

# Performance and Combustion Characteristics Analysis of HCCI Engine Operation with Diesel Like Fuels

N. Shahangian<sup>1\*</sup>, M. Keshavarz<sup>1</sup> and S.A.Jazayeri<sup>2</sup>

<sup>1</sup> Iran Heavy Diesel Engine. Mfg.Co(DESAs), Performance Analysis Department, 83 Vahid Dastgerdi St, Tehran - Iran  
<sup>2</sup> Khaje Nasir Toosi University of Technology, Pardis St, Vanaq Sq, Tehran - Iran  
e-mail: navid.shahangian@gmail.com - keshavarz@d87.ir - jazayeri@kntu.ac.ir

\* Corresponding author

**Résumé — Analyse de performance et caractéristiques de combustion du moteur HCCI avec les carburants similaires au gasoil** — La technologie HCCI est considérée comme une solution prometteuse pour réduire les émissions de polluants, mais seuls quelques prototypes expérimentaux exploitent ce concept. Dans la combustion HCCI de DME et *n*-heptane, on distingue deux phases de réaction d'allumage, la première à plutôt basse température et la deuxième à haute température. La seconde est responsable de l'essentiel des pertes thermiques. Dans cette étude, un modèle adimensionnel et thermocinétique de combustion à une zone est développé. Le logiciel MATLAB est utilisé pour prédire les caractéristiques des moteurs HCCI utilisant deux types de carburants diesel : le diméthylether et le *n*-heptane. Les effets de la température et de la pression d'admission, de la prise en charge des carburants et de l'addition des gaz EGR sur les caractéristiques de l'auto-allumage l'optimum de la combustion et les performances des moteurs HCCI ont été considérés.

**Abstract — Performance and Combustion Characteristics Analysis of HCCI Engine Operation with Diesel Like Fuels** — HCCI is considered a very promising solution to reduce engine pollutant emissions, however so far only experimental prototypes have been inspired by this concept. HCCI combustion of both DME and *n*-heptane fuels display a distinct two-stage ignition reaction with the first stage taking place at fairly low temperatures and the second stage taking place at high temperatures. The second stage is responsible for the main stage of the heat release process. In this study, a single-zone, zero-dimensional, thermo-kinetic combustion model has been developed. MATLAB software is used to predict engine performance characteristics of HCCI engines using two types of diesel fuel: Dimethyl ether and *n*-heptane. The effects of intake temperature and pressure, fuel loading and addition of EGR gases on auto-ignition characteristics, optimum combustion phasing, and performance of the HCCI engines are considered in this study.

## INTRODUCTION

The Homogeneous Charge Compression Ignition (HCCI) engines have been vigorously studied in the last decade because of their high thermal efficiency and ultra low NO<sub>x</sub> and particulate matter (PM) emissions in comparison with the SI (Spark Ignition) and CI (Compression Ignition) engines [1].

The basic idea is to employ a sufficiently lean premixed air-fuel mixture to keep flame temperatures below 1900 K to keep NO<sub>x</sub> and particulate production low. Despite this potential advantage, there are some problems with HCCI combustion such as controlling burn rate, excess rate of heat release at high loads, excess CO and UHC emissions particularly at partial loads, and difficulty with cold start. For lean burn operation, the production of NO<sub>x</sub> in HCCI engines has been reported to be under 10-ppm and these engines have shown higher thermal efficiency than the conventional engines [2]. Various types of fuels have been examined in so many research reports using detailed chemical kinetics computation for the HCCI engine operation [3] such as *n*-Butane/dimethyl ether [4], iso-octane and *n*-heptane [5-10].

Studies on reaction kinetics of dimethyl ether have been conducted in a shock tube, which is a constant volume apparatus [11]. Also to study the oxidation of *n*-heptane, experimental results of ignition behind reflected shock waves and in a rapid compression machine were used to develop and validate the reaction mechanism of *n*-heptane at both low and high temperatures [12].

Many studies on dimethyl ether as an alternative fuel or additives to base fuel have shown that the use of ether may help the simultaneous reduction of both NO<sub>x</sub> and particulate matters in diesel engines [13]. This is attributed to its high oxygen content and absence of carbon-carbon bonds. The HCCI combustion process is dependent on chemical reactions and it is not easy to control the auto-ignition process under different load and engine speed conditions. HCCI combustion of both DME and *n*-heptane, display a distinct two-stage ignition reaction. The first stage is associated with low temperature reactions (LTR) and releases a relatively small amount of energy. The second stage associated with high temperature oxidation releases most of the energy and is considered as the main Combustion Stage (MCS).

*N*-heptane has a cetane number equal to most common diesel fuels and has similar ignition characteristics. So to compare the performance and combustion characteristics of a diesel fuel with DME, *n*-heptane mechanism was used which has been developed and tested through extensive comparisons between computed and experimental data [12]. And all chemical processes important in diesel ignition have been validated for this fuel.

In this paper a single-zone detailed chemistry combustion model has been implemented into a 4-stroke engine fueled with both DME and *n*-heptane. Cantera [14], which is an open-source object oriented software package for problems

involving chemically reacting flows and has an interface with MATLAB, is used to predict engine performance characteristics.

First the analysis result is compared to the experimental one in terms of pressure trajectory and also the significance of the cool flame combustion heat release in comparison to the main one for both fuels. Then the effects of equivalence ratio, intake temperature and pressure, and EGR on the characteristics of auto-ignition and its different stages by low and high temperature reactions, rate of heat release, performance and operating regime of the HCCI engines are investigated and presented in detail.

## 1 MODEL DESCRIPTION

In this study a single-zone model, which uses CANTERA library for calculation of the time evolution of the homogeneous reacting gas mixture in the combustion chamber, has been developed to study engine performance and auto-ignition characteristics of the DME and *n*-heptane oxidation. This is because of the simplicity of zero-dimensional model and its ability to predict overall performance characteristics of the HCCI engines [15-17].

## 2 MODELING APPROACH

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 summarized as:

$$\dot{Q} - p \frac{dV}{dt} = \sum_{i=0}^s \bar{u}_i \frac{dn_i}{dt} + n \sum_{i=0}^s n_k \frac{d\bar{u}_k}{dt} \quad (1)$$

From conservation law of chemical species:

$$\frac{d[x_k]}{dt} = \dot{w}_k - \frac{[x_k]}{V} \frac{dV}{dt} \quad (2)$$

The pressure is found from the ideal gas law:

$$p = \left( \sum_{k=1}^s [x_k] \right) \bar{R}T \quad (3)$$

To present the variation of mixture temperature:

$$\frac{dT}{dt} = \frac{\dot{Q} - \left( \sum_{k=1}^s [x_k] \bar{R}T \right) \frac{dV}{dt} - V \sum_{k=1}^s u_k \dot{w}_k}{V \sum_{k=1}^s [x_k] \bar{C}_{v,k}} \quad (4)$$

Combination of the above equations results in a system of ordinary differential equations. The unknowns in Equation (4) 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.

