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Study of the Combustion Process of a Homogeneous Charge Compression Ignition (HCCI) Engine and a Partially Premixed Combustion (PPC) Mode of a Compression Ignition Engine Using Natural Gas as an Alternative Fuel

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ABSTRACT

In order to investigate a viable approach to achieving high efficiencies and low nitrogen oxide (NO_X) emissions, this paper presents the application of a homogeneous charge compression ignition (HCCI) engine and the partially premixed combustion (PPC) mode applied to a heavy diesel engine. The effect of carbon dioxide (CO_2) fraction on combustion parameters was analyzed and discussed in detail. For this purpose, on the one hand, ANSYS CHEMKIN-Pro software was used to perform simulations of a closed homogeneous reactor under conditions relevant to HCCI engines, and on the other hand, ANSYS-Fluent software was used by adding a CO_2 fraction varying from 20% to 58% to methane fuel to study 2D flow simulation by applying a PPC combustion mode to predict the distribution of various output parameters such as in-cylinder temperature, in-cylinder pressure and emissions. In comparison with the two presented models, it was found that the HCCI engine showed a lower NO_X level than the PPC mode and this was due to the lower in-cylinder temperature in the HCCI engine.

1. Introduction

In the context of the reduction of polluting emissions and fuel consumption of internal combustion engines, the researchers and engineers in engine community pay more attention to the advanced combustion modes based on the conventional diesel (CI) engine and SI engine, such as homogeneous charge compression ignition (HCCI) [1-4] and premixed charge compression ignition (PCCI) [5-7].

The homogeneous charge compression ignition (HCCI) engines employ a relatively new mode of combustion technology, in which auto-ignition takes place when the lean mixture of air and fuel reaches its chemical activation energy and is fully controlled by chemical kinetics [8-9] rather than

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spark or injection timing. The HCCI mode is faster [10] compared to conventional compression ignition (CI) and spark ignition (SI) combustion methods. Whereas the working principle of the HCCI process is similar to that of the SI engine, in that the fuel and air are mixed before being induced into the cylinder. Plus, it uses homogeneous fuel-air mixtures as in the case of the SI engine and typically uses a high compression ratio that allows the mixture to auto-ignite as in the case of the diesel engine. In addition, the lean combustion technology is employed mainly in HCCI. Undoubtedly, auto-ignition of the air-fuel mixture is necessary for the occurrence of ignition and fuel selection is a very important factor that significantly affects on the combustion process and thus on the engine performance. For this reason, the auto-ignition of HCCI may be controlled by changing the fuel properties [11]. Furthermore, the addition of an ignition inhibitor in the fuel can make it more chemically reactive. Therefore, the chemistry and properties of the fuel play an important role in determining combustion characteristics [12].

Soylu [13] examined the combustion characteristics of natural gas HCCI engine using detailed chemical kinetics. The study highlighted that, if the initial conditions of the mixture are known precisely at intake valve closing, the auto-ignition timing is controllable. In other research studies, it was concluded that the auto-ignition in HCCI engines is affected by several factors such as the fuel auto-ignition chemistry and thermodynamic properties, alternative fuel, combustion duration, wall temperatures, concentration of reacting species, residual rate, degree of mixture homogeneity, intake temperature, compression ratio (CR), equivalence ratio (ϕ), amount of exhaust gas recirculation (EGR), engine speed, and other engine parameters [14-15]. Moreover, the HCCI mode is characterized by low temperature (LTC), lean combustion that is generated at several spots throughout the cylinder due to the lean nature of the combustion, and the little or no flame propagation ensures independence from turbulence [16].

Lu *et al.,* [17] investigated the effect of RON (research octane number) fuels, EGR rate, equivalence ratio, intake charge temperature, coolant temperature and engine speed on the HCCI ignition timing, combustion duration, cycle-to-cycle variation, and emissions. It was found that the cycle-to-cycle variation decreases with the increase of equivalence ratio and cetane number. It was also found that the combustion phase advances, and the combustion duration shorten with the increase of intake charge temperature and the coolant out temperature and the decrease of engine speed. Furthermore, the NO_X emissions increase notably once the equivalence ratio exceeds a "critical value"; this is also supported by another study, Sindhu *et al*., [18]. They reported that, at a higher equivalence ratio, more fuel is burned in the cylinder and therefore more heat is released which leads to higher gas temperatures and pressures on one hand, and takes a toll on the thermal efficiency of the engine on the other hand.

The paper of Xiongbo Duan *et al*., [3] reviewed the fundamental understanding of controlling strategies of the ignition timing and combustion phase in homogeneous charge compression ignition (HCCI) engine and different controlling strategies as well as their effects. They reported that alternative fuels show some superior properties for controlling the ignition timing and combustion phase of the HCCI engine compared with the traditional diesel and gasoline fuels. Moreover, the strategies of different external and in-cylinder mixture preparation methods and the different strategies of controlled auto ignition by HCCI combustion were discussed in the paper reviews presented by Harisankar Bendu *et al*., [1]. Through this review, the authors concluded that the combination of equivalence ratio and charge temperature decides the auto-ignition characteristics of the fuel for HCCI combustion.

In many respects, the most fundamental principle in the study of combustion is the need to distinguish between two basically different arrangements of fuel; premixed (homogeneous) and non-premixed (heterogeneous). Premixed systems are those in which the gaseous fuel is

thoroughly mixed with air before combustion begins [19]. Many researchers have used different premixed strategies in order to reduce emissions and improve the engines performance. The premixed compression-ignited combustion system is one of the examples that have been developed to early injection to form a premixed lean mixture prior to auto-ignition [20]. In a premixed charge compression ignition (PCCI) engine, spontaneous ignition occurs at unspecified points and then the flame rapidly develops throughout the combustion chamber [21].

