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A COMPUTATIONAL AND EXPERIMENTAL INVESTIGATION OF THE EFFECTS OF SECOND INJECTION TIMING ON A DI-HCCI ENGINE FUELED WITH GASOLINE-ETHANOL BLENDS

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ABSTRACT

In this study, experimental and computational investigation of a homogeneous charge compression ignition (HCCI) combustion engine were carried out using gasoline-ethanol blends and two stage direct injection (TSDI) strategy. First injection was fixed in intake stroke while second injection was varied close to the compression top dead center (TDC). For this reason, a diesel engine was modified to work as an electronically controlled DI-HCCI engine. The test fuels were prepared as pure gasoline and two different gasoline–ethanol blends with 10% (E10) and 20% (E20) of ethanol by mass. CFD simulations were performed using AVL's Fire code and CFD results were compared against the experimental results of the DI-HCCI engine. The effects of various second injection timings on HCCI combustion were investigated at constant engine speed and same energy input conditions for high equivalence ratio conditions. Combustion temperature and NO_x emissions were investigated visually using CFD model results. Both experimental and CFD studies showed that retarding second fuel injection timing reduces the peak in-cylinder pressure and rate of heat release. Combustion phases and NO_x emissions were able to be controlled by changing second injection timing.

INTRODUCTION

HCCI combustion which is consistently being improved and many researchers recently concentrate on its evolution is a candidate of being amongst the future's new engine technologies due to its low NO_x emissions and high thermal efficiency compared to conventional gasoline and diesel engines.

HCCI operation has similarities to both SI and CI combustion modes. The air-fuel mixture is prepared before the compression stroke as in SI engine and the pre-mixed mixture is compressed until the auto-ignition point. In SI engines, premixed charge is ignited by means of a spark plug and combustion takes place as turbulent flame propagation. In CI engines, highly pressurized fuel is injected on compressed air, auto-ignites and combustion proceeds as diffusion flame within the cylinder. In HCCI engines, pre-mixed mixture is prepared as in an SI engine and the whole mixture is ignited by compression as in a CI engine. Hence, HCCI combustion is an auto-ignition combustion and reactions leading to ignition and combustion depends on chemical kinetics of air-fuel mixture [1]. This auto-ignition process is governed by the chemical kinetics of air-fuel mixture. Therefore, there is not a control mechanism to precisely change the ignition timing of HCCI combustion.

HCCI combustion is challenging in terms of controlling auto-ignition timing and combustion phase. Two main parameters concerning the control of both auto-ignition timing and combustion phase are time-temperature history of the cylinder charge and mixture reactivity. The methods that control time-temperature history include intake temperature, intake pressure, variable compression ratio, variable valve timing to implement residual-affected HCCI with rebreathing, re-induction and retention (also known as negative valve overlap-NVO) methods [2], external and cooled EGR and direct injection timing. After the closing of intake valve, time-temperature history and fuel concentration can only be controlled with timing, rate and number of injections. Mixture reactivity can be altered by blending two or more fuels, changing air-fuel ratio, using fuel additives and fuel pre-conditioning.

Combustion phasing can be controlled and emissions can be reduced properly by changing number of injections (single or double) and ratio of the injected fuel amount in different injections. Two stage direct injection (TSDI) strategy allows us to achieve desired fuel/air mixture concentration in the cylinder owing to flexible controlling of fuel injection timing and ratio in DI-HCCI engines. Canakci and Reitz [3] investigated effects of double injection technique on a gasoline DI-HCCI engine

using high intake air temperature and compression ratio (16.1). They concluded that double injection technique was able to control the start of combustion (SOC). In addition, they observed significant reduction in NO_x emissions, as well as high thermal efficiency was obtained by using optimal injection timings and ratios. Das et al. [4] investigated the effects of double injection technique in a single-cylinder diesel DI-HCCI engine by applying pilot injection in intake stroke and main injection close to TDC. They observed that retarding main injection towards compression reduces maximum pressure and retards combustion phase. They also found that NO_x emissions are lower compared to baseline emissions and decreased simultaneously by retarding main injection timing. Marriott and Reitz [5] investigated the effects of injection timing on a gasoline direct injection (GDI) engine with high compression ratio and high intake air temperature without spark assist. They were able to control combustion phasing by changing injection timing from early intake stroke to late compression stroke.

Mixture reactivity in HCCI combustion can be changed by using various fuel mixtures and additives. Alcohols such as methanol and ethanol can be used in engines with high compression ratio and provide higher thermal efficiency since they have higher octane rating than gasoline. Alcohols have great lean burn properties and promise great potential for reducing exhaust gas emissions. They are renewable fuels and can be produced from variety of sources. Therefore, they can stop dependence on fossil fuels. Earl [6] investigated usability of ethanol and methanol in internal combustion engines. He observed that mixtures of ethanol and methanol with gasoline resist more to auto-ignition than pure alcohol and can be used in higher compression ratios. He stated that effect of alcohols on reducing combustion end temperatures causes reduction in NO_x emissions and their higher oxygen content helps to reduce unburned HC (UHC) and CO emissions. Chen et al. [7] investigated the combustion of different blended of ethanol-gasoline mixtures in a high-temperature constant volume vessel using single hole injector and spark plug. They discovered that it gets harder to start combustion and flame propagation becomes more dependent on spark energy as ethanol fraction increases in mixture since ethanol has less lower heating value (LHV) than gasoline. They also revealed that higher latent heat of vaporization of ethanol leaded to decrease combustion temperature and shorten ignition delay time. Zhang et al. [8] investigated the effect of intake air temperature on HCCI combustion characteristics and emissions using ethanol, methanol and gasoline as fuels. They observed that NO_x emissions were almost zero for ethanol and methanol while they increased for gasoline as intake air temperature increases.

HCCI combustion and other combustion phenomena can be examined more in detail by using CFD simulations thanks to its advanced level calculations and giving opportunity to investigate visually. Wang et al**.** [9] conducted a 3D- CFD study of a gasoline HCCI engine with a detailed chemistry model to investigate two-stage injection strategy. They compared single injection with two-stage (split) injection and observed that late injection advances ignition timing and builds a stratified charge in the cylinder which allows controlling ignition timing and combustion rate. Syed et al. [10] analyzed the effect of pressure, temperature, dilution and equivalence ratio on auto-ignition timings of gasoline-ethanol mixtures by using semi-detailed chemical mechanism. They found that auto-ignition timing retarded at low temperatures and advanced at high temperatures as ethanol fraction in the mixture increased. Increase in pressure and equivalence ratio advanced ignition while dilution of mixture retarded ignition. They also observed that ethanol's charge cooling effect influenced auto-ignition timing more dominantly compared to chemical kinetic effects in gasoline-ethanol mixtures. Ghorbanpour and Rasekhi [11] experimentally and computationally investigated the effects of injection timing, air-fuel equivalence ratio, injection rate shape and EGR on HCCI combustion as well as using poor and rich fuel mixture in a diesel engine. They discovered that it is possible to get lower emissions and better performance, and to optimize HCCI combustion by changing all these parameters.

It is seen in the literature that TSDI technique is an effective parameter to control HCCI combustion and alcohol-gasoline fuel blends can be utilized to get better combustion characteristics and lower emissions. However, there are not enough CFD studies about using TSDI technique and ethanol-gasoline mixtures in DI-HCCI engines. In this study, we investigated the effects of second injection timing and gasoline-ethanol blends on DI-HCCI combustion using CFD technique.

EXPERIMENTAL STUDY

In this study, a naturally aspirated, water cooled, single cylinder DI diesel engine was converted to a DI-HCCI engine fueled with 97 octane gasoline and its blends with ethanol. Fuel properties of gasoline and ethanol were evaluated in Alternative Fuels R&D Center at Kocaeli University and can be found in previous study [12]. Test engine specifications are shown in Table 1. Schematic diagram of the test system is shown in Fig. 1. The engine is coupled to a DC electrical dynamometer. K type thermocouples were used during the experiments for measuring intake air, fuel, oil, exhaust gas and cooling water inlet-outlet temperatures. Intake charge temperature was controlled in closed-loop at 100 ± 2 °C to provide steady engine operating conditions. Engine coolant temperature was held at 75 ± 2 °C in order not to exceed maximum pressure rise rate. Air consumption was measured using an orifice-meter and a differential pressure manometer, and an intake surge tank was installed to eliminate cyclic fluctuations.