### 2.1 Chemical kinetics model

The production rate of each species is calculated according to:

$$\dot{w}_i = \sum_{k=1}^{N_r} (v_{i,k}'' - v_{i,k}') (PR)_k \quad (5)$$

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

$$(PR)_k = K_{f,k} \prod_{i=1}^{N_s} [x]_i^{v_{i,k}'} - K_{r,k} \prod_{i=1}^{N_s} [x]_i^{v_{i,k}''} \quad (6)$$

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

$$K_k = A_k T^{\beta_k} \exp\left(\frac{-E_k}{R_u T}\right) \quad (7)$$

All the above equations related to chemical kinetics and rate expressions are derived from Chemkin Theory Manual [20].

The Arrhenius constants for both forward and reverse reactions and thermodynamic properties of each species are from LLNL combustion Chemistry Group [11, 12, 21]. The data obtained from the website are believed to be reliable. The mixture gas-constant is calculated by Cantera as a function of the mixture composition.

The detailed mechanism of DME oxidation considering upwards of 354 reactions and 82 species, and reduced mechanism of *n*-heptane oxidation made up of 770 reversible elementary reactions among 159 species have been used to predict oxidation process of the fuels using the Cantera package. Free cost availability of the Cantera software makes it a suitable alternative compared to the costly CHEMKIN package.

### 2.2 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 because of its simplicity and wide acceptance [22].

The empirical constants of Woschni equation in this study have been derived from Reference [22].

$$h = 129.8 B^{-0.2} p^{0.8} T - 0.55 (2.28 S_p + f(p))^{0.8} \quad (8)$$

$$f(p) = 3.34 \times 10^{-4} \frac{V_d T_r}{p_r T_r} (p - p_{mot}) \quad (9)$$

The motored pressure is derived from following differential equation:

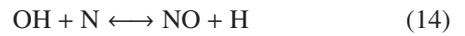
$$\frac{dp_{mot}}{dt} = \frac{\gamma_{mot} - 1}{V} \frac{dq_{ht,mot}}{dt} - \gamma_{mot} \frac{p_{mot}}{V} \frac{dV}{dt} \quad (10)$$

Finally, the cylinder pressure derived from ideal gas law.

$$p = \rho RT \quad (11)$$

### 2.3 NOx formation model

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. In order to model NOx formation for the HCCI combustion, extended Zeldovich mechanism has been used. Extended Zeldovich Mechanism is:



## 3 MODEL VALIDITY

Figures 1 and 2 show the comparison of zero-dimensional thermo-kinetic model with experimental results conducted on the engines fuelled with DME [15] and *n*-heptane [6], respectively. Table 1 shows the specifications of the engines used in relevant references.

The predicted pressure by the single-zone HCCI model is rather larger than the actual measurement and the maximum pressure occurs earlier. The difference is related to the zero-dimensional model, which can't take into account in cylinder temperature and mixture distributions that caused all chemical species in the cylinder to react instantaneously. The calculated ignition timing, however, agrees well with the measured result as shown in Figures 1 and 2.

TABLE 1  
Specification of the engine used in References [6, 15]

Specification	Engine 1	Engine 2
Bore (mm)	115	82.55
Stroke (mm)	115	114.3
Compression ratio	17.0:1	10.0:1
Intake valve close	45 CA ABDC	36 CA ABDC
Exhaust valve open	55 CA BBDC	40 CA BBDC
Speed (rpm)	1400	600

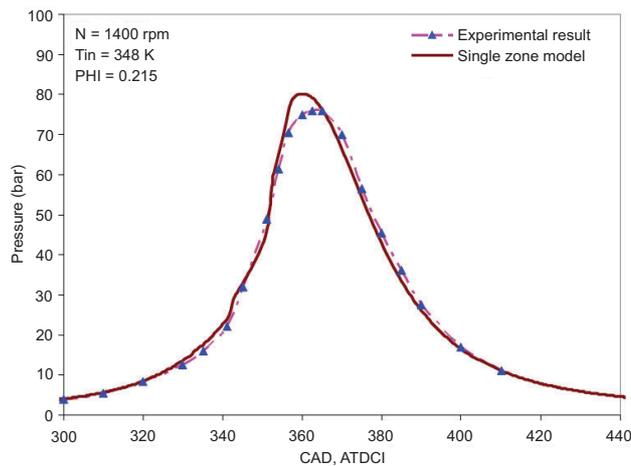


Figure 1

Comparison of pressure profiles using DME fuel.

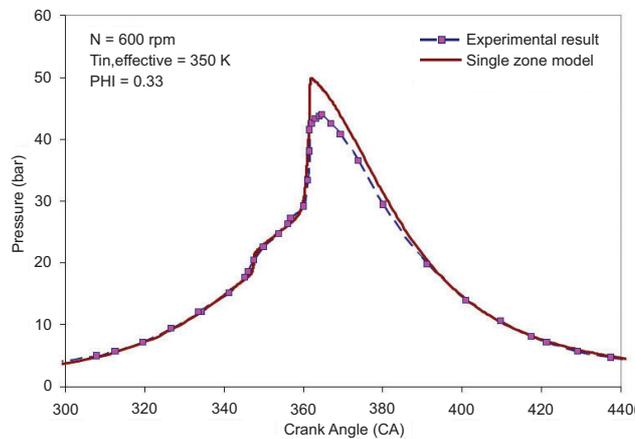


Figure 2

Comparison of pressure profiles using *n*-heptane fuel.

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 [15]. The difference between experimental result and the calculated pressure trajectory by single-zone model in the first step pressure rise can be explained by inhomogeneities of temperature distribution within the cylinder in real engine operating conditions [12, 13]. So the model can be used for investigation of performance analysis, combustion characteristics, and evaluation of HCCI combustion.

The specification of the RK215 industrial heavy-duty diesel engine, which is considered for calculating the results of the single-zone HCCI model, is summarized in Table 2. For knock phenomenon consideration, maximum rate of

pressure rise per crank angle ( $dp/d\Theta$ ) has been assumed 20 bars per crank angle [24, 25].