Admittedly, partially premixed combustion (PPC) is another promising advanced combustion mode for future engines [22], in which it is possible to obtain low NO_X and low soot by using diesel fuel [23]. Furthermore, the PPC mode can be considered as a hybrid combustion process between HCCI combustion and diesel combustion, which has been widely applied in recent years [24-28]. Therefore, PPC is controlled by inlet conditions and the injection process [22]. Sharath *et al*., [26] made a comparison of PCCI and PPC modes using the ANSYS-Fluent software. It was concluded that the PPC mode is a better viewpoint in engine design.

The effect of different research octane number (RON) on the performance, emissions and combustion characteristic of a spark ignition (SI) engine was carry out by Teoh *et al.,* [29]. The results showed that the high octane fuel leads to reduce the emission of CO and UHC, while the low octane fuels caused a lower emission of CO_2 and NO_X. It is known that more than 90% of the weight of natural gas is methane, which has a very high octane number up to 120. For this reason, methane is currently introduced in various places and applications [30, 31] and is considered one of the alternative fuels. Additionally, alternative fuel is promising green technologies for reducing engine emissions and therefore air pollution. In addition, NO emissions can be reduced by 35% compared to pure diesel fuel when 50% methane is added to the mixture [32].

The effect of the biogas composition on the emissions of CO and NO_X was investigated numerically by Mokrane *et al*., [27], and it was concluded that the concentration of carbon dioxide (CO_2) in the biogas has an important effect on reducing NO_X and CO emissions. Meanwhile, Lee *et al.,* [33] concluded that when the CO_2 fraction changed from 0% to 50%, carbon monoxide (CO) and unburned hydrocarbons (UHC) emissions increased, while NO_X emissions decreased. Thus, several fundamental research topics were introduced to explore different aspects of the combustion process, such as laminar flame speed [34-37]. Therefore, the flame speed definition is dependent on the propagation of the flame in the unburned mixture as perceived by the observer [38]. Typically, the laminar flame speed is determined from a premixed flame. This is the only type of flame in which flame propagation can be empirically determined. Thus, premixed laminar flames are generally used in combustion models to simulate turbulent flows [39, 38].

It is necessary to recycle the exhaust gases in the combustible gas results in remarkably changing the fundamental flame properties, including the laminar flame speed, adiabatic flame temperature and flame structure [40, 41], and thereby affecting the pollution emissions formation [42]. The chemical effect of the CO_2 dilution gas produced the greatest impacts on the laminar flame speed, adiabatic combustion temperature and key radicals formation of the methane/air [43]. Therefore, it was importance to investigate the effects of the dilution gases on the combustion process of premixed methane/air mixture. Many studies have been conducted on the premixed laminar methane/air flames to investigate the fundamental influences of dilution gases, among them CO_2 [44-46].

The present study is a real application of HCCI engine and PPC mode of a direct injection diesel F8L413 engine which has a higher compression ratio in light of methane is used as a fuel under lean mixture conditions. Therefore, this study mainly focuses on the effect of the carbon dioxide CO_2 on the HCCI engine performance and its effect on the laminar flame speed of the methane/air mixture in partially premixed combustion mode incorporated with an auto-ignition model.

2. Calculation Model

2.1 Present Work

The simulation is confined to phases between intake valve close (IVC) to exhaust valve open (EVO) to reduce the computational time. This paper includes two parts:

In the first part, a simulation in the "Internal Combustion Engine" module from ANSYS CHEMKIN-Pro software [47] was carried out. ANSYS CHEMKIN-Pro was used to perform the thermodynamic and chemical kinetics analysis [48]. In this part, the ϕ varied from 0.3 to 0.6, the intake charge temperature of the mixture at IVC timing (T_{IVC}) was set at 500K and the amount of carbon dioxide (CO_2) added to methane (CH_4) fuel is 10% and 50%. The engine parameters are specified by the user directly in the CHEMKIN interface for the internal combustion HCCI engine reactor model [48]. Heywood [49] provides equations that describe the volume (to first order) as a function of time, based on the engine parameters and specifications of the single cylinder HCCI engine shown in Table 1. The calculation starts with an intake valve close (IVC) value of 52 deg aBDC and ends at an exhaust valve open (EVO) value of 67 deg bBDC. The single-zone model allows relatively short computation. Methane is the main component of natural gas, thus the mechanism we have selected is the GRI-Mech 3.0 (325 reactions, 53 species) to describe the combustion process [50]. The heat transfer correlation has as parameters: a=0.035, m=0.7, c=0.0; the temperature of the wall was taken equal to 400K; the Woschni correlation of average cylinder gas velocity has as parameters: C_{11}=2.28, C_{12}=0.308, C_2=3.24 x 10^{-3} and finally the swirl speed ratio was taken equal to 0.0.

The zero-dimensional single-zone HCCI thermodynamic simulation model used in this part was based on the following assumptions

i. Only the closed cycle from IVC to EVO was taken into account in the model;
ii. Temperature and pressure have a uniform distribution;
iii. The heat exchange is done with the walls and is taken into account by the modified Woschni model [51];
iv. The fuel is premixed with air before entering the cylinder and is compressed during the compression stroke;
v. There are no spark plugs or injectors to support (assist) the combustion; the mixture is ignited automatically by auto-ignition;
vi. Mixing in the cylinder was considered an ideal gas.

The second part of the work presents a combustion simulation of a single cylinder engine using a CFD tool, to carry out numerically the combustion process in the combustion chamber. For PCCI engines, the fuel and the air are mixed before entering the combustion chamber. At the time of the ignition or spark, the mixture is supposed to be homogeneous and the combustion process is known as "premixed combustion". Since the premixed combustion mode does not predict any species, it could result in over prediction of the peak temperature and pressure. For this reason, the PPC mode was used to predict the NO_X level rate, which will have better prediction of peak temperature and pressure [52]. This model of ANSYS-FLUENT predicts equilibrium composition and can be used for premixed combustion. The geometry was built and meshed in preprocessor Gambit 2.4.6 and then it was exported to ANSYS-Fluent. ANSYS-Fluent was incorporated with an auto-ignition model for simulation and prediction. In this part, the CO_2 concentrations were varied in the mixture (CH_4/CO_2) between 20% and 58% to study their effect on the combustion process and parameters such as in-cylinder pressure, in-cylinder temperature…etc. The C-equation model was used for the PPC mode. For modeling turbulence, the Renormalization Group Theory (RNG) k-ε model with standard wall function was used. Use was made of the PRESTO discretization scheme

for discretizing pressure and the first order upwind scheme for the discretization of the model equations. The PISO (Pressure-Implicit with Splitting of Operation) algorithm was selected for the pressure-velocity coupling.