A water-cooled transducer (Kistler, model 6061B) was installed on cylinder head to measure the cylinder gas pressure. A swirl type, single-hole gasoline direct injector was installed on the cylinder head to inject the fuel. Injection pressure was fixed at 10 MPa by using a low pressure common rail system. First and second injection timings and quantity of fuel per cycle (Q_{cyc}) were controlled by means of a designed electronic control unit, which was synchronized with crank angle sensor.

Exhaust emissions were acquired by two exhaust gas analyzers (Bosch, model BEA 350 for CO and UHC; Bosch,

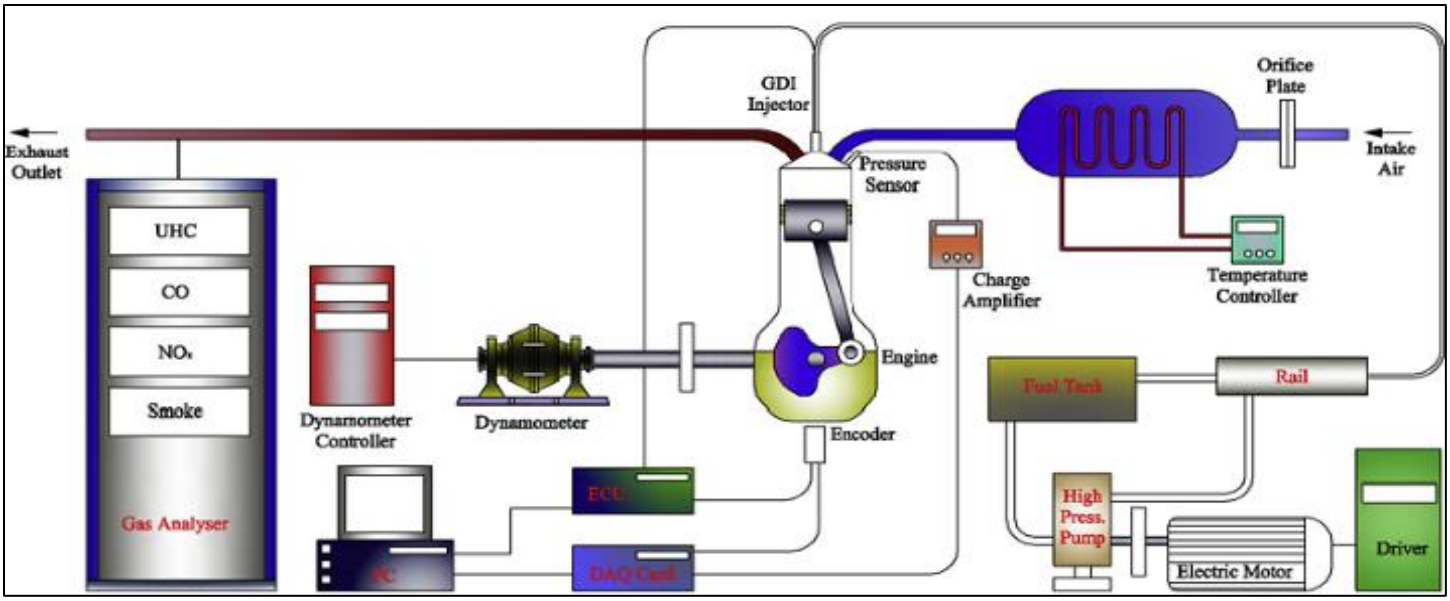


FIG. 1. SCHEMATIC DIAGRAM OF THE EXPERIMENTAL SETUP

model RTM 430 for smoke emissions; Capalec, model Cap 3200 for NO_x emissions). Each of the analyzers were calibrated before starting experiments.

Two different common rail fuel systems for gasoline and diesel fuel were mounted on the test engine. But, only one gasoline direct injector was used for both fuels. Firstly, diesel fuel was used to warm the oil temperature to 60 ± 2 °C. Then the fuel was switched to gasoline with the use of TSDI strategy. Before each experimental case, intake air, coolant and fuel temperatures were fixed to eliminate their effects on combustion. Experiments were carried out for the same energy input (different amounts of fuels were selected to provide 710 J constant energy input per cycle) and engine speed was limited at 1100 ± 20 rpm to avoid knocking. Different second injection timings were used in the experiments. Crank angle positions are shown according to compression TDC (360 °CA) in the graphs.

TABLE 1. ENGINE SPECIFICATIONS

Engine	Super Star 7716 Model Diesel Engine
Type	DI, natural aspirated, 4 stroke, water cooled
Cylinder number	1
Volume (cm^3)	770
Compression ratio	17:1
Intake valve open (bTDC)	22
Intake valve close (aBDC)	60
Exhaust valve open (bBDC)	66
Exhaust valve close (aTDC)	16

CFD MODELLING

HCCI combustion and emission characteristics were calculated using 3D CFD simulation program AVL Fire. Combustion, spray, turbulence, species, emissions etc. calculations were performed using this CFD tool.

Extended Coherent Flame Model-Three Zone (ECFM-3Z) was used for modelling the combustion. Fig. 2 shows detailed scheme of the model [13]. The model comprises flame surface density transport equation and a mixing model that describes non-uniform turbulent premixed as well as diffusion combustion process. Processes are achieved within three mixing zones namely the unmixed fuel zone, the mixed air/fuel zone, and unmixed air (+ EGR) zone. Turbulent mixing occurs between unmixed air and unmixed fuel zones, and auto-ignition happens in the mixed zone as shown in the figure.

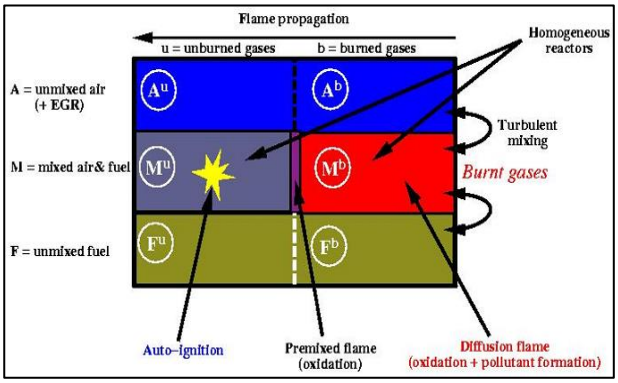


FIG. 2. ZONES IN ECFM-3Z MODEL

The k-ε model was used for modelling turbulence and transient flows were modelled using PISO algorithm. Extended Zeldovich mechanism [14] was used for modelling NO_x emissions. The fuel spray breakup was modeled using the wave breakup model with the value of model constants C1 and C2 set as 0.61 and 18 respectively. Temperature and velocity of the

fuel at the injector nozzle were set to 330 K and 150 m/s respectively. A single hole injector with cone angle 30° was used in the experiment and entered into the simulation parameters.

1/8 sector mesh with 15 subdivisions in angular direction was selected to reduce computational time. Simulation was performed with a time step size of 0.25 °CA from intake valve closing to exhaust valve open, i.e. "closed cycle". It is assumed that fuel-air mixture formed homogeneously in the cylinder at the start of simulation which is 120 °CA after first injection. Boundary conditions are selected as wall type for piston, liner and cylinder head, symmetry type for axis, and periodic type for segment. Grid density sensitivity analysis for HCCI combustion was done by Kong and Reitz [15]. They discovered that a denser mesh provides more accurate results. Because of that, mesh structure of the computational domain (Fig. 3) was created with average cell sizes of 0.6 mm between -30 and 30 °CA to precisely investigate spray and combustion and 0.8 mm for the remaining crank angles. Computational grid around spray region was intensified in order to accurately calculate fuel injection as shown in Fig 3. 3D mesh has 48105 and 170625 cells at TDC and BDC, respectively.

