperature Reaction
<i>LTR</i>	:	Low Temperature Reaction
<i>Imep</i>	:	Indicated Mean Effective Pressure

Nomenclature

<i>A</i>	:	Arrhenius coefficient
<i>A</i>	:	Third-body coefficient
<i>C_v</i>	:	Specific heat in constant volume
<i>E</i>	:	Activation energy
<i>f</i>	:	forward
<i>K</i>	:	Rate constant
<i>N_s</i>	:	Total umber of chemical species
<i>n_i</i>	:	Number of moles of each species
<i>Q</i>	:	Heat transferred via system boundaries
<i>T</i>	:	Time, unspecific internal energy
<i>X</i>	:	Mole fraction
<i>B</i>	:	Arrhenius coefficient
<i>γ</i>	:	Specific heats ratio
<i>ν'</i>	:	Forward stoichiometric coefficient
<i>ν''</i>	:	Reverse stoichiometric coefficient
<i>ω_i</i>	:	Production rate,
<i>f</i>	:	Forward
<i>i</i>	:	Species index
<i>K</i>	:	Reaction index
<i>mot</i>	:	Motoring
<i>R</i>	:	Reverse

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