Table 1
Simulated engine specifications

Characteristics	Specification
Type of engine	4-stroke, compression ignition
Nominal max speed	2650 rpm
Bore (mm)x Stroke (mm)	120 x 125
Displacement (cm3)	11310
Compression ratio	18: 1
Connecting rod length (mm)	238
Exhaust valve open (EVO)	67 deg before Bottom Dead Center (bBDC)
Exhaust valve close (EVC)	27 deg after Top Dead Center (aTDC)
Intake valve open (IVO)	22 deg before Top Dead Center (bTDC)
Intake valve close (IVC)	52 deg after Bottom Dead Center (aBDC)

2.2 Charge Compression Ignition (HCCI) Model (CHEMKIN-Pro set up)

The CHEMKIN-Pro software is designed for modeling different chemically reacting flow configurations [53]. Therefore, CHEMKIN-Pro was used as the calculation solver.

2.2.1 Governing equations

The governing equations for temperature and species as follows

i. Internal Energy/Temperature:

$$\rho C_v \frac{dT}{dt} = -\sum_{k=1}^{kgas} \dot{\omega}_k W_k u_k - \frac{P}{V}\frac{dV}{dt} - \frac{h_g (T - T_w) A_w}{V} \quad (1)$$

ii. Species conservation equation with constant mass:

$$\rho \frac{dY_k}{dt} = \dot{\omega}_k W_k \quad (2)$$

with

Y_k : Mass fraction of the k_{th} species, dimensionless;

C_v : Constant-volume specific heat capacity of the mixture, J/kg/ K;

T : Temperature, K;

r : Mass density of a gas mixture, kg/m^3;

u_k : Specific internal energy of the k_{th} species, J/kg;

W_k : Molecular weight of the k_{th} species, kg/mole;

$\dot{\omega}_k$: Chemical production rate of the k_{th} species due to gas-phase reactions, mole/cm^3/s;

h_g : Heat transfer coefficient, W/m^2/K;

A_w : Surface area, m^2.

The complete stoichiometric combustion reaction for a lean mixture is written

$$C_xH_y + \frac{a_{st}}{\phi}(O_2 + 3.76N_2) \rightarrow xCO_2 + \frac{y}{2}H_2O + \gamma O_2 + 3.76\frac{a_{st}}{\phi}N_2 \quad (3)$$

with

$$a_{st} = x + \frac{y}{4}$$

2.2.2 Engine operating parameters

The indicated work (Wi) by cycle in kJ is given by

$$W_i = \int P\,dV \quad (4)$$

Indicated mean effective pressure (IMEP) was calculated by the equation below

$$IMEP = \int \frac{W_i}{V_d} \quad (5)$$

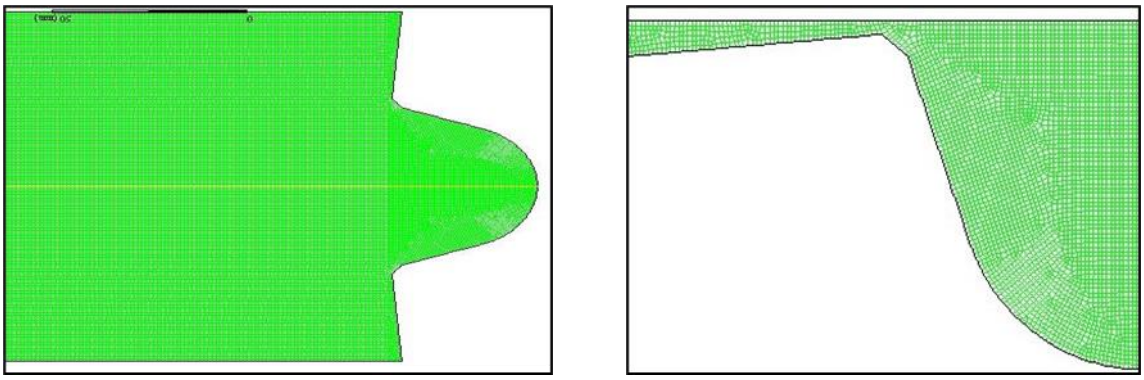
The indicated thermal efficiency (h_i) is given by

$$h_i = \frac{W_i}{m_f\,LHV} \quad (6)$$

with
LHV: Lower heating value, MJ/kg;
m_f : Fuel consumption per cycle.

2.3 Partially Premixed Combustion (PPC) Mode

A mesh motion preview was carried out in order to bring the piston to the IVC position. In this case, the piston reaches the bottom dead center (BDC) at a crank angle of 540 deg. The intake valve closes at 592 deg (52 deg aBDC) and the piston reaches the top dead center (TDC) at 720 deg. The exhaust valve opens at 67 deg bBDC. The piston reaches BDC at 900 deg. This covers 360 deg, which is equal to two strokes between which the IVC and EVO take place. In this case, the step size chosen was 0.25 deg of the crank angle and the number of steps came to 928, bringing the crank angle from 360 deg to 592 deg. The valves were not considered because this simulation was carried out between the closing of the inlet valve (IVC) and the opening of the exhaust valve (EVO). The simulation was carried out between the crank angles 592 deg and 833 deg, i.e., between IVC and EVO. The crank angle duration is 241 deg. In order to carry out the calculation for 241 deg with a step size of 0.25 the total number of steps is 964. The computational domain of the two-dimensional combustion chamber geometry of the F8L413 engine is shown in Figure 1.