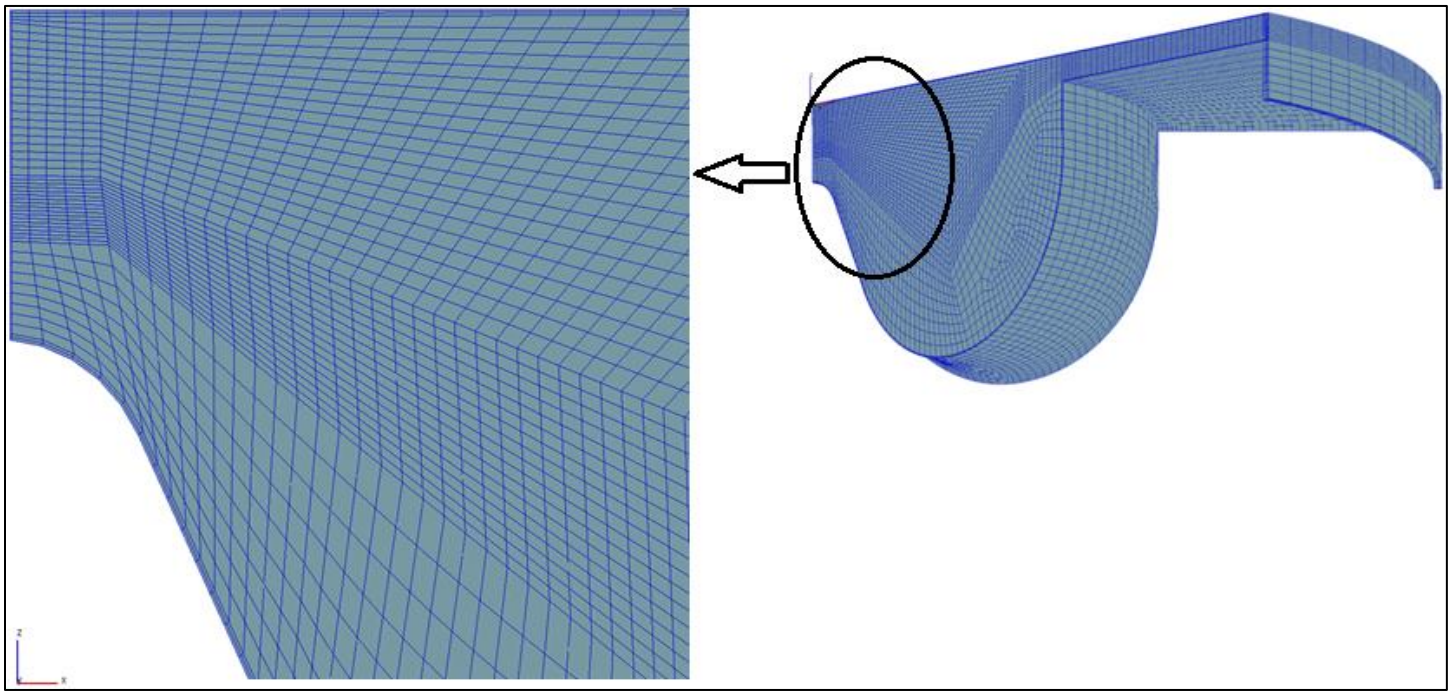


FIG. 3. COMBUSTION CHAMBER COMPUTATIONAL MESH WITH 45° SECTOR GRID AT TDC

RESULTS AND DISCUSSION

Effects of second injection timing on combustion characteristics and emissions of gasoline, E10 and E20 were investigated using CFD simulations and validated against experimental results. First injection timing was kept constant at 120 °CA aTDC for all cases to form the homogeneous charge. Second injection timings were changed between 330 and 345 °CA with 5 °CA intervals. 80% of fuel was injected during the first injection while the 20% of fuel was injected during the second injection (Injection ratio (IR), which is the proportion of first injection mass (I_1) to second injection mass (I_1) is 4) to control ignition timing. 16.5 °CA total injection duration was measured from injection signal and adapted to simulation cases. Rate of heat release (ROHR), in-cylinder gas pressure, NO and CO mass fractions were analyzed numerically while in-cylinder temperature distribution and NO mass fraction were analyzed visually.

Effects Of Second Fuel Injection Timings on HCCI Combustion

Effects of various second injection timings on the cylinder gas pressure and rate of heat release (ROHR) as shown in Fig. 4 and 5, respectively. And also experimental results were compared with the computational results. Different amount of fuels are injected for the different mixtures to ensure constant energy input. It can be seen that experimental and modeling results showed similar trend. Retarding second injection timing retarded combustion phase and caused to decrease maximum cylinder gas pressure (P_{max}) and maximum rate of heat release (MRHR). As can be seen from the experimental and computational results, second injection timing can be used in the control of combustion phasing. Partial rich mixture is formed and combustion phase can be controlled by performing second injection close to compression TDC. In addition, NO emissions could be reduced as a result of reduced cylinder gas pressure and temperature.

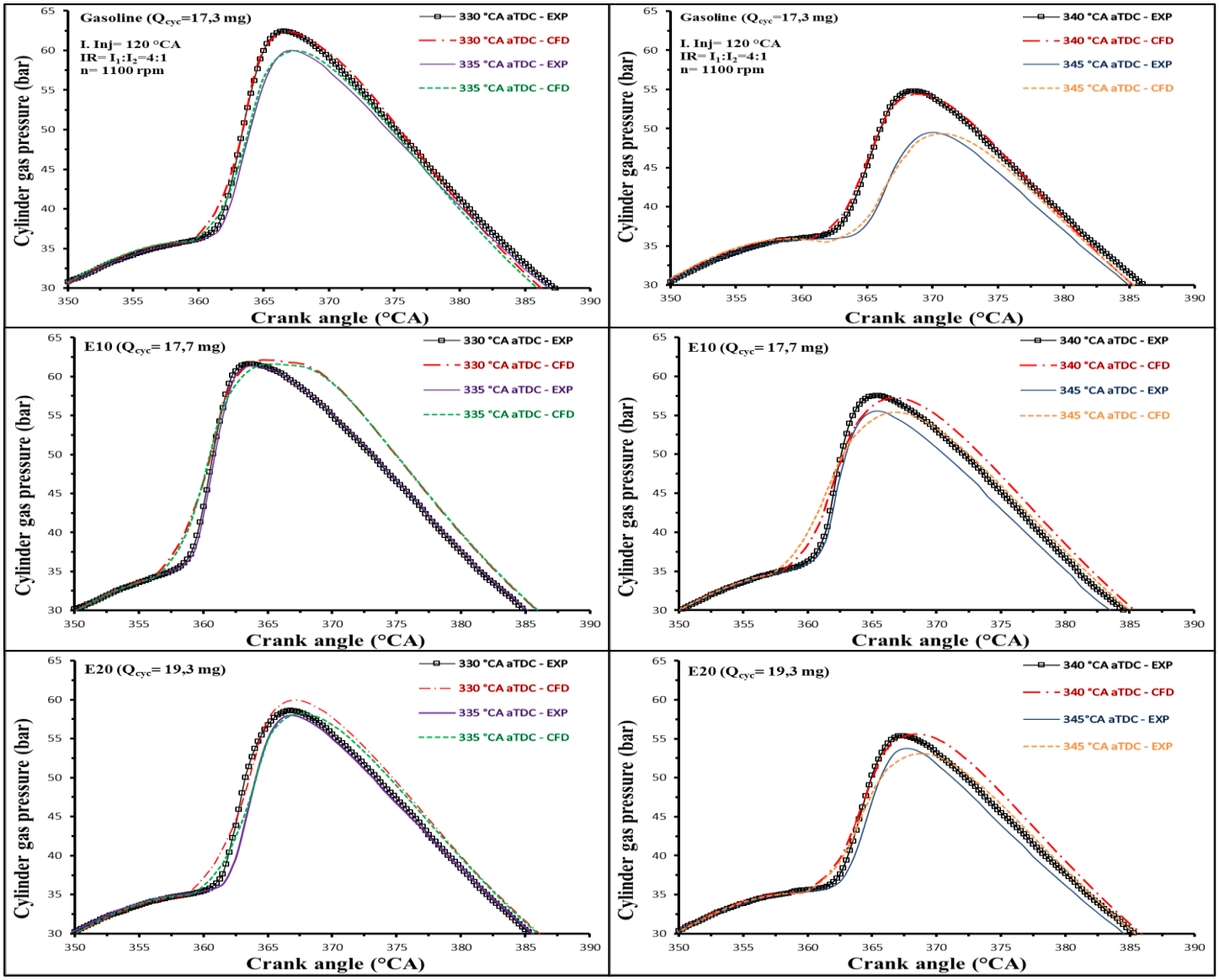


FIG. 4. COMPARISON OF CYLINDER GAS PRESSURE FOR CFD AND EXPERIMENTAL STUDIES

As can be observed in Figs. 4 and 5, ROHR and cylinder gas pressure values decreased and combustion phase moved towards expansion stroke as second injection timing retarded. It is because as second injection timing gets close to compression TDC, its charge cooling effect increases and there will be insufficient time for vaporization.