TABLE 2

Specification of the considered diesel engine

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

### Oxidation mechanism

HCCI combustion of most diesel-like fuels display a distinct two-stage heat release. In the first stage of combustion the first peak of heat release will appear which is described by low temperature chemical reactions. High temperature chemical reactions, which are responsible for the main heat release, follow the low temperature reactions. At lower temperatures, degenerative chain branching process controls ignition process. Figures 3 and 4 show the changes in temperature, rate of heat release and rate of pressure rise of DME and *n*-heptane modeled by single-zone model where  $\text{PHI} = 0.25$  and  $T_{in} = 330$  K. In this paper, all initial conditions of the mixture have been considered at intake valve close (IVC) situation.

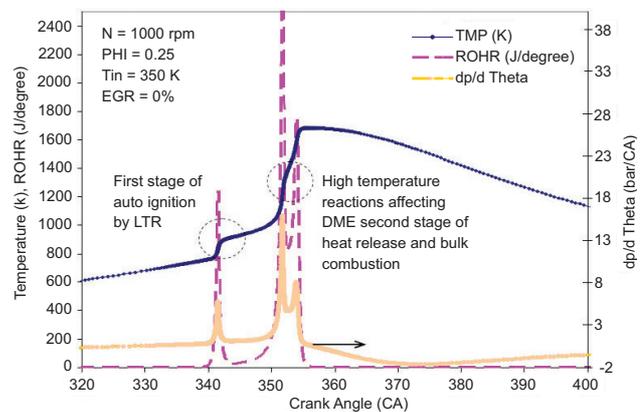


Figure 3

Temperature trajectory, rate of heat release and rate of pressure rise for DME oxidation where  $T_{in} = 330$  K and  $\text{PHI} = 0.25$ .

Results show that for the same initial conditions, DME present higher ROHR especially in the first stage of heat release by LTR and the maximum rate of pressure rise for this oxygenated fuel raises up to 15 bar/CA while this value is restricted to 5 bar/CA for *n*-heptane.

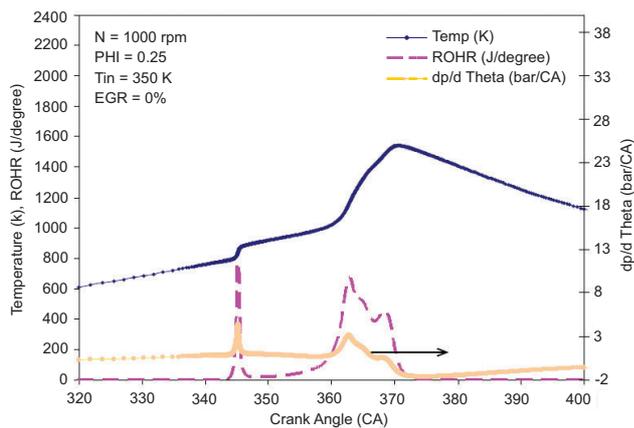


Figure 4  
Temperature trajectory, rate of heat release and rate of pressure rise for *n*-heptane oxidation where PHI = 330 K and PHI = 0.25.

Heat release curve of DME and *n*-heptane oxidation is the result of two-stage auto-ignition: low temperature reaction (LTR) and high temperature reaction (HTR). LTR appears in the range of 750-800 K and HTR above 1000 K. In the LTR region the concentrations of CH<sub>2</sub>O, CO, and H<sub>2</sub>O<sub>2</sub> are increased [15], also the three-stage heat release is the result of higher initial temperature, which corresponds to hot flame combustion.

There is a period in conversion of LTR and HTR with negative-temperature-coefficient region (850-1000 K) called NTCR [26]. When the temperature increases above 1000 K, HTR is dominant which is divided in two stages. First stage of HTR is controlled by hydrogen peroxide decomposition, which is the main source of OH in the HTR.

The heat release rate of the second stage of the HTR is dominated by oxidation process of CO to CO<sub>2</sub>. At temperatures exceeding about 1400 K, exothermic oxidation reaction of OH and CO occurs. Thus at lean concentration of the fuels and low incylinder temperature, CO can't be completely converted to CO<sub>2</sub> [15, 26].

#### 4 ENGINE OPERATING CHARACTERISTICS ASSESMENT

In this section the effect of initial temperature and pressure, equivalence ratio, and EGR on combustion characteristics and operating regime of HCCI engine powered with DME are investigated. In all cases the temperature, equivalence ratios and the amount of residual gases in intake valve close (IVC) situation have been assumed as the initial conditions. Figures 5 and 6 show the effect of initial temperature of the mixture on cylinder pressure and heat release rate using DME. Figures 7 and 8 also show the effect of using different charge temperature on pressure trajectory and rate of heat release, respectively.

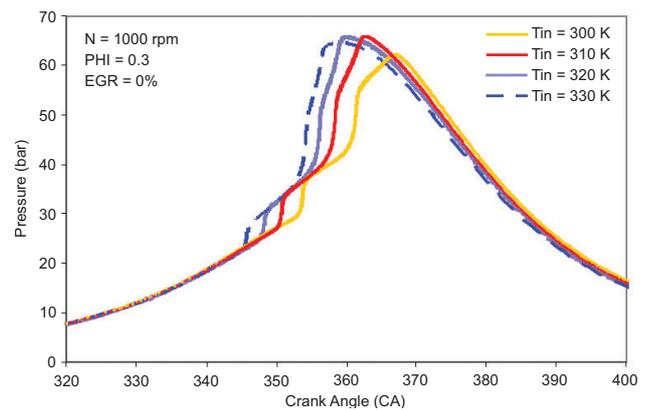


Figure 5  
Effect of initial temperature of the mixture on pressure trajectory where PHI = 0.3 for DME.

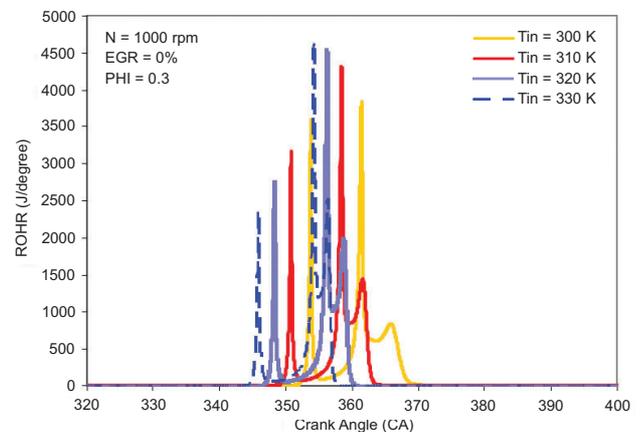


Figure 6  
Effect of initial temperature of the mixture on rate of heat release where PHI = 0.3 for DME.