(a) (b)

Fig. 1. The computational domain of the two-dimensional combustion chamber geometry of the F8L413 Deutz engine (a) Meshed and mirrored model at the crank angle 592 deg (b) Meshed half-geometry in preprocessor Gambit

The "axis" type boundary condition must be used in the center of the axisymmetric geometry. Since the geometry is symmetric, the software takes this fact into account for the axis. Therefore, the user-defined function (UDF) is used to modify the laminar flame speed so that it is more realistic (it recomputes the flame speed based on the pressure, the temperature and the mixture fraction inside the cylinder) [52]. Another UDF provides a tool for initializing the flow field with a swirl ratio. Because the combustion and power stroke are relevant to this internal combustion flow, the initial condition normally involves swirl flow. The last UDF was used to calculate indicated work. In partially premixed combustion, we find premixed and non-premixed conditions. The model uses the extended Zeldovich mechanism to calculate production of thermal NO_X, with local concentrations of O and OH obtained by a partial equilibrium assumption. Turbulent fluctuations were taken into account by using a presumed probability density function (PDF) approach [54, 27].

Table 2 summarizes the combustion model. Concerning governing transport equations, we can find details in [52].

Table 2
Combustion model

Model	Partially premixed combustion
Premixed model	C-equation
Turbulence model	(RNG) k-ε
Turbulent flame speed model	Zimont
State relation	Chemical equilibrium
Energy treatment	Non-adiabatic
Equilibrium operating pressure (Pa)	3000000
PDF options	Inlet diffusion and compressibility effects
Temperature (K)	300

The two dimensional in-cylinder, transient and reacting flow system in a partially premixed combustion (PPC) is modeled by solving a set of governing equations from the law of conservation of mass, momentum, energy and species. The simulation starts at IVC and ends at EVO. Therefore, there are no valves involved. A pure layering approach was used on a 2D axisymmetric geometry. The numerical model was solved by considering pressure-based, transient and axisymmetric swirl solver and the effect of turbulence was taken into account. For turbulence modeling, an (RNG) k-ε model is used. In this study, for NO_X modeling, we used the ANSYS-Fluent prompt model. The dynamic mesh option was enabled, and then layering in the mesh methods group box was selected. The engine parameters were entered in-cylinder settings dialog box option as follows: crank shaft

speed: 2000rpm; starting crank angle: 360 deg; crank period: 720 deg; crank angle step size: 0.25 deg; piston stroke: 125mm; connecting rod length: 238mm.

Most existing modelling techniques have been formulated specifically for one combustion regime (non-premixed, premixed or partially premixed) [55].

2.3.1 Premixed combustion model [55]

In premixed combustion, fuel and oxidizer are mixed at the molecular level prior to ignition. Combustion occurs as a flame front propagating into the unburnt reactants. The reason for this is that premixed combustion usually occurs as a thin, propagating flame that is stretched and contorted by turbulence. Cannot be used in conjunction with the pollutant (i.e., soot and NO_X) models. However, a perfectly premixed system can be modeled with the partially premixed model, which can be used with the pollutant models.

2.3.2 Non-premixed combustion [55]

In non-premixed combustion, fuel and oxidizer enter the reaction zone in distinct streams. This is in contrast to premixed systems, in which reactants are mixed at the molecular level before burning.

2.3.3 Partially premixed combustion [55]

Partially premixed combustion systems are premixed flames with non-uniform fuel oxidizer mixtures (equivalence ratios). Such flames include premixed jets discharging into a quiescent atmosphere, lean premixed combustors with diffusion pilot flames and/or cooling air jets, and imperfectly premixed inlets. The partially premixed model is a combination of the non-premixed model and the premixed model. The premixed reaction-progress variable, c, determines the position of the flame front. Behind the flame front (c=1), the mixture is burnt and the equilibrium or laminar Flamelet mixture fraction solution is used. Ahead of the flame front (c=0), the species mass fractions, temperature, and density are calculated from the mixed but unburnt mixture fraction. Within the flame (0 <c< 1), a linear combination of the unburnt and burnt mixtures is used.

2.3.4 C-equation model theory [55]

A scalar variable representing the progress of reaction from unburnt to burnt is denoted by c. The transport equation for c describes the spatial and temporal evolution of the reaction progress in a turbulent flow field. Ahead of the flame, c is defined as zero in the unburnt reactants, and behind the flame c is unity in the burnt products. Within the flame brush c varies between zero and one. The flame brush propagates upstream at a modeled turbulent flame speed. Fluent offers two models for the turbulent flame speed, namely the Zimont model [56-58] and the Peters model [59], as detailed in Peters Flame Speed Model.

One of the approaches to model partially premixed turbulent combustion is the transported PDF (Probability Density Function) model. This method is very precise and remains valid in all combustion regimes. However, the description of finite chemical kinetics phenomena requires taking into account a number of species, which further increases the dimension of the attached PDF and may in practice make the calculation impossible.

The composition PDF transport equation is derived from the Navier-Stokes equations as [60]

$$\frac{\partial}{\partial t}(\rho \mathrm{P})+\frac{\partial}{\partial x_i}(\rho u_i \mathrm{P})+\frac{\partial}{\partial \psi_k}(\rho S_k \mathrm{P})=\frac{\partial}{\partial x_i}\left[\rho\langle u_i^{"}|\psi\rangle \mathrm{P}\right]+\frac{\partial}{\partial \psi_k}\left[\rho\langle\frac{1}{\rho}\frac{\partial J_{i,k}}{\partial x_i}\middle|\psi\rangle \mathrm{P}\right] \tag{7}$$

where

P : Favre joint PDF of composition;
ρ : Mean fluid density;
u_i : Favre mean fluid velocity vector;
S_k : Reaction rate for species;
ψ : Composition space vector;
$u_i^{"}$: Fluid velocity fluctuation vector;
$J_{i,k}$: Molecular diffusion flux vector.