Maximum ROHR values decreased and combustion phase retarded with the increase in ethanol fraction in the blends. This is because ethanol has less LHV and higher latent heat of vaporization than gasoline as can be seen from Table 2. Ethanol also has higher laminar flame speed than gasoline [16]. For this reason, start of combustion occurred earlier compared with gasoline fuel as can be seen from the breaking points of the ROHR and pressure curves. Compared to E10 blend, higher amount of injected fuel in E20 increased latent heat of vaporization further and higher amount of heat was absorbed from surroundings. Therefore, higher latent heat of vaporization leads to reduction in cylinder charge temperature near TDC and restrains development of laminar flame speed.

CO and NO_x emissions were given in Fig. 6 and compared for experimental and CFD simulation results. NO_x emissions from combustion are primarily and mostly in the form of NO [17]. Therefore, NO emissions calculated from CFD simulations are assumed as total NO_x emissions. By retarding second injection, cooling effect increased and leaded to reduction in cylinder temperature. As a result of this, fuel could not find time to evaporate, reactions worsened and CO emissions increased due to incomplete combustion. Higher latent heat of vaporization of ethanol-gasoline blends prevented sufficient evaporation more for complete combustion and increased CO emissions further. CO emissions were acquired in a 0,03-0,25% difference from experimental results.

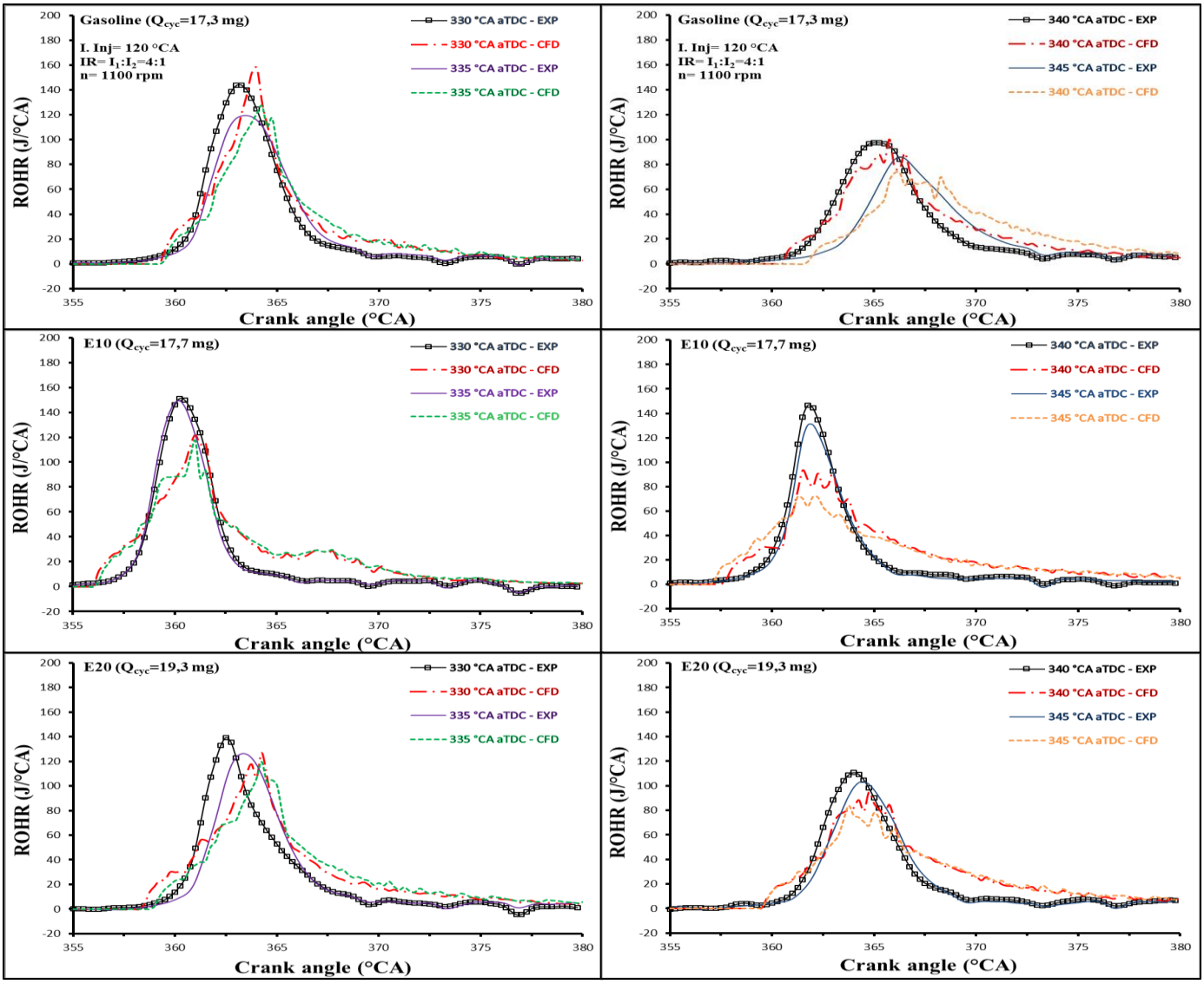


FIG. 5. COMPARISON OF ROHR FOR CFD AND EXPERIMENTAL STUDIES

The effects of second injection timing on NO_x emissions and were compared numerically for experimental and simulation results in Fig. 6. NO_x emissions decreased with retarded second injection timing as shown in the figure. As well known, NO_x emissions are formed by oxidation of N_2 gas in the presence of oxygen. But also for NO_x formation reactions to accelerate, higher combustion temperatures more than 1800 K are critical [18]. NO_x emissions reduced significantly as second injection timing retarded since cooling effect of fuel increased and maximum cylinder gas temperature reduced. CFD simulation results for NO_x emissions exhibited the same descending trend with nearly 200 ppm overprediction.

Even though gasoline-alcohol mixtures contain more oxygen due to the presence of oxygen within ethanol's chemical bonds, it seems that in-cylinder pressure and temperature affect NO_x emissions more. When E10 blend was used, oxygen content and higher laminar flame speed enhanced air-fuel reactions, advanced combustion phase and increased cylinder pressure and temperature values. This caused maximum values of NO_x emissions for E10 blend. When E20 blend was used, minimum NO_x emissions were obtained from experiments. Higher ethanol ratio and amount in the blend decreased volatility and increased cooling effect. Much higher Q_{cyc} for E20 blend caused more heat absorption from surroundings and reduction in maximum ROHR values. As a result, NO_x emissions decreased due to lower cylinder temperatures.

Mass fraction of gasoline at different piston positions inside combustion chamber was given according to various second injection timings visually in Fig. 7. The other images for gasoline-ethanol mixtures were almost the same, so only one image for gasoline mass fraction is considered in this work.