It can be clearly seen that increasing initial temperature significantly advances the beginning of LTR for both fuels and consequently advances the start of auto-ignition which enhances maximum pressure of the cylinder and the heat release rate.

Figure 9 shows the effect of different charge temperature on maximum rate of pressure rise for both fuels. At lower charge temperature values at IVC, maximum rate of pressure rise is strongly affected by low temperature reaction. This affects the first stage of heat release causing a step pressure rise at lower IMEP. But at higher initial temperatures where higher IMEP is achievable, HTR strongly affects the second stage of pressure rise during bulk combustion.

Tables 3 and 4 show the effect of four different initial temperatures of the mixture on performance characteristics of HCCI engine for PHI = 0.3 for DME and *n*-heptane, respectively.

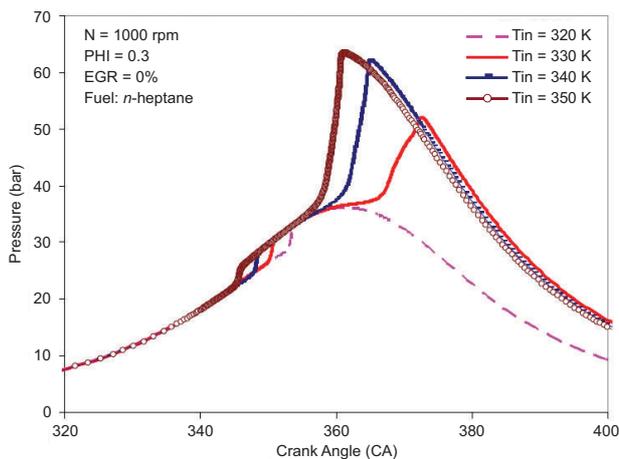


Figure 7  
Effect of different charge temperature on pressure trajectory for *n*-heptane.

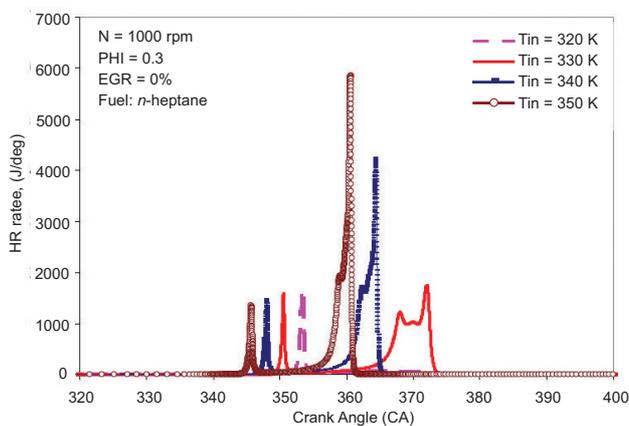


Figure 8  
Effect of initial charge temperature on rate of heat release for *n*-heptane.

In these tables the regions with maximum power ratios have been presented so the values related to lower initial temperatures, which show incomplete combustion and lower thermal efficiency, are avoided. It can be concluded that increasing initial temperature significantly increases the rate of heat release and maximum temperature of the cylinder for both fuels. In the case of DME, when increasing the initial temperature from 300 to 330 K, the rate of pressure rise is increased up to 17.5 bar/CA.

When the initial temperature is lower than 300 K, the maximum incylinder temperature is not sufficient to complete the oxidation of CO to CO<sub>2</sub> so incomplete combustion takes place. This is because only at temperatures exceeding 1400 K can the CO be oxidized to CO<sub>2</sub> in hot-flame combustion [15]. The last of three peaks on the ROHR curve is also caused by CO oxidation [27]. In the case of *n*-heptane

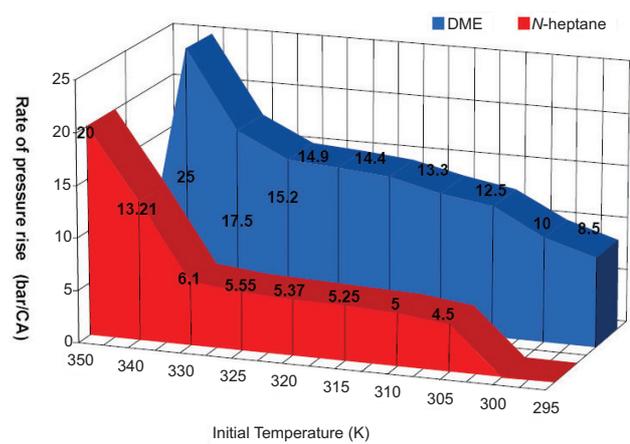


Figure 9  
Rate of pressure rise while using DME and *n*-heptane.

higher initial temperature should be applied to trigger the second stage of heat release by HTR.

TABLE 3

Effect of initial temperature on performance characteristics while using DME where PHI = 0.3

T0 (K)	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Start of LTR (ATDC)	Imep (bar)	Ipower (kW)
300	63	10	1600	-6	4.6	39
310	65.5	13.3	1650	-9	4.34	36.13
320	67	15	1690	-12	4.09	34.05
330	69	17.5	1700	-15	3.9	32

TABLE 4

Effect of initial temperature on performance characteristics while using *n*-heptane where PHI = 0.3

T0 (K)	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Start of LTR (ATDC)	Imep (bar)	Ipower (kW)
325	36.32	5	1200	-9	3.03	25.21
330	52	6.1	1630	-9.5	4.33	36.09
340	62.1	13.21	1722	-12	4.15	34.58
350	63.37	20	1758	-14.5	3.93	32.77

Figures 10 and 11 show the cylinder pressure and heat release rate with different equivalence ratios for initial temperature of 300 K and initial pressure of 100 kPa for DME.

It can be seen that increasing equivalence ratio has minor effect on the onset of the first peak in the ROHR and initiation of LTR for both fuels. The onset of the second peak in the ROHR is advanced significantly and the equivalence ratio, in which the first stage of ignition timing is near TDC, is larger. Figures 12 and 13 show the effect of different equivalence ratios on pressure and ROHR diagram while using *n*-heptane as the fuel.

