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Numerical Investigation of Combustion in HCCI Diesel Engine Fuelled with Biodiesel Blends

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***Abstract*—Homogeneous Charge Compression Ignition (HCCI) is an advanced combustion technology being considered for internal combustion engines due to the potential for high fuel conversion efficiency and extremely low particulate matter (PM) and Nitrogen Oxides (NOx) emissions. In HCCI engines, there is no direct control method for auto ignition time. A common method to indirectly control the ignition timing in HCCI combustion engines is altering engine's parameters which can affect the combustion. Previous research has indicated that fuel chemistry has a strong impact on HCCI combustion. This work introduces a new predictive multi-zone model for the description of combustion in HCCI engines. A multi zone model with reduced fuel chemistry was developed to simulate the combustion process in HCCI engines and predict engine performance. In this work, a parametric study on Diesel/Biodiesel blends(D80B20) HCCI combustion is conducted in order to identify the effect of equivalence ratio values (0.1786, 0.27, 0.37, and 0.4762) on combustion and engine performance parameters. Two kinds of parameters will be discussed. First, in-cylinder pressure, temperature and net heat release rate diagrams at altering Diesel/Biodiesel dose (0%, 20%, 40%, 60%), then the second category, the variation of start of combustion and combustion duration which are performance parameters of HCCI Diesel Engine.**

Keywords*—HCCI engine, Multi-zone model, Biodiesel, Chemical Kinetics Mechanism

I. INTRODUCTION

THE HCCI combustion process is characterized that combining the advantages of both spark-ignition (SI) engines and compression ignition direct injection (CIDI) engines[1]. In HCCI combustion engines, the air/fuel homogenous mixtures are compressed and self-ignited occurs in the cylinder when the mixture temperature and pressure reach fuel ignition, the auto ignition takes place simultaneously at multiple locations throughout the entire combustion chamber. The mixture auto-ignites uniformly without any external ignition device such as the spark plugs or fuel injectors. The principle of HCCI engine operates a diluted and HCCI combustion processes and ignition is controlled by chemical kinetic reaction rates of the mixture [2, 3]. Therefore, controlling the timing of ignition and burning rate is more difficult in an HCCI engine compared to a conventional diesel engine.

The reactivity of fuels and auto ignition is the important parameter that affects HCCI combustion characteristics. Consequently, the combustion of HCCI will be influenced by controlling the temperature, pressure, and composition of the fuel and air mixture. The HCCI combustion process has the potential to improve thermal efficiency and reduce nitrogen oxides (NOx), soot emission [4]. However, there are many challenges remaining before applied HCCI to commercial use such as controlling start of combustion as a result, lack of ignition control mechanism and a limited operation range of HCCI engine. Some methods are used to realize the control method of the mixture autoignition and overcome the disadvantage of HCCI, such as heating the intake air [5], increasing the compression ratio [6] and reactivity of multi fuel [7]. Fuel flexibility from the most important characteristic of HCCI. Many types of research focused on the effects of different fuel physical and chemical properties on the combustion. The use of multiple types of fuel has the potential to the expansion of the HCCI operating rang and controlling combustion rate of HCCI [8]. The basic idea is to use different types of fuel with different self-ignition characteristics such as diesel fuel and Biodiesel. Biodiesel is one of the "alternative" fuels that contribute to the solution of energy problems in the future.

It can be seen that HCCI combustion process has many benefits in raising the thermal efficiency and reduce emissions. HCCI offers flexible use of multiple fuels to reduce dependence on fossil fuels. The study is carried out using a multi-zone model. This model is a simplified way to represent the HCCI combustion process. Kongsereeparp [9] developed a segregated multi zone model. Work and heat transfer between zones were considered but there was no mass transfer between them. Temperature differences between the cylinder wall, piston crown and cylinder head were considered, too. Various fuels with different octane numbers were used as engine fuel. Results showed that the model could predict in-cylinder pressure, accurately. But the results were not reported about emissions prediction.

A new multi zone model was developed by Kodavasal et al. [10]. In this model there were no mass and heat exchanges between zones. It is noted even though the zones have had constant mass distribution, their volume fractions have changed at different time steps. Heat has transferred from all of zones to walls. Gasoline was used as HCCI engine fuel and model has had a satisfactory accuracy in pressure prediction. There were no reported results for emissions.