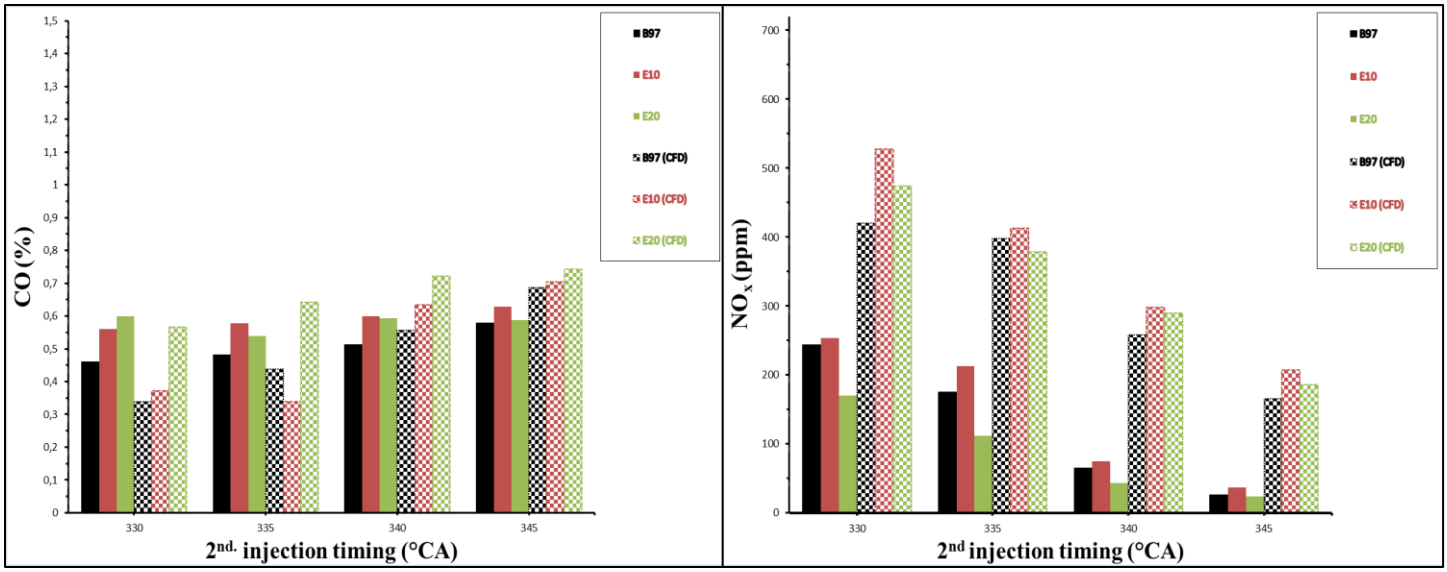


FIG. 6. COMPARISON OF CO AND NO_X EMISSIONS FOR CFD AND EXPERIMENTAL STUDIES WITH REFERENCE TO 2ND INJECTION TIMING

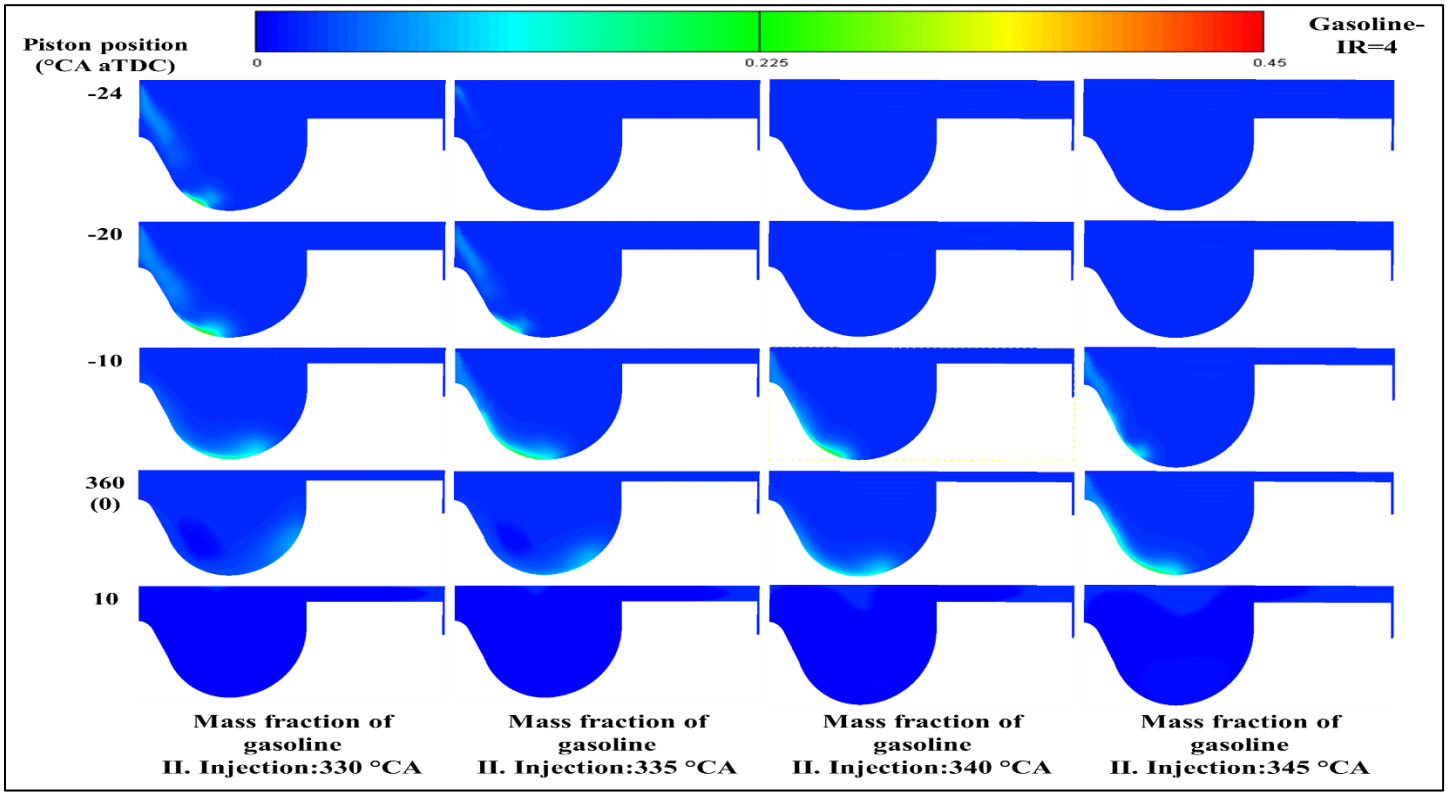


FIG. 7. MASS FRACTION OF GASOLINE INSIDE COMBUSTION CHAMBER AT VARIOUS 2ND INJECTION TIMINGS

For early second injection times, injected fuel was partly accumulated on the surface of piston bowl as observed from Fig. 7. Since these regions are rich in terms of fuel, they cause inhomogeneous fuel-air mixture. NO_x emission formation is triggered by high temperature combustion of this inhomogeneous mixture. Latter second injections, especially 340 and 345 °CA injections, ended just before the beginning of combustion and fuel could not find enough time to evaporate and accumulate on the bowl. As a result, high temperature combustion and NO_x formation were avoided. On the other side, CO emissions increased due to partly non-premixed and incomplete combustion.