In Eq. (7), the terms on the left-hand side are closed, while those on the right-hand side are not and require modeling. The first term on the left-hand side is the unsteady rate of change of the PDF, the second term is the change of the PDF due to convection by the mean velocity field, and the third term is the change due to chemical reactions. The principal strength of the PDF transport approach is that the highly-non-linear reaction term is completely closed and requires no modeling. The two terms on the right-hand side represent the PDF change due to scalar convection by turbulence (turbulent scalar flux), and molecular mixing/diffusion, respectively.

The turbulent scalar flux term is unclosed, and is modeled in ANSYS Fluent by the gradient-diffusion assumption

$$-\frac{\partial}{\partial x_i}[\rho\langle u_i^{"}|\psi\rangle \mathrm{P}]=\frac{\partial}{\partial x_i}\left(\frac{\rho\mu_t}{Sc_t}\frac{\partial \mathrm{P}}{\partial x_i}\right) \tag{8}$$

where

μ_t : is the turbulent viscosity and
Sc_t : is the turbulent Schmidt number.

3. Results and Discussion

This study investigated the mechanisms of auto-ignition reactivity under operation parameters in which the fuel was natural gas. Therefore, it is important to understand how these parameters influence the auto-ignition process of HCCI engine on the one hand, and on the other hand, the focus of this paper was on PPC internal combustion engine (ICE) conditions. The mixture air-fuel enters the cylinder at an intake charge temperature (T_{IVC}) and intake charge pressure (P_{IVC}). In the compression stroke, the volume of the chamber reduces because the piston moves from BDC to TDC. Furthermore, the mixture is compressed, so the pressure and temperature of the fuel-air mixture gradually increases, leading to ignition. The effect of ϕ and CO_2/CH_4 fraction rate on the performance characteristics was assessed.

3.1 Combustion Parameters

Figure 2 shows the effect of equivalent ratios (ϕ=0.3, 0.45, 0.5, 0.6) on different combustion parameters using ANSYS CHEMKIN-Pro software. It can be seen that an increase in ϕ led to increased values of in-cylinder pressure (see Figure 2(a)), in-cylinder temperature (see Figure 2(b)), net heat release rate (see Figure 2(c)), CO molar fraction (see Figure 2(d)), UHC (see Figure 2(e)) and NO_X emissions (see Figure 2(f)). According to the ϕ=0.3 to 0.6, predicted peak in-cylinder temperatures range from 2107.61K to 2693.70K as shown in Figure 2(b). It can be concluded from Figure 2(a), that with higher ϕ, more heat is released which in turn leads to increase in-cylinder pressures [18].

Figure 2(c) shows the net heat release rate (NHRR) profiles per crank angle (CA) for various ϕ at T_{IVC}=500K. It can be observed that the peak of the NHRR per CA increases rapidly when the ϕ goes from 0.3 to 0.6. These results are in agreement with those found in the literature. It can be seen that the NHRRs have a smaller peak around 6.57 deg bTDC for ϕ=0.3 while the peak occurs at a higher value of around 4 deg bTDC for ϕ=0.6. Furthermore, growing the ϕ causes the combustion to start later which hence increases the temperature and pressure of the cylinder (see Figure 2(b) & 2(a)). It shows also how the NHRR is extremely advanced, so that the pressure peak occurs around the TDC position [61]. The explanation is that for a higher ϕ more fuel is burned in the cylinder and therefore more heat is released, which leads to higher gas temperatures and pressures [18].

Equivalence ratios ϕ=0.3, 0.45, 0.5 and 0.6 were chosen and the predicted CO, UHC and NO_X levels are shown and presented in Figure 2(d), 2(e) and 2(f), respectively. The upward trend in NO_X levels can clearly be seen as the ϕ is increased. Furthermore, higher ϕ leads to higher indicated specific fuel consumption (ISFC) and IMEP because more fuel is injected and burning rates are higher, leading to a decrease in the ηi. The explanation is that for higher equivalence ratios, the heat losses are higher, thereby decreasing the thermal efficiency. It was concluded that, increasing the ϕ takes a toll on the thermal efficiency of the engine [18].

Figure 3 shows the variation of in-cylinder temperature and NO_X emissions with different CH_4 fractions in the mixture (50%:CH_4- 50%:CO_2), (90%:CH_4- 10%:CO_2). However, when the CO_2 fraction rate decreased in the mixture, this led to an increase in-cylinder temperature and NO_X emissions rate. This can be explained by the fact that when the temperature is high in the combustion chamber it contributes to a higher emission of nitrogen oxides.

Figure 4 shows the engine parameters (in-cylinder pressure, work done, laminar flame speed, NO emissions) and the effects of four compositions that were studied (CH_4:42%, CO_2:58%), (CH_4:60%, CO_2:40%), (CH_4:80%, CO_2:20%), (CH_4:100%) using ANSYS-Fluent software. It can be seen from Figure 4(a), increasing the peak pressure values with the reduction of CO_2 fraction and increasing the CH_4 fraction. This is due to faster combustion and improved thermal efficiency because of a higher CH_4 concentration [62, 27].