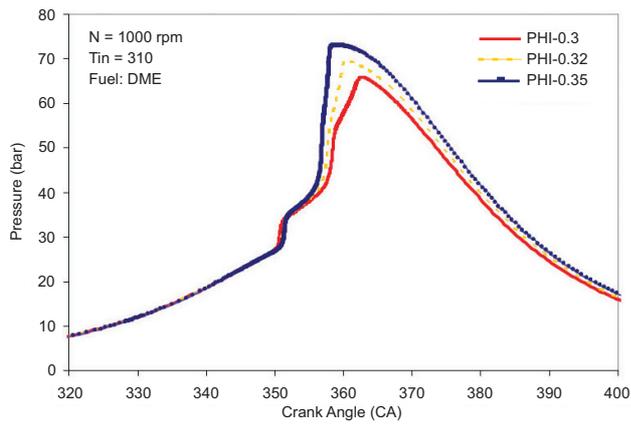


Figure 10  
Effect of different equivalence ratio on pressure trajectory where  $T_{in} = 310$  K while using DME as the fuel.

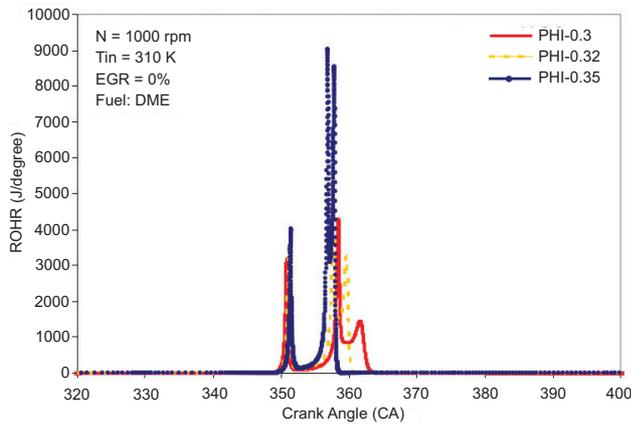


Figure 11  
Effect of different equivalence ratios on the rate of heat release where  $T_{in} = 310$  K while using DME as the fuel.

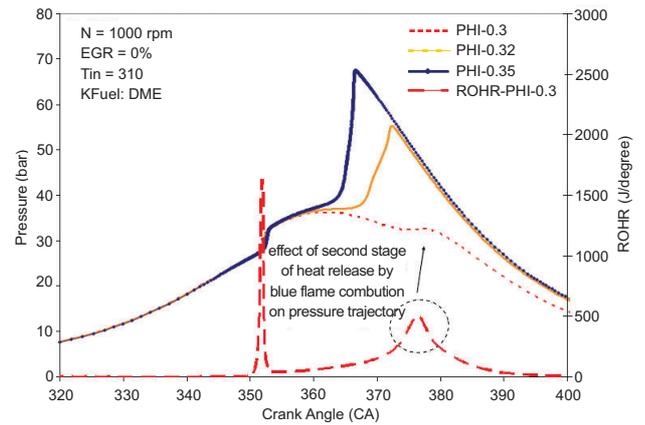


Figure 12  
Effect of different equivalence ratio on pressure trajectory where  $T_{in} = 325$  K while using *n*-heptane as the fuel.

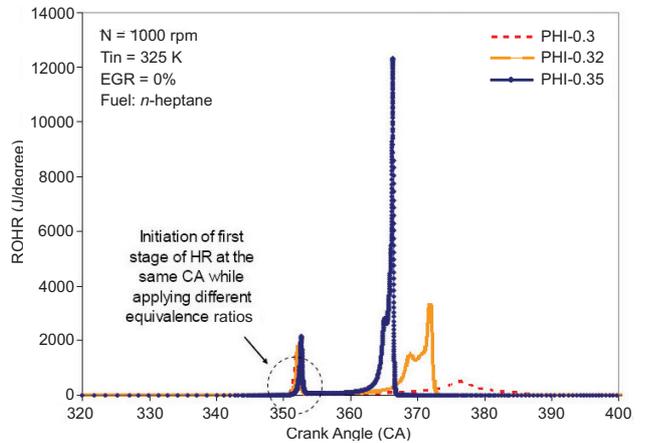


Figure 13  
Effect of different equivalence ratio on ROHR where  $T_{in} = 325$  K while using *n*-heptane as the fuel.

Comparing the results it can be concluded that the NTCR region in the case of *n*-heptane is obviously affected by equivalence ratio and longer ignition delay between two stages of HR is seen for this fuel. DME fuel, however, is less sensitive to the equivalence ratio variation but with increasing the value of Phi, 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. Tables 5 and 6 show the effects of various equivalence ratios on performance characteristics of HCCI engines fueled with DME and *n*-heptane where initial temperature is 310 K and 325 K, respectively.

Results of the DME fuel suggest that at equivalence ratios more than 0.32, where  $T_{in} = 310$  K, engine tends to knock. However, at this initial temperature, the maximum rate of

TABLE 5  
Effects of various equivalence ratios on performance characteristics of HCCI engine where  $T_{in} = 310$  K while using DME

PHI	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Start of LTR (ATDC)	Imep (bar)	Ipower (kW)
0.3	65.9	13.8	1630	-10	4.34	36.13
0.32	70	15.2	1700	-11	4.63	38.57
0.35	73.5	28	1820	-11	6	43

pressure rise for a maximum equivalence ratio of 0.35 would be 5 bar/CA for *n*-heptane fuel. So higher initial temperatures for achieving complete combustion and higher IMEP should be considered for this alkane fuel.

In the case of DME fuel, at high equivalence ratios (*e.g.* 0.38) with the same initial temperature of 310 K, the rate of pressure rise would reach as high as 40 bars per crank angle and the maximum temperature of the cylinder exceeds

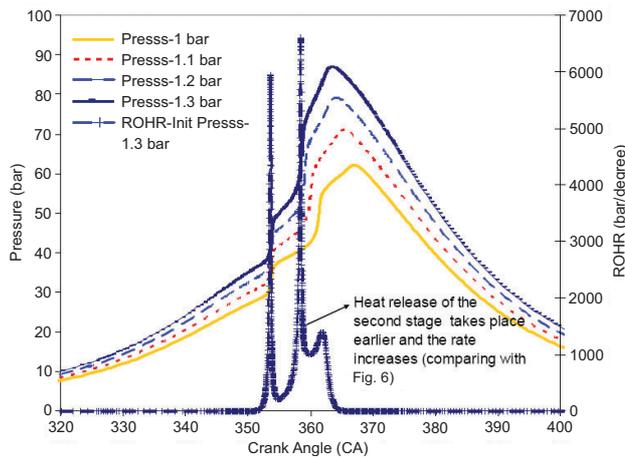


Figure 14  
effect of different boost pressure on pressure trajectory for DME fuel where  $\text{PHI} = 0.3$ ,  $T_{in} = 300 \text{ K}$  for DME fuel.