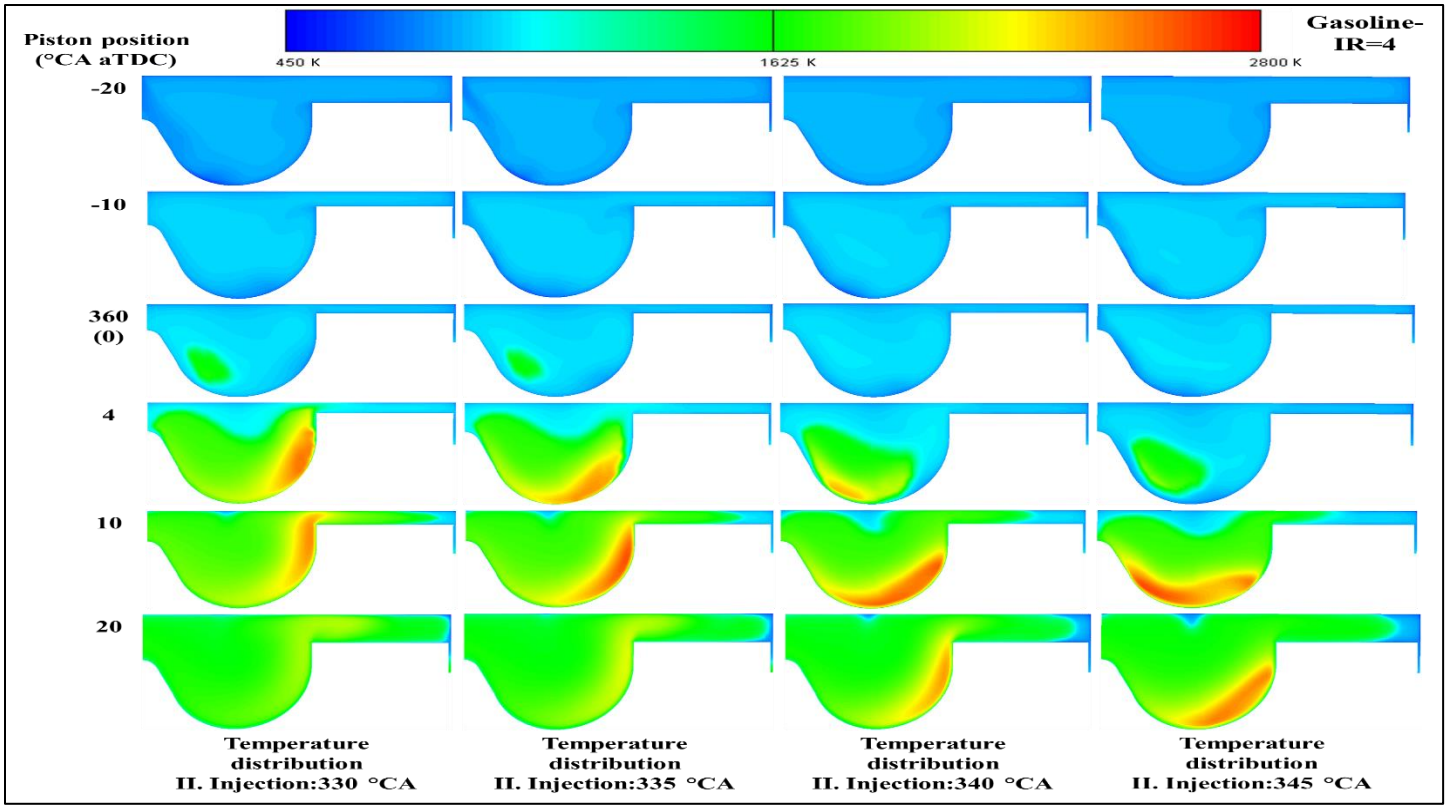


FIG. 8. EFFECTS OF 2ND INJECTION TIMING ON COMBUSTION CHAMBER TEMPERATURE DISTRIBUTION (GASOLINE)

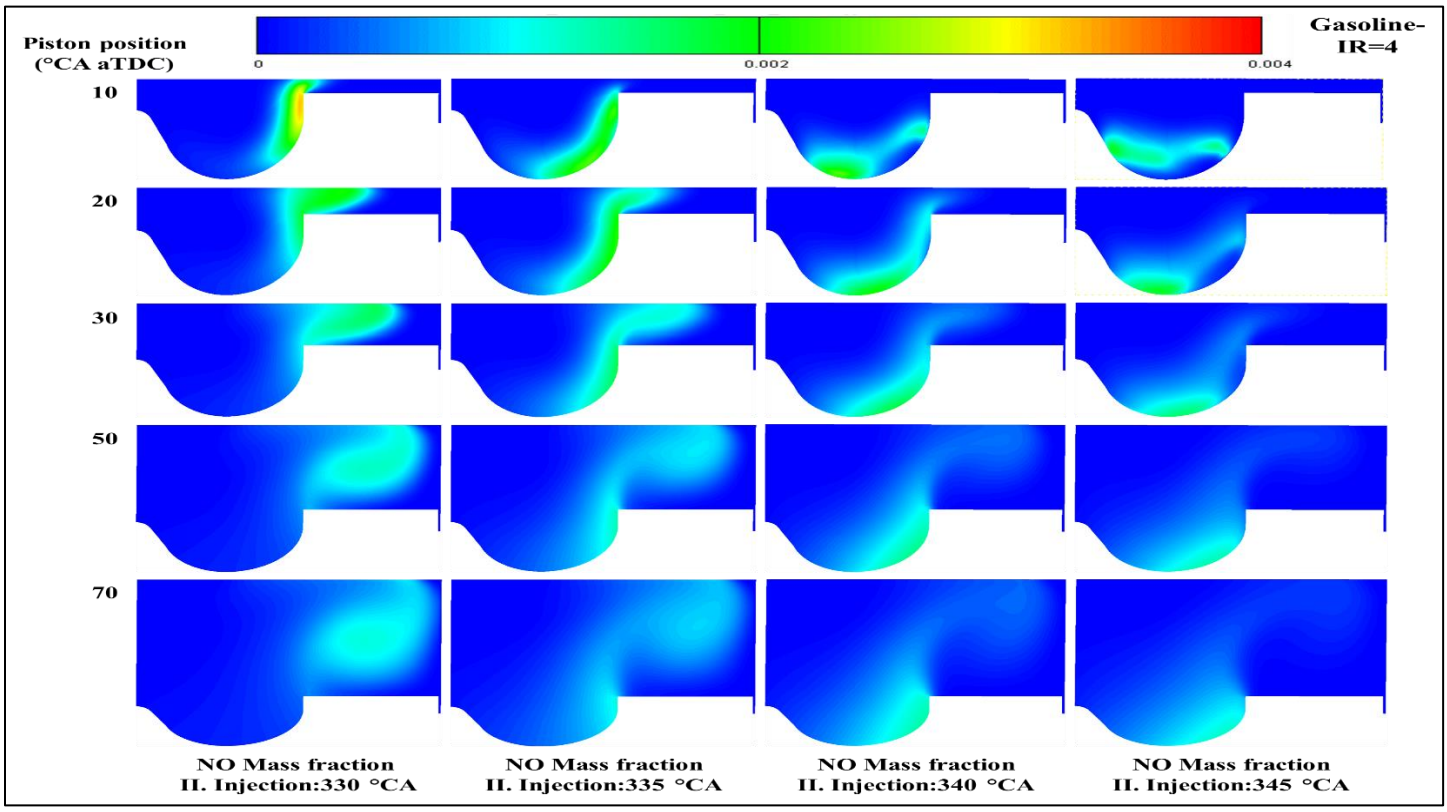


FIG. 9. EFFECTS OF SECOND INJECTION TIMING ON NO_X EMISSIONS (GASOLINE)

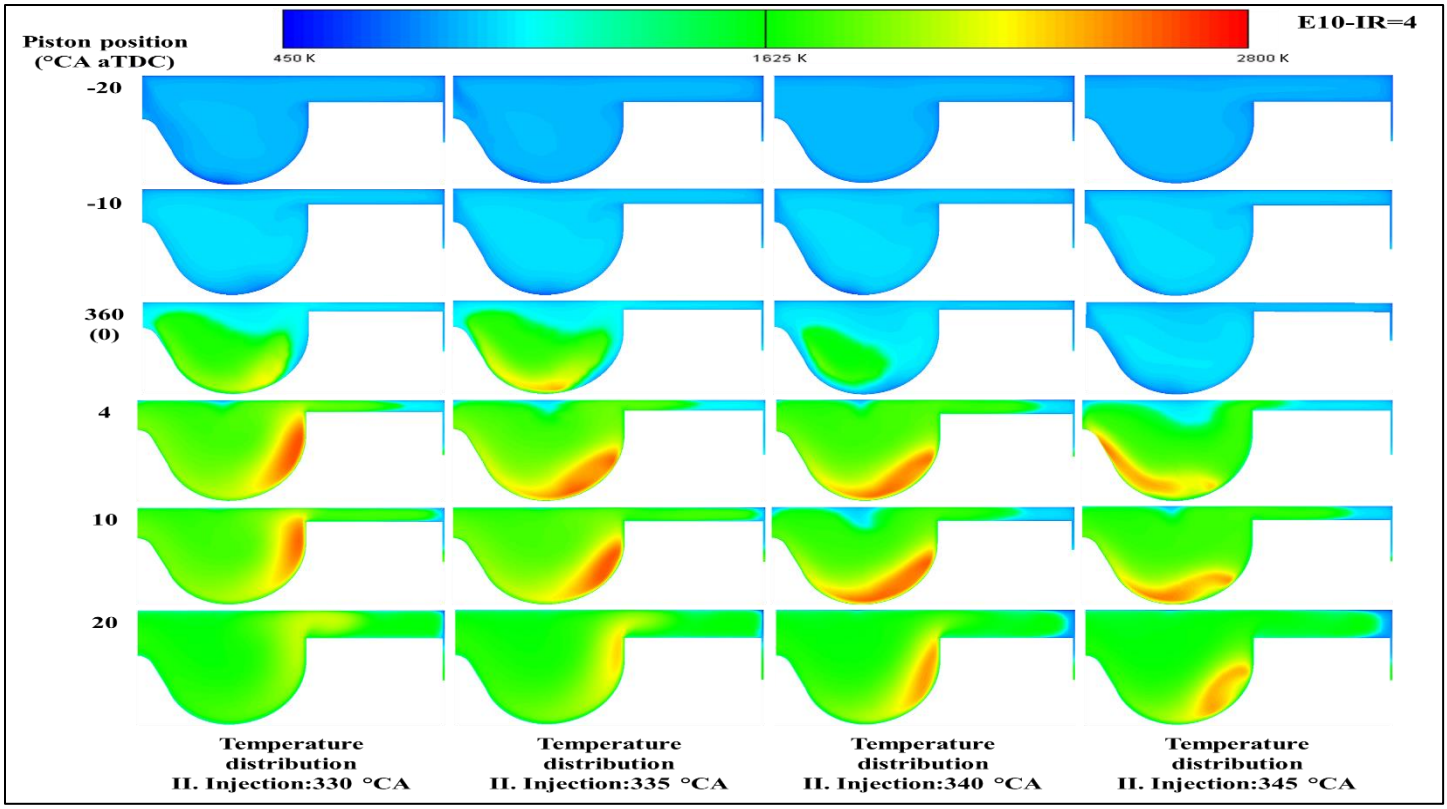


FIG. 10. EFFECTS OF SECOND INJECTION TIMING ON COMBUSTION CHAMBER TEMPERATURE DISTRIBUTION (E10)