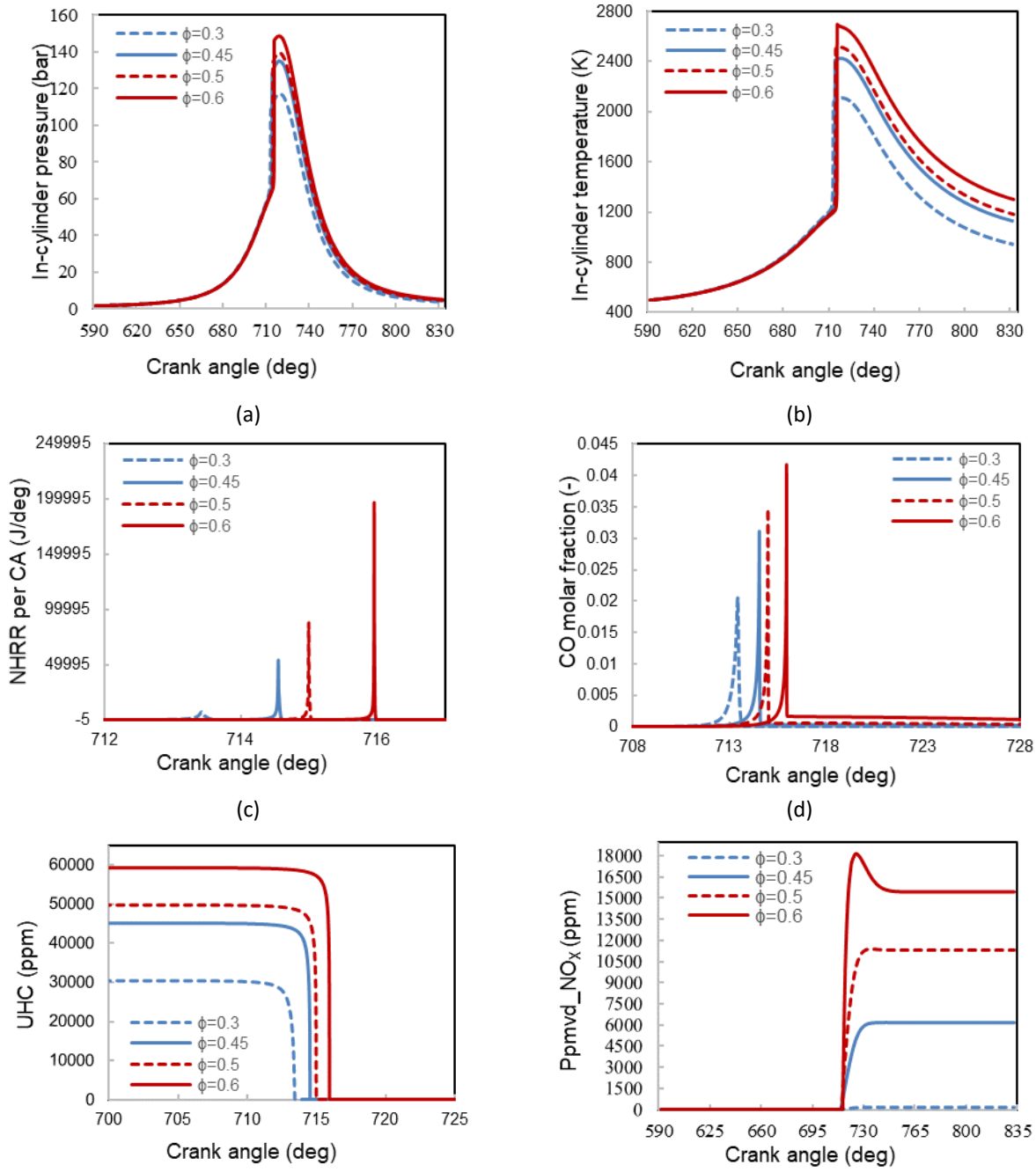


Fig. 2. Variation of (a) cylinder pressure; (b) cylinder temperature; (c) NHRR; (d) CO molar fraction; (e) UHC and; (f) NO_X emissions with crank angle according to the ϕ. Intake conditions (P_{IVC}=1.8bar, T_{IVC}=500K, CR=18, engine speed=2000rpm)

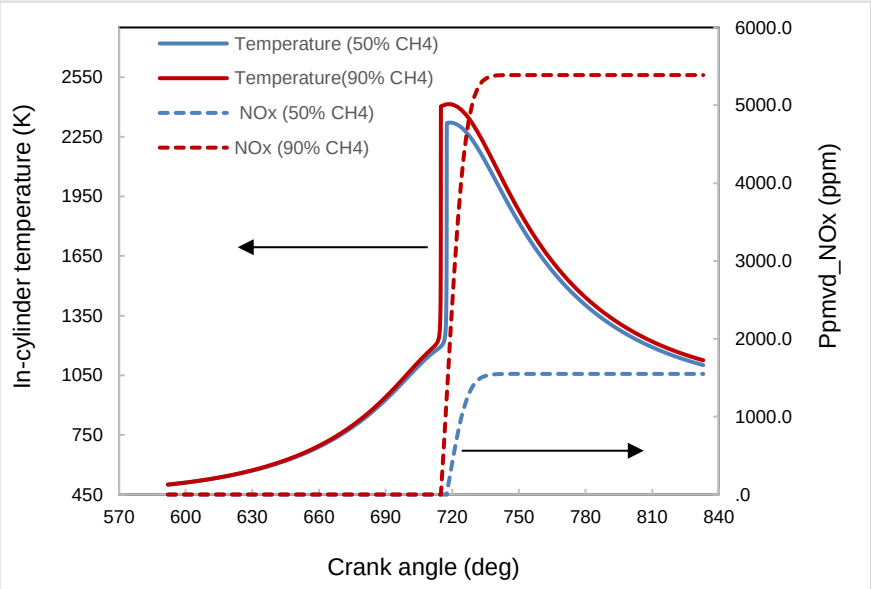


Fig. 3. Variation of cylinder temperature and NO_X emissions with crank angle according to the different methane compositions. Intake conditions (P_{IVC}=1.8bar, CR=18, ϕ=0.45, engine speed=2000rpm)

The decrease in CO_2 in the mixture led to an advanced combustion phase and an increase in the duration combustion, as shown in Figure 4 and Figure 6. The maximum laminar flame speed was observed as 25.46m/s (15.5 deg bTDC) for pure methane, while it reached at 24.72m/s for (CH_4:60%, CO_2:40%) in the same position (see Figure 4(c)). It is clear that adding CO_2 to methane causes a decrease in speed. Figure 4(d) shows the NO_X level increases with the increase in CH_4 concentration in the mixture. This is due mainly to the temperature increase, see Figure 5. This figure shows the temperature distribution contour near TDC (7 deg aTDC). It is concluded that a reduction in the peak cylinder temperature is due to addition of the CO_2 fraction to the mixture. Increasing the CO_2 concentration from 20% to 58% led to decreases at 380K in temperature distribution. We can also notice that the cylinder temperature distribution is actually uniform throughout the combustion chamber (see Figure 5). This is because the flame has dominated the whole combustion chamber. It can be explained by auto-ignition in several spots and the absence of flame propagation.