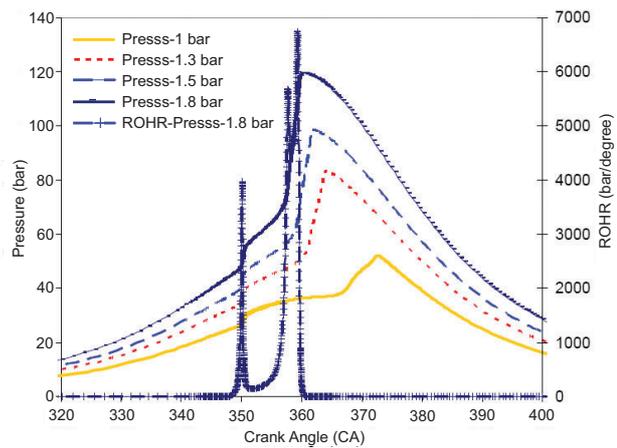


Figure 15  
Effect of different boost pressure on pressure trajectory for *n*-heptane where  $\text{PHI} = 0.3$ ,  $T_{in} = 330 \text{ K}$ , for *n*-heptane.

1900 K. Consequently, this point can't be considered as an operating point for the engine.

TABLE 6

Effects of various equivalence ratios on performance characteristics of HCCI engine where  $T_{in} = 325 \text{ K}$  while using *n*-heptane

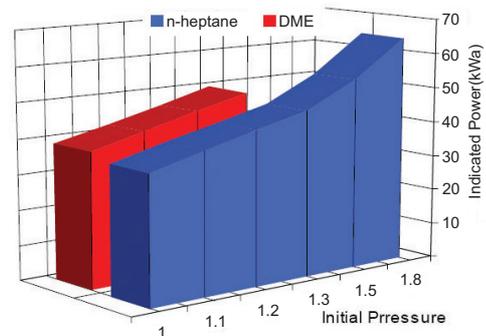
PHI	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Start of LTR (ATDC)	Imep (bar)	Ipower (kW)
0.3	36.32	4.45	1200	-9.5	3.03	25.21
0.32	39.5	5.5	1690	-10	4.71	40
0.35	67.42	21.5	1822	-10	5.2	43

Also at equivalence ratios less than 0.25, the rate of pressure rise would be less than 5 bars per crank angle and the maximum in cylinder temperature (less than 1200 K in this case) wouldn't be enough for CO oxidation. Incomplete combustion occurs and, consequently, power output is decreased.

At low loads, the fuel consumption will suffer due to the poor combustion efficiency and improper combustion phasing. To achieve higher Imep at low loads, increasing initial pressure is proposed. Figures 14 and 15 show the effect of various boost pressure on pressure trajectory for DME and *n*-heptane fuels for initial temperature values of 300 K and 330 K, respectively.

Figure 15 shows the effect of applying different boost pressure on Indicated power for both DME and *n*-heptane. For both fuels the knock limitation for evaluating the values have been considered.

Results show that increasing intake pressure values don't have any significant effect on first stage of heat release by LTR, but HTR is advanced [13] and the rate of heat release is enhanced greatly with higher boost pressures.



	1	1.1	1.2	1.3	1.5	1.8
n-heptane	36.097	39.92	43.55	47.134	54.235	64.83
DME	38.268	42.029	45.78	49.53		

Figure 16  
Effect of applying different boost pressure on Ipower for DME at 300 K and *n*-heptane at 330 K where  $\text{PHI} = 0.3$ .

Figure 16 shows that, in the case of DME where the initial temperature is 300 K, the maximum allowable initial pressure would be less than 1.5 bars. For *n*-heptane, the boost pressure is restrained to less than 1.8 bars where the initial temperature is 330 K. Out of these regions the rate of pressure rise per crank angle would increase to over 20 bar/CA which for both fuels is an indication of knock phenomenon.

Tables 7 and 8 show the effect of different boost pressure on performance characteristics of HCCI engine for DME and *n*-heptane fuels, respectively.

It can be investigated that higher Imep is achievable at higher boost pressures of the mixture, and for the case of DME, the effect of boost pressure on the second stage of pressure rise is stronger. So after 0.3 bar additional pressure the rate of pressure rise would increase up to 20 bar/CA,

TABLE 7

Effect of different boost pressure on performance characteristics where PHI = 0.3 and Tin = 300 K for DME

Pressure (bar)	Max Pressure (bar)	Max dp/d Theta (bar/CA)	Max Temp (K)	Imep (bar)	Ipower (kW)
1	64.1	8	1650	6.04	50.3
1.1	74.1	14.1	1680	6.68	55.6
1.3	90.4	20	1690	7.91	60.59

TABLE 8

Effect of different boost pressure on performance characteristics where PHI = 0.3 and Tin = 330 K for n-heptane

Pressure (bar)	Max Pressure (bar)	Max dp/d Theta (bar/CA)	Max Temp (K)	Imep (bar)	Ipower (kW)
1	52	5	1630	4.33	36
1.3	83.5	10	1712	5.66	55.6
1.8	119.5	20	1732	7.91	60.59

which shows the sensitivity of this oxygenated fuel to charge pressure ratio.

But n-heptane is less sensitive to boost pressure, so higher level of pressure ratio can be applied for this alkane fuel, e.g., 1.8 bar in this case when considering knock limitation.

Another parameter that can affect the combustion phasing is the amount of EGR. 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" [28].

In addition to the thermal effect, the inert gases contained in the EGR can be used to control the heat release rate due to its impact on chemical reaction rate, which can delay the second stage of auto-ignition, reduce the heat release rate, and thus lower peak cylinder pressure [29].

Increasing the EGR amount causes the decrease of oxygen in the mixture that can lower the rate of heat release. The rate of low temperature chain branching reaction then becomes lower due to decrease in oxygen amount [25]. Also, the mean specific heat of the mixture with EGR is higher than the one with no EGR. This enhances the above point and these two factors together delay bulk combustion [30,31].