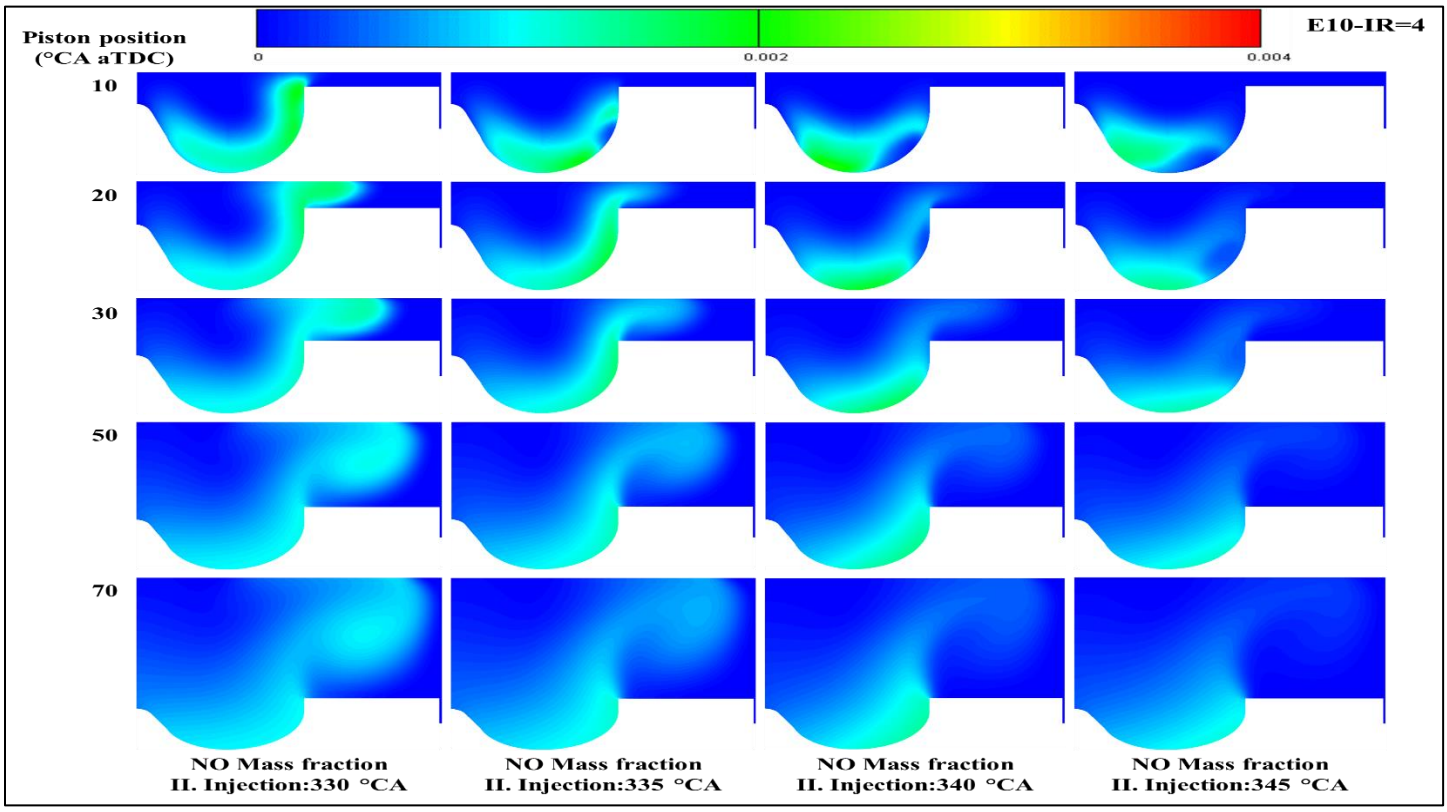


FIG. 11. EFFECTS OF SECOND INJECTION TIMING ON NO_X EMISSIONS (E10)

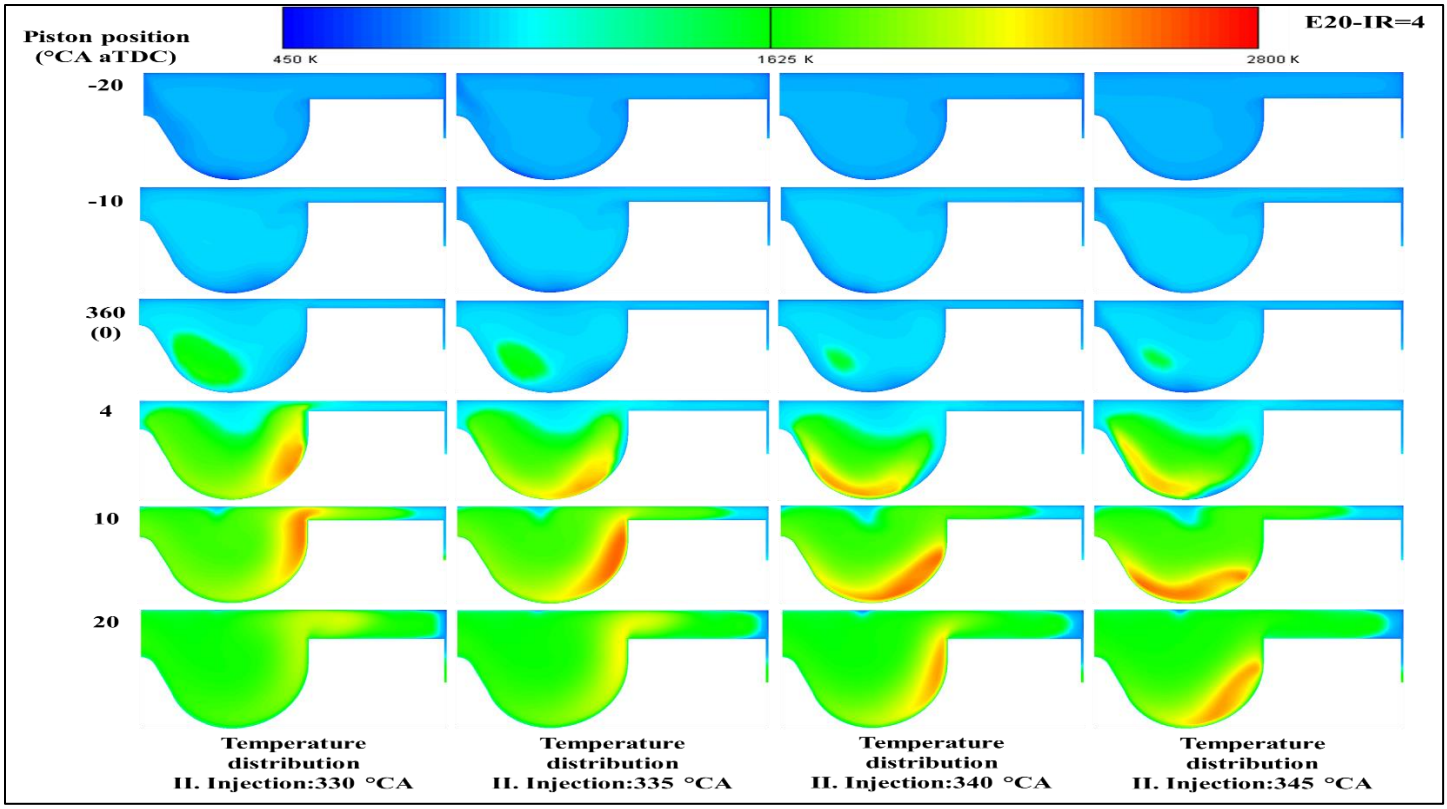


FIG. 12. EFFECTS OF SECOND INJECTION TIMING ON COMBUSTION CHAMBER TEMPERATURE DISTRIBUTION (E20)