The mixture with 80% CH_4 burns more rapidly compared to 60% CH_4, which burns more rapidly than the mixture with 42% CH_4 and so forth. This is explained by the higher thermal efficiency due to higher CH_4 concentration [27]. We notice that combustion is homogeneous in the combustion chamber due to the dilution of the fuel by CO_2 [27]. The lower the dilution, the faster the auto-ignition and occupying the maximum of the volume of the combustion chamber.

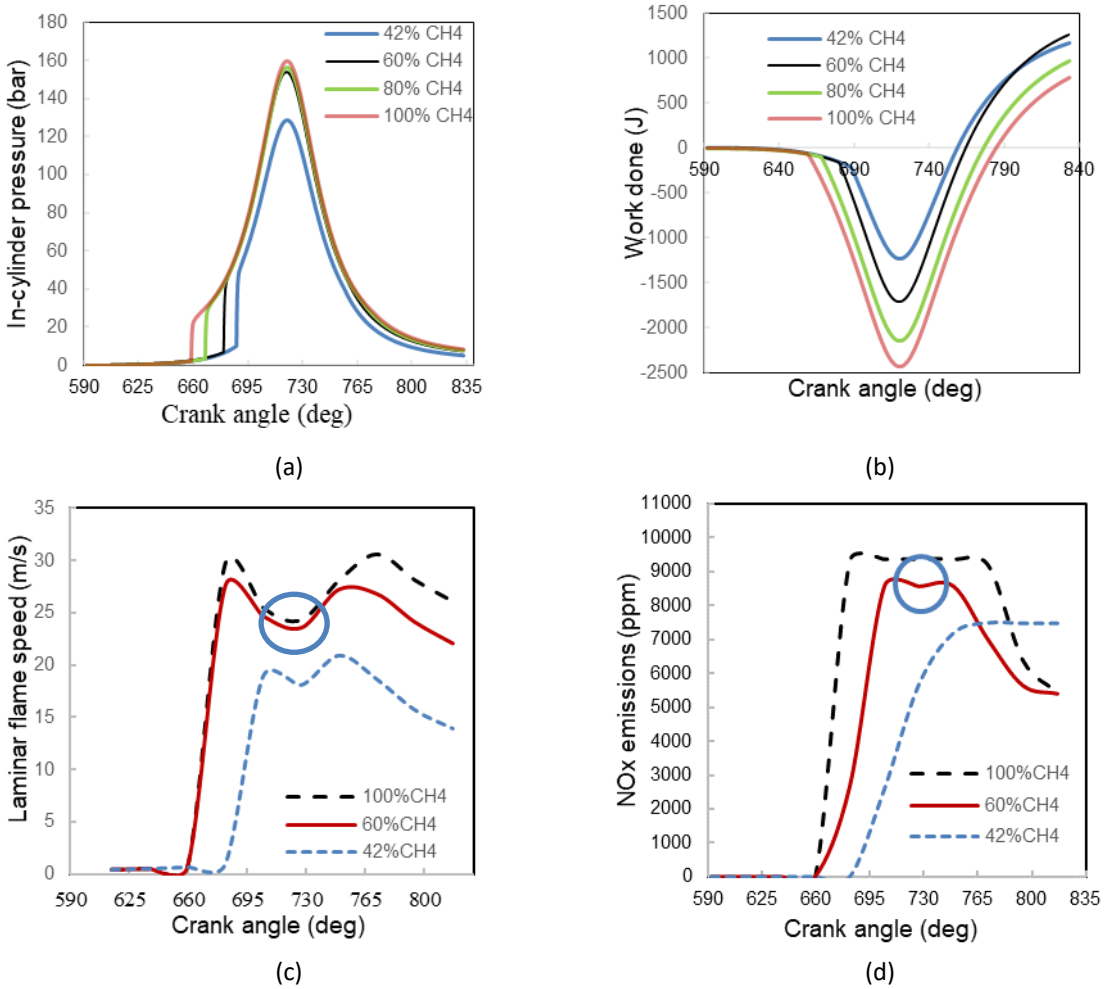


Fig. 4. Effect of different methane compositions on calculated (a) cylinder pressure; (b) work done; (c) laminar flame speed and; (d) NO emissions with crank angle according to the different methane compositions

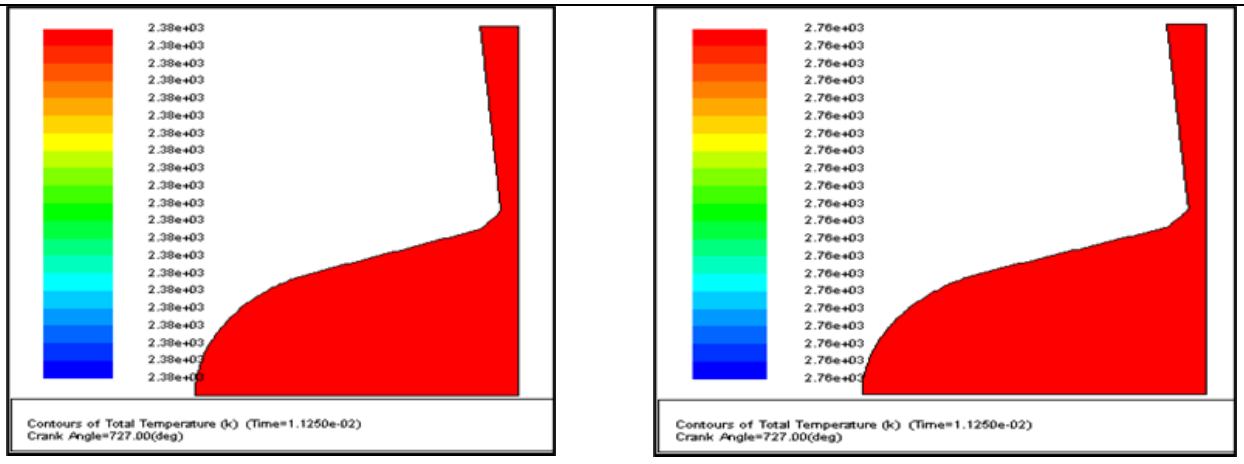


Fig. 5. The contour of temperature distribution for different concentrations of CO_2 in mixture