Guo et al. [11] developed another multi zone model, which was contained boundary layer, crevice and some core zones. Heat transfer was considered between zones but there was no mass transfer between them. The multi zone model was able to reasonably capture the experimentally measured cylinder pressure variations over a range of operation conditions. It also provided qualitative trends of CO emissions. The numerical simulation over predicted the combustion completeness at ultra-high air/fuel ratios and higher engine speeds. Some differences were detected between the experimental and numerical data for NOx emissions.

The main purpose of this paper is to develop a multi zone model for HCCI engine to predict the engine combustion,

performance and emission characteristics accurately for different types of fuels in a wide range of operating conditions. More attention was paid on zones configuration, accurate estimation of trapped conditions and heat and mass transfer between neighboring zones.

II. METHODOLOGY

A. Engine simulation model

Engine closed loop is simulated by a multi-zone model. Multi-zone model is coupled with a single-zone model for gas exchange process simulation. Temperature and composition are assumed to be uniform in each zone and pressure is assumed to be uniform throughout the cylinder at each time step. Model is clarified in detail in published literature [12, 13]. Zone configuration is shown in Fig. 1[12]. Model contains four types of zones including core, boundary layer, crevice and outer zones that are located between core and boundary layer. Heat and mass transfers are considered between zones and there is heat transfer between boundary layer zone and combustion chamber walls. For each zone, first law of thermodynamics equation and chemical kinetic equations are solved, simultaneously. Eqs. (1–8) are the governed equations [14].

$$\frac{dU_i}{dt} = -\frac{dW_i}{dt} + \frac{dQ_i}{dt} \quad (1)$$

$$\frac{dU_i}{dt} = C_v^i \frac{dT_i}{dt} + m_i \sum_{j=1}^{n_s} u_{j,i} \frac{dY_{j,i}}{dt} + \sum_{j=1}^{n_s} u_{j,i} Y_{j,i} \frac{dm_i}{dt} \quad (2)$$

$$\frac{dW_i}{dt} = P \frac{dV_i}{dt} \quad (3)$$

$$\frac{dQ_i}{dt} = \frac{dQ_{i,cond}}{dt} + \frac{dQ_{i,conv}}{dt} + \frac{dQ_{i,mtran}}{dt} \quad (4)$$

$$\frac{dQ_{i,cond}}{dt} = -KA_i \frac{\partial T}{\partial Z} \quad (5)$$

$$\frac{dQ_{BL,conv}}{dt} = h(T_{wall} - T_{BL})A_{wall} \quad (6)$$

$$\frac{dQ_{i,mtran}}{dt} = \frac{dm_{in,i}}{dt} H_{in} - \frac{dm_{out,i}}{dt} H_{out} \quad (7)$$

$$\frac{dY_{k,i}}{dt} = \frac{\dot{\omega}_{k,i} Mw_k}{\rho_i} \quad (8)$$

B. Chemical Kinetic Mechanism Operating Condition and Validation

A skeletal mechanism with 115 species and 460 reactions for a tri-component biodiesel surrogate, which consists of methyl decanoate, methyl 9-decenoate and n-heptane, was developed to reduce computational costs for 3-D engine simulations. The detailed mechanism for biodiesel developed by Lawrence Livermore National Laboratory (LLNL) was employed as the starting mechanism. The rate constants for the n-heptane and larger alkane subcomponents in the detailed mechanism were first updated. The detailed mechanism was then reduced with direct relation graph (DRG), isomer lumping, and DRG-aided sensitivity analysis (DRGASA), which was improved to achieve a larger extent of reduction. The reduction was performed for pressures from 1 to 100 atm and equivalence ratios from 0.5 to 2 for both extinction and ignition applications.

The initial temperatures for ignition were from 700 to 1800 K, covering the compression ignition (CI) engine conditions. Extensive validations were performed against 0-D simulations with the detailed mechanism and experimental data for spatially homogeneous systems, 1-D flames and 3D-turbulent spray combustion. The skeletal mechanism was able to expect various combustion characteristics precisely such as ignition delay, flame lift-off length, and equivalence ratio at flame lift-off location under different ambient conditions. Compared with the detailed mechanism that consists of 3299 species and 10806 reactions, the skeletal mechanism features a reduction by a factor of around 30 in size while still conserving good accuracy and comprehensiveness [15].