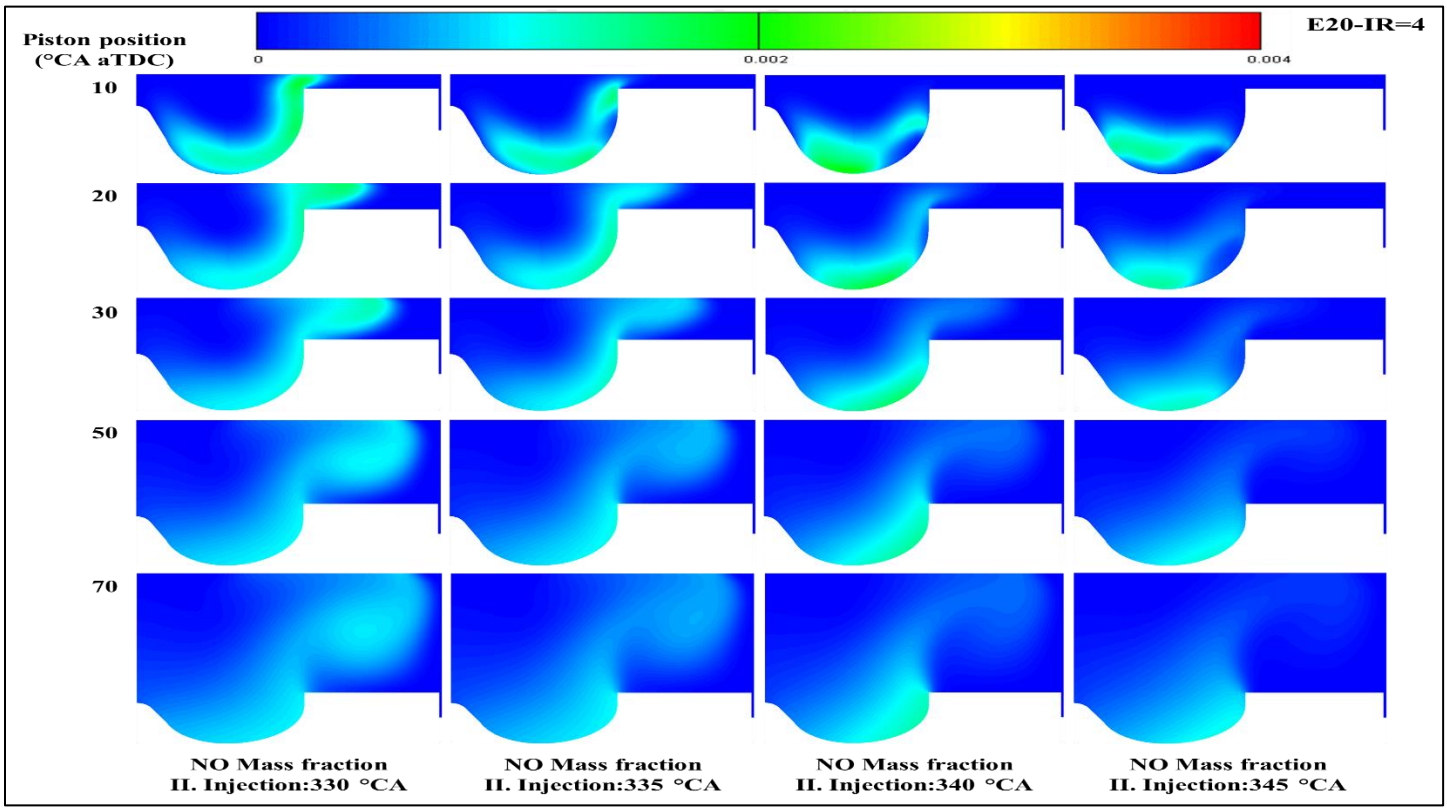


FIG. 13. EFFECTS OF SECOND INJECTION TIMING ON NO_X EMISSIONS (E20)

In-cylinder temperature distribution and NO mass fractions were given visually at changing CA positions and various second injection timings, respectively for gasoline, E10 and E20 in Figs. 8-13. It can be seen from the images that the second injection timing has distinctive effect on temperature distributions and NO_x emissions. Cylinder charge cooling effect can be observed better from the temperature distribution images of -20 and -10 °CA aTDC piston positions. The areas around injected fuel show more blue color than others which demonstrates cooling effect. At earlier injection times, red and green color distribution becomes wider which indicates a higher average temperature. It can be seen from 0-4 °CA aTDC temperature distribution images that combustion started at fuel-rich regions and formed high temperatures inside combustion chamber. Further reduction of combustion temperature is observed for later injection times since cooling effect of fuel increased and evaporation process worsened.

The second fuel injection timing has a dominant effect on NO_x emissions. From the NO mass fraction images, it can be seen that NO_x emissions formed with stratified charge which is obtained by late second fuel injection [19]. Formed between initially homogeneous mixture and injected fuel, the stratified charge results in higher local temperatures which triggers the production of NO_x emissions. Stratified appearance of NO_x emissions can be conveniently seen from the images at 50 and 70 °CA aTDC. As the second injection timing is retarded, higher cooling effect and decreased temperature caused to decrease NO_x emissions. Since combustion started later and maximum temperature values was reached at latter crank angles for gasoline fuel, NO_x emissions were seen more at piston crown region due to proceeding of injected fuel inside combustion chamber. Earlier start of combustion for E10 caused maximum temperature values to occur earlier and NO_x emissions were seen mostly at piston bowl region. More latent heat of vaporization of E20 blend retarded combustion phase and NO_x emissions were seen closer to piston crown region compared to E10 blend. It can be concluded from cylinder temperature distribution and NO mass fraction images that NO_x emissions are formed in the presence of high temperature inside the cylinder.

CONCLUSIONS

In this study, the effects of second injection timing on HCCI combustion and emissions were investigated using gasoline-ethanol blends. HCCI combustion was simulated by 3D-CFD modeling of test engine and simulation results were compared against experimental results. Both experimental and modeling results showed that second injection timing is significant effective in controlling HCCI combustion and emissions. The conclusions can be summarized as follows:

(1) HCCI combustion and emission characteristics can be controlled by means of various second injection timings.
(2) Retarding second fuel injection timing delayed the combustion phase, decreased P_{max}, MRHR and NO_x emissions while it increased CO emissions. CO emissions were affected slightly, while NO_x emissions were affected significantly by retarding second injection timing.
(3) P_{max}, MRHR and NO_x emissions decreased and start of combustion retarded by increasing the ethanol content in the blends.
(4) CFD model was able to predict HCCI combustion and emission process under high equivalence ratio conditions. Visual results show how injection, combustion and NO_x formation occur in HCCI combustion with TSDI strategy.
(5) Calculated pressure curves and P_{max} values agree well with the experimental results. MRHR values were obtained for all cases with approximately 10-20 J/°CA difference from experimental results, except for E10 blend which has lower MRHR values.
(6) In-cylinder images of temperature distribution demonstrate that combustion begins in the fuel rich zone between injected fuel and initially homogeneous mixture. It can be observed from NO mass fraction and temperature distribution images that NO_x emissions formed in the areas where high temperature combustion occurred.

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NOMENCLATURE

aBDC	= After bottom dead center
aTDC	= After top dead center
bBDC	= Before bottom dead center
bTDC	= Before top dead center
BDC	= Bottom dead center
CI	= Compression ignition
CFD	= Computational fluid dynamics
DI	= Direct injection
GDI	= Gasoline direct injection
EGR	= Exhaust gas recirculation
LHV	= Lower heating value
HCCI	= Homogeneous charge compression ignition
IR	= Injection ratio
MRHR	= Maximum rate of heat release
NVO	= Negative valve overlap
P_{max}	= Maximum cylinder gas pressure
Q_{cyc}	= Fuel quantity per cycle
ROHR	= Rate of heat release
SI	= Spark ignition
TDC	= Top dead center
TSDI	= Two stage direct injection

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