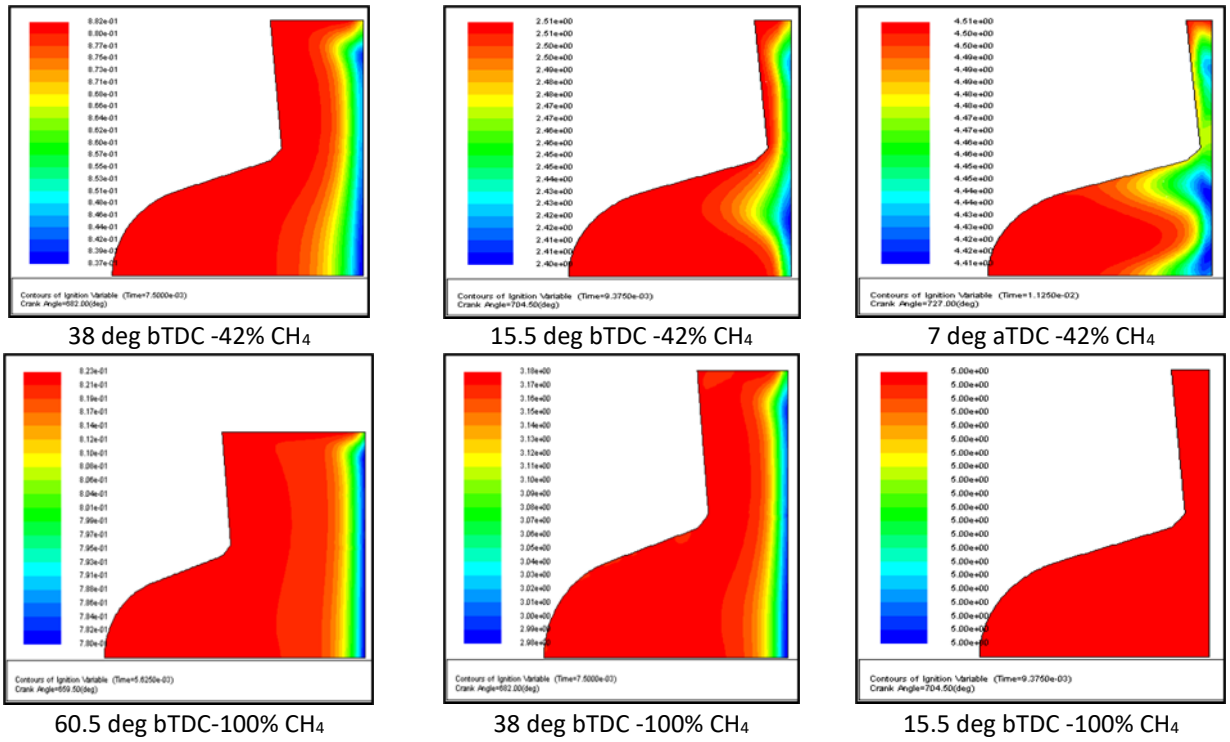


Fig. 6. The contour of ignition variable for different concentrations of CO_2 in mixture

3.2 Model Validation

During last two decades, there have been some studies on the performance and engine emissions. The effect of the biogas composition on the emissions of CO and NO_X was investigated numerically by Mokrane *et al*., [27] and it was concluded that the concentration of carbon dioxide (CO_2) in the biogas has an important effect on reducing NO_X and CO emissions. Furthermore, we found a study made by Sharath *et al*., [26] made a comparison of PCCI and PPC modes using the ANSYS-Fluent software. It was concluded that the PPC mode is a better viewpoint in engine design. Meanwhile, Lee *et al*., [33] concluded that when the CO_2 fraction changed from 0% to 50%, carbon monoxide (CO) and unburned hydrocarbons (UHC) emissions increased, while NO_X emissions decreased. We can find more information about the subject of this study in previous papers [63-66].

4. Conclusions

In this paper, the characteristics of HCCI engine and PPC mode were numerically investigated by ANSYS CHEMKIN-Pro software and ANSYS-Fluent, respectively to study the effect of carbon dioxide (CO_2) fraction on engine performance parameters. The study yielded the following conclusions

i. For a higher equivalence ratio, more fuel is burned in the cylinder and therefore more heat is released, which leads to higher gas temperatures and pressures on the one hand and on the other hand takes a toll on the engine's thermal efficiency.
ii. The quantity of NO_X emission increases as the ϕ increases due to the high combustion temperature.
iii. The auto-ignition phenomenon in the engine is the reaction kinetics of fuel under the transient temperature and pressure conditions by the piston movement.

iv. It was clear that HCCI combustion was more practical for very lean mixture. Furthermore, it was found that the peak in-cylinder pressure and temperature increased with the equivalence ratios variation and the pressure peak occurred around the TDC position.
v. The concentration of CO_2 in the mixture has an important effect on reducing temperature in the cylinder and thus leads to a decrease in NO_X emissions in the PPC mode. Moreover, the temperature is uniform throughout the combustion chamber.
vi. The HCCI engine model has a low temperature compared to the PPC mode.

The results revealed that the CO_2 fraction is important and valuable. These can improve the combustion and performance characteristics of the HCCI engine on the one hand, and on the other hand, flame propagation was absent and the temperature distribution was uniform throughout the combustion chamber of the PPC mode.

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