Figures 17, 18, and 19 show the variation of cylinder pressure, cylinder temperature and heat release rate with three EGR amounts where phi = 0.33 and Tin = 315 K for DME fuel.

These figures show that increasing the amount of EGR leads to extension of heat release rate duration and, therefore, operating regime in which more initial temperature can be used for a constant equivalence ratio to achieve controlled auto-ignition.

Figures 20 and 21 also show the effect of different EGR amount on cylinder pressure and heat release rate respectively for n-heptane where phi = 0.35 and initial temperature is equal to 335 K.

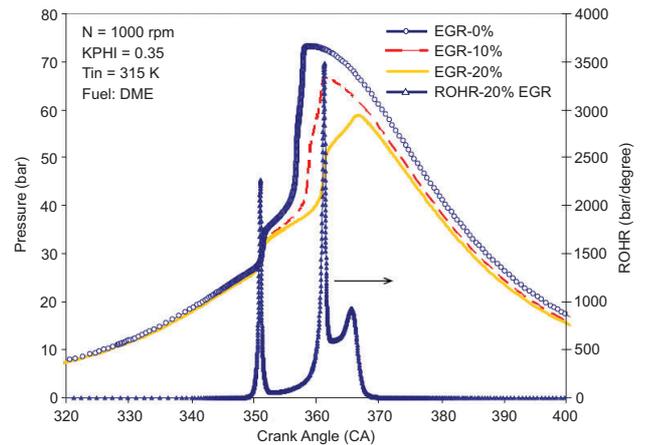


Figure 17

Effect of various EGR amount on in cylinder pressure trajectory where Tin = 300 K and PHI = 0.35.

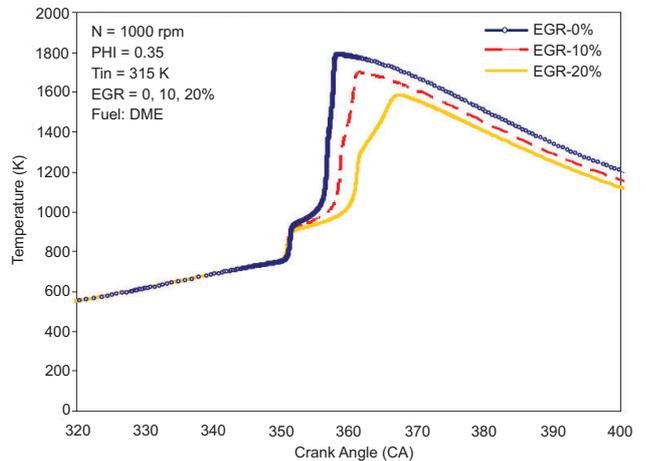


Figure 18

Effect of various EGR amount on in cylinder temperature where Tin = 315 K and PHI = 0.35.

For this alkane fuel the maximum amount of EGR would be restricted to 15% since above this amount the incomplete oxidation of CO in the main stage of HR makes the combustion incomplete. At lower equivalence ratios, e.g. 0.25, for the case of DME, with low intake temperatures, the exothermic oxidation reaction of OH and CO can't be completed and lower power density is achieved.

So for this oxygenated fuel, 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. For both fuels, the first condition with 0% EGR gives over 20 bar/CA rate of pressure rise, so increasing the amount of EGR in both cases, would put these points between the boundaries of knock and incomplete combustion.

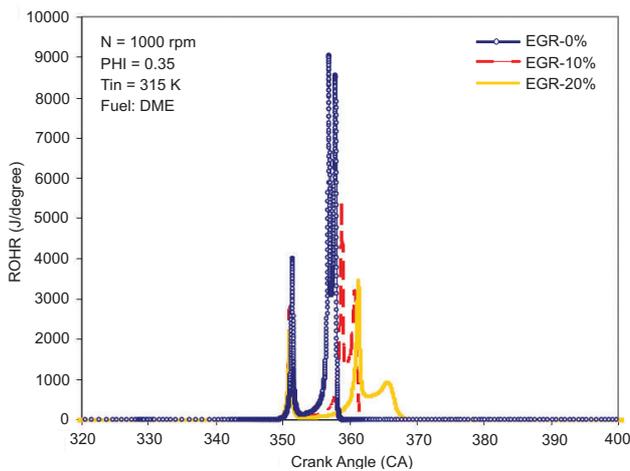


Figure 19

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

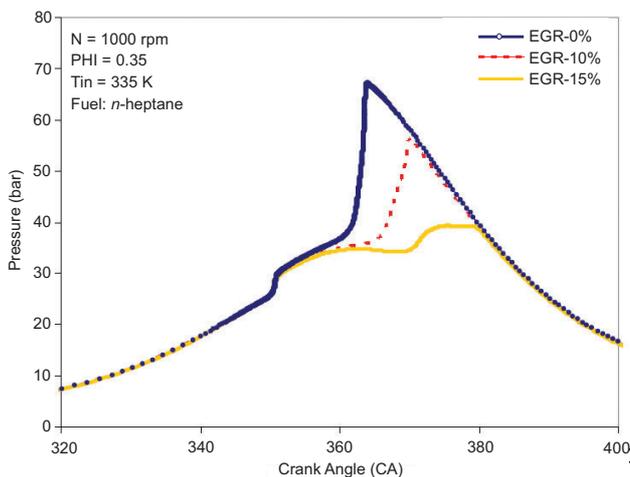


Figure 20

Effect of different EGR amount on pressure trajectory for *n*-heptane fuel.

Table 9 shows the effect of EGR amount on performance characteristics of DME fuel where  $\text{PHI} = 0.35$  and  $T_{in} = 315$  K. The results show that increasing the amount of EGR by 20% will reduce the cylinder pressure by up to 30 percent and the rate of pressure rise by up to 63%.

Results show that when the amount of EGR or trapping residual gases in to the combustion chamber is increased by 20%, the maximum in cylinder temperature is reduced up to 11% showing significant effect on thermal  $\text{NO}_x$  emission production.