C. Wall Heat Transfer

Wall heat transfer affects the thermal stratification inside the cylinder and the combustion behavior of HCCI engines. In order to provide a trustworthy prediction of the interaction with the boundaries, the present multi-zone model adopts a wall-function model for estimating the heat exchanged with the cylinder walls and the piston surface. The worldwide Woschni relationship for the heat exchange has been suggested for HCCI engine studies [16, 17], despite the fact that the conditions in the HCCI combustion differ fundamentally from those considered in the first work went for CI engine. However, the engine wall heat transfer sub-model has been activated and the convective heat flux and coefficient are represented by Eqs. (9-11) as the following [16, 17],:

$$\dot{Q} = hA(T - T_{wall}) \quad (9)$$

$$h = 129.8\, B^{-0.2} P^{0.8} T^{-0.55} \omega^{\,0.8} \quad (10)$$

$$\omega = [(C_{11} - C_{12} \frac{\gamma_{swiral}}{\bar{S}_p})]\bar{S}_p + C_2 \frac{V_d T_i}{P_i V_i}(P - P_{motored}) \quad (11)$$

TABLE 1
VALUES OF HEAT TRANSFER SUB-MODEL COEFFICIENT [16, 17]

Coefficient	Values
Coefficient “a”	0.035
Coefficient “b”	0.71
Coefficient “c”	0.0
C_{11}	2.28
C_{12}	0.0
C_2	0.00334
Prandtl Number “pr”	0.7

where B is the cylinder bore, P is the cylinder pressure, T is the cylinder temperature, ω is the average cylinder velocity gas, S_p is the mean piston speed, C_{11}, C_{12} and C_2 are modeling parameters. The model coefficients are represented in Table 1. Also, γ_{swiral} is the swirl velocity, V_d is the displacement volume, $P_{motored}$ is the motored cylinder pressure, T_i, V_i and P_i are the initial temperature, volume and pressure inside the

cylinder, respectively. The model that describes the combustion process in the HCCI engine was based on the first law of thermodynamics, the mass balance, and variable of the in-cylinder volume, simultaneously. The model assumptions for all the chemical species are an ideal gas, constant masses, neglecting the kinetic and potential energy, and uniform in the temperature in the whole thermodynamics system. The predictions of the heat transfer crossing through the combustion chamber boundary to the surroundings and the work exchange at the combustion chamber due to the variation of pressure and volume have been considered. All the used governing equations are solved simultaneously during the simulation run and all the details of the model can be found in the original reference text [18].

III. MODELING

Computer simulation of engines is a significant tool in analyzing the effect of input variables like intake pressure, temperature, and fuel mixture. It also reduces the need for expensive engine tests for engine study. A zero-dimensional, multi-zone combustion model has been utilized in the present study [19, 20]. The principle aim of the employed model is to recognize the auto-ignition and combustion history throughout the engine stroke, starting from the suction and ending to the heat rejection stroke. This model can predict all the combustion process such as auto-ignition events, ignition delay, and heat transfer losses through the engine cylinder wall. The model is made under assumption of the charge inside the engine cylinder is homogenous in temperature in each proposed zone.

The simplest HCCI modeling Single zone models assume that the thermodynamic state of the mixture is uniform inside the combustion chamber. No variations in the temperature, pressure, or mixture composition are considered. In-cylinder fluid motion is neglected, Cylinder charge was considered to behave as an ideal gas. The package used to model combustion and chemical kinetics of the HCCI combustion is called CHEMKIN-PRO. This software is one of the most known packages for solving complex chemical kinetics problems and allows the user to calculate species concentrations, heat release rate, temperature, and pressure history of the combustion.

The engine geometry was divided into different regions configuration. There are three main regions inside the engine cylinder containing crevice region, boundary layer region, and core region. The mass inside the cylinder is separated into zones for the chemical kinetic examination. Every zone has the identical immediate pressure, although all zones have entity temperature and chemical composition. Ten zones model have been suggested for this investigation. The suggestion of the mass distribution for this work is set as represented in Table 2. The zone mass percentage is kept constant during the whole chemical kinetic process inside the engine cylinder [21].

TABLE 2
ZONE CONFIGURATION USED FOR 10 ZONES MODEL.

Zone Number		**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
10 Zones model	**Mass %**	0.5	0.5	1	1	2	3	7	20	30	35
	Area %	5	5	5	10	10	15	15	15	10	10

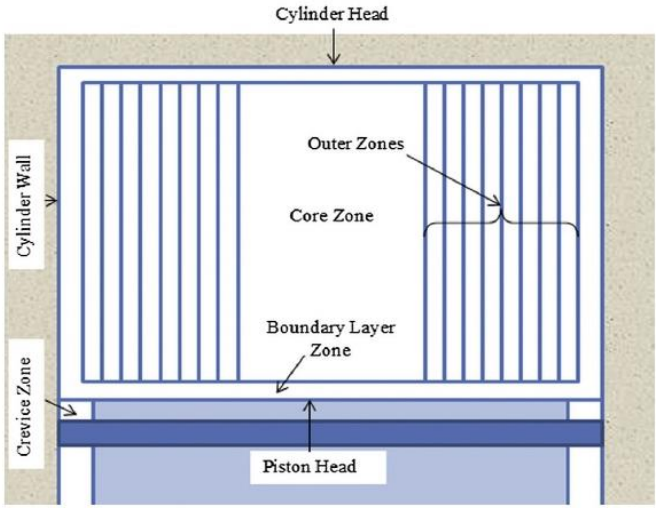

Fig. 1 Geometry of zones [12]

However, the temperature histories of each zone inside the engine have been used to validate the assumption of zone configuration. The average temperature of multi-zones model was numerically calculated by using the multi-zone model.

TABLE 3
ENGINE CIRCUMSTANCES FOR THE MEASURE EXPERIMENTAL AND NUMERICAL RUNS

Fuel–air equivalent ratio ϕ	0.1786	0.27	0.37	0.4762
Engine load relative to maximum load %	15 %	35%	55%	75%
Engine operating conditions	Low load	Moderate load	High load	knocking
Engine power (KW)	0.855	1.995	3.135	4.275
BMEP (KPa)	82.88	193.38	303.88	414.38

IV. RESULTS AND DISCUSSIONS

In this work, a single cylinder four stroke HCCI engine with specification as described in table 4 was tested to evaluate the combustion parameters of biodiesel fuels mathematically.

TABLE 4
DIESEL ENGINE SPECIFICATION

Engine Parameter	**Specification**
Engine type	"DEUTZ FL 511/A."
No. of cylinder	1 cylinder
Bore	100 mm
Stroke	105 mm
Displacement	825 cm^3
Compression ratio	17
Power	7.7 HP =5.7 KW
Engine speed	1500 RPM (Fixed)
Cooling type	Air cooling
Direction of rotation	Counter- clockwise
Weight	116 Kg
Oil Capacity, approx.	2.4 L

Lubrication system	Forced circulation
Piston crown clearance	1– 1.2 mm
Inlet valve opens	32° before TDC
Inlet valve closes	59° after BDC
Exhaust valve opens	71° before BDC
Exhaust valve closes	32° after TDC
Injection release pressure	115 bar

Fig. 2 depicts the variation of the in-cylinder zone temperature histories from simulation work with respect to the crank rotation angle for 10-zones model at moderate load. The first aim of the proposed work is to find out the combustion parameters of HCCI diesel engine fueled with 20% Biodiesel blend. From the simulation result of the 20% Biodiesel HCCI combustion chemistry analysis, it was found that, the two-stage heat release or two stage combustion process involving low temperature oxidation (LTO) stage followed by high temperature oxidation (HTO) stage separated by a time delay between them is attributed to negative temperature coefficient (NTC).

The first stage of heat release is associated with low temperature kinetic reactions (Low Temperature Oxidation, LTO) and the second that much stronger one (main reaction) is the High Temperature Oxidation (HTO). About 7-10% of the energy is released during the LTO and the rest is released during HTO. Ignition delay can be defined as the time interval between the start of fuel injection and the start of combustion. The Start and end of combustion can be defined as the crank angle when 10% and 90% of the cumulative heat release (HR) have taken place respectively. The combustion duration is often defined as the time between 10% and 90% cumulative heat releases. The start of combustion was controlled using equivalent ratio for all fuel mixtures.

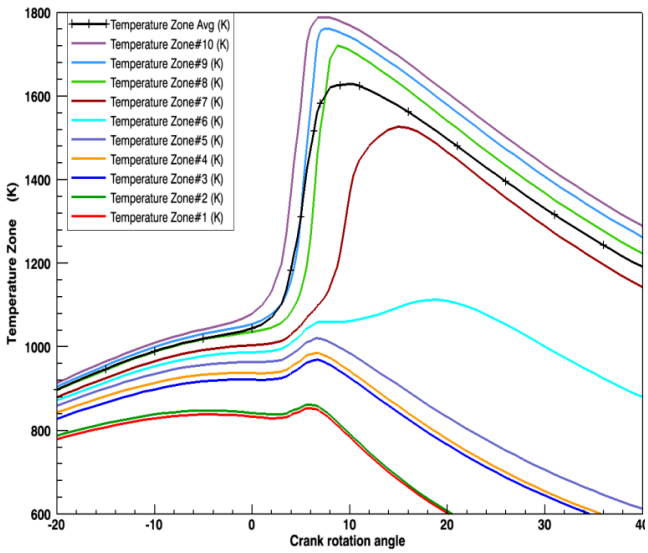

Fig. 2 The variation of the in-cylinder zones temperature for 10 zones model.

Table 5, Fig. 3 and Fig. 4 represent the Combustion parameters for 10 zone model for B20 % at different cases of equivalence ratio. From Fig. 3 we find that the value of maximum first stage of NHR, maximum second stage of NHR, maximum pressure and maximum temperature increase as a result of increasing equivalence ratio and this is expected as a result of increasing engine load. The combustion duration (CD) decreases with increasing equivalence ratio as represented in Fig. 3 and this is expected as a result of increasing engine load. Fig. 4 represent the rest of combustion parameters of 10 zone model with increasing equivalence ratio at B20 % and we find that the value of SOC is being negative because ignition occurs before TDC. the value of SOC is defined in both experimental and simulation data by measuring the crank angle corresponding to 10% of the cumulative heat release during the stage of the high temperature combustion process.

The second aim of the proposed work is the numerical investigation of the combustion parameters of HCCI diesel engine fueled with Diesel/Biodiesel blends (D100B0, D80B20, D60B40, D40B60).

Fig. 5 represent the Variation of the calculated pressure profile for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of maximum pressure decreases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the poor calorific values of biodiesel in comparison with diesel fuel. But for the same blend ratio, the value of the maximum pressure increases with increasing the equivalence ratio because of increasing engine load.

Fig. 6 represents the variation of the calculated Temperature profile for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of maximum temperature decreases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the poor calorific values of biodiesel in comparison with diesel fuel. But for the same blend ratio, the value of the maximum temperature increases with increasing the equivalence ratio because of increasing engine load.

Fig. 7 represents the variation of the Net Heat Release profile for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of both first and second peak of Net Heat Release decreases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the poor calorific values of biodiesel in comparison with diesel fuel. But for the same blend ratio, the value of both first and second peak of Net Heat Release rate increases with increasing the equivalence ratio because of increasing engine load.

Fig. 8 represents the variation of the value of maximum pressure for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of maximum pressure decreases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the poor calorific values of biodiesel in comparison with diesel fuel. But for the same blend ratio, the value of the maximum pressure increases with increasing the equivalence ratio because of increasing engine load.

TABLE 5

COMBUSTION PARAMETERS FOR 10 ZONES MODEL AT 20% BIODIESEL AT CASES OF EQUIVALENCE RATIO.

Equivelent Ratio (Φ)	1st stage of NHR		2nd stage of NHR		Max. Pressure		Max. Temperature		SOC	CD
	value	CA˚	value	CA˚	Value bar	CA˚	value ˚K	CA˚	CA˚	value
Φ_1=0.1786	18.83	-2.26˚	38.27	4.25˚	58.46	2˚	1456.9	9˚	-9˚	27.3
Φ_2=0.27	47.49	-6˚	107.485	6.424˚	66.56	6.5˚	1628.9	10˚	-15˚	16.88
Φ_3=0.37	56.39	-9˚	202.68	2.53˚	71.3	9˚	1852.6	13˚	-14˚	9.5
Φ_4=0.4762	102.58	-5.22˚	311.36	4.98˚	89.44	3˚	1983.3	16.8˚	-14˚	5.83

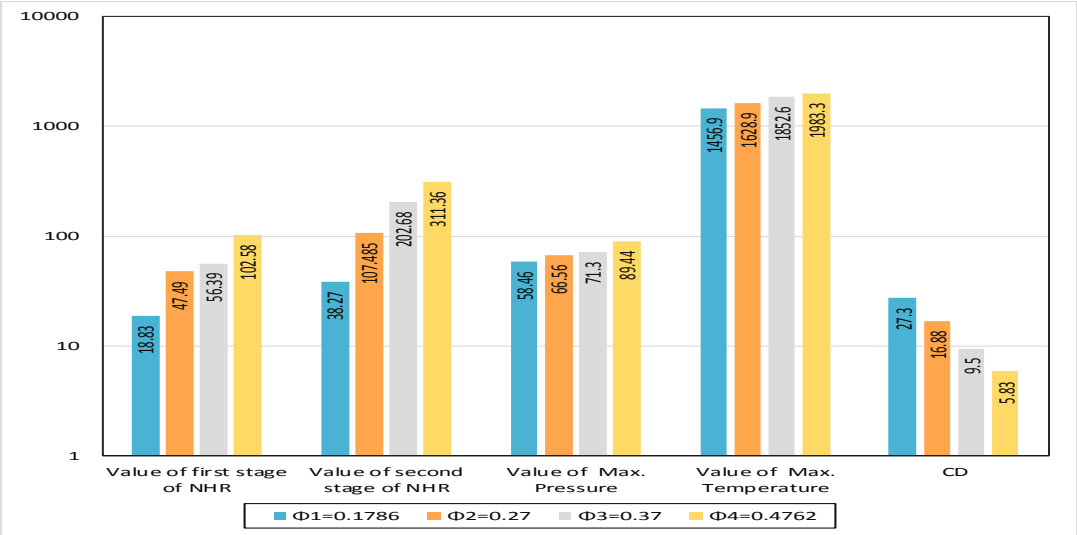

Fig. 3 variation of values of first stage of NHR, second stage of NHR, maximum pressure, maximum temperature and combustion duration for 10 zones model at cases of equivalence ratio.

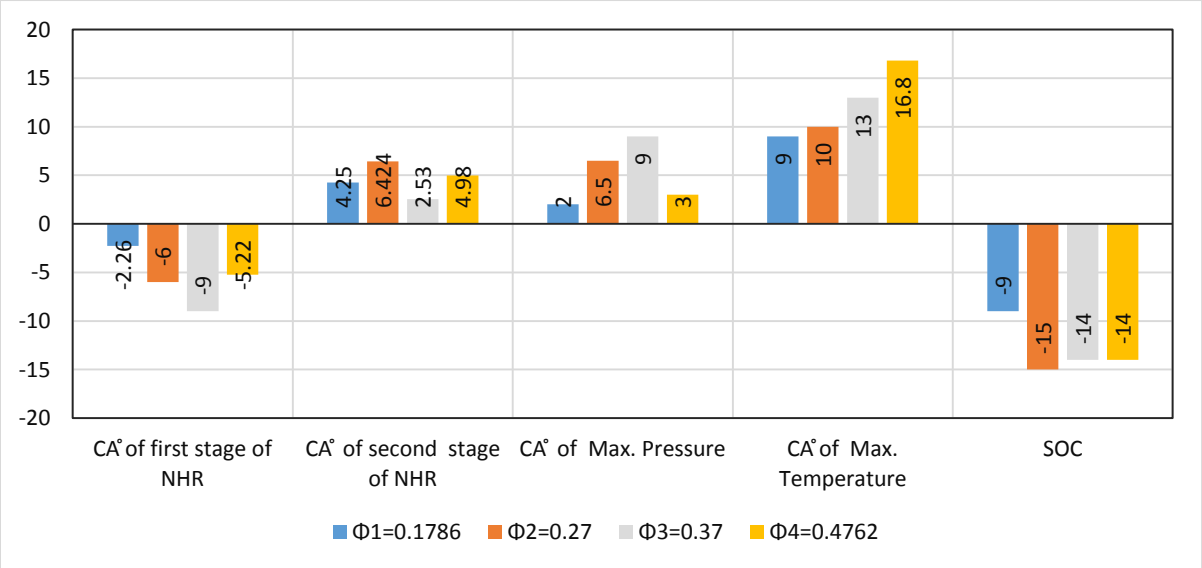

Fig. 4 variation of position of first stage of NHR, second stage of NHR, maximum pressure, maximum temperature and start of combustion for 10 zone model at cases of equivalence ratio.

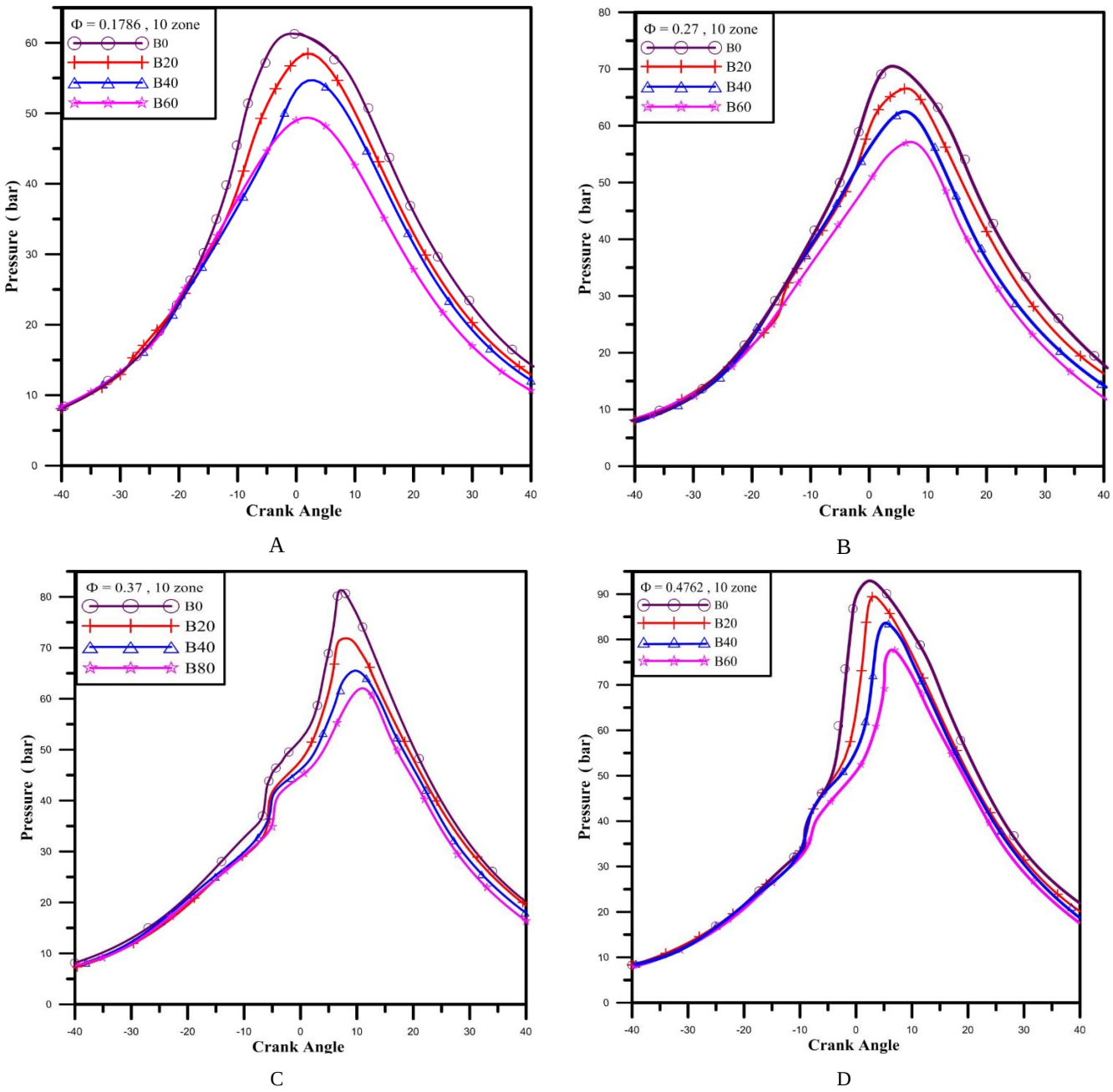

Fig. 5 Variation of the calculated pressure for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. However, the temperature histories of each zone inside the engine have been used to validate the assumption of zone configuration. The average temperature of multi-zones model was numerically calculated by using the multi-zone model.

Fig. 9 represents the variation of the maximum Temperature for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of maximum temperature decreases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the poor calorific values of