Once knocking occurs, the exhaust  $\text{NO}_x$  will increase sharply which is shown in the first case where  $\text{PHI} = 0.35$ ,  $T_{in} = 315$  K, and  $\text{EGR} = 0\%$ . When the engine is working

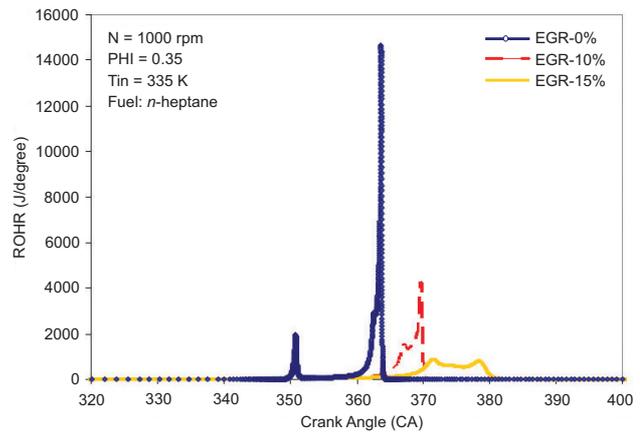


Figure 21

Effect of EGR amount on ROHR for *n*-heptane.

TABLE 9

Effect of EGR amount on performance characteristics where  $T_{in} = 315$  K and  $\text{PHI} = 0.35$  for DME fuel

PHI, 0.35 (EGR %)	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Imep (bar)	Ipower (kW)
0	74	30	1827	5.07	42.2
10	66	18	1700	4.7	39.5
20	58.7	11	1580	4.3	36.5

TABLE 10

Effect of EGR amount on performance characteristics where  $T_{in} = 335$  K and  $\text{PHI} = 0.35$  for *n*-heptane fuel

PHI, 0.35 (EGR %)	Pmax (bar)	Max dp/d Theta (bar/CA)	Tmax (K)	Imep (bar)	Ipower (kW)
0	66.9	26.5	1847	5.047	42.2
10	56.3	11.2	1715	4.64	39.5
20	40	6	1550	4.39	36.5

at higher EGR amounts,  $\text{Imep}$  and engine power density are decreased and an increase in the amount of  $\text{I}_{sc}$  is predicted.

Table 10 shows the effect of different EGR amount on performance and combustion characteristics of HCCI engine fuelled with *n*-heptane where  $\text{PHI} = 0.35$  and  $T_{in} = 335$  K. Figures 19 and 20 show that amount of EGR does not have any significant effect on the first stage of heat release, but the maximum rate of heat release is decreased remarkably for both cases. 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 [30].

Figures 22 and 23 show the effect of different amount of EGR, temperature and equivalence ratios on  $\text{IMEP}$  for DME and *n*-heptane fuels, respectively. Increasing the equivalence ratio causes the engine to go toward the uncontrolled auto-ignition.

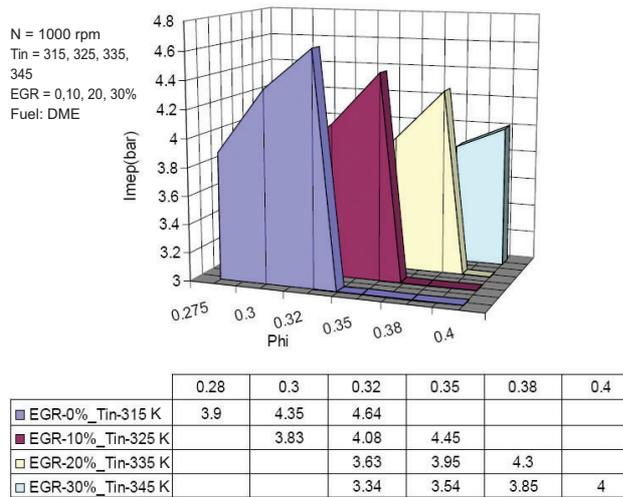


Figure 22  
Effect of various amount of EGR on extending the operating regime for DME.

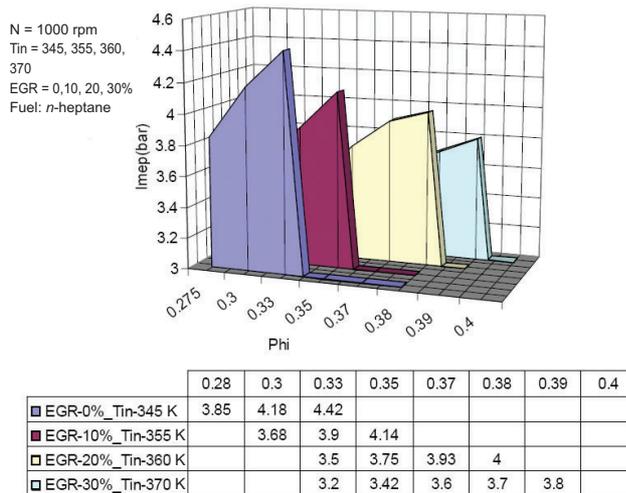


Figure 23  
Effect of various amount of EGR on extending the operating region for n-heptane.

These figures further show that increasing the amount of EGR would increase the operating region between knock and misfire specially at higher phi values when considering higher initial temperatures. But the needed initial temperature is elevated with increasing the amount of EGR.

### CONCLUSION

The results could be summarized as follows:

- The first inflection in the calculated pressure trajectory of both DME and n-heptane is due to strong low temperature kinetics reaction of HCCI combustion of diesel surrogate

fuels. Results show that the role of cool flame in HCCI operation of DME is much stronger than n-heptane.

- At the same equivalence ratio, increasing initial charge temperature affects the first step of pressure rise in DME oxidation more strongly. A gradual increase in the rate of pressure rise is predicted in the case of n-heptane, and after reaching a certain temperature, the rate of pressure rise would increase drastically.
- Result show that, HCCI combustion with DME fuel is less sensitive to the variation of phi but with increasing the value of Phi, 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.
- In the middle range of IMEP, wide range of intake mixture temperatures, when considering knock and misfire boundaries, can be applied for both fuels.
- At the same equivalence ratio, higher boost pressures can be applied to n-heptane to achieve higher Imep because the effect of boost pressure on the second stage of heat release is stronger in the case of DME. It was shown that after just 0.3-bar additional charge pressure, the rate of pressure rise increased up to 20 bar/CA, which confirmed the sensitivity of this oxygenated fuel to charge pressure ratio.
- To achieve higher IMEP, using high boost pressure ratios (up to 2 bar) with high amount of EGR (up to 30%) is suggested in the case of DME fueled HCCI engine.
- For DME fuel, with increasing the charge temperature to 65°C and the EGR amount to 30%, up to 4 bars Imep can be achieved.
- For n-heptane higher value of IMEP (up to 4 bar) can be achieved with high level of EGR (up to 30%) with higher equivalence ratio (up to 0.39) and enhanced temperature which reaches up to 370 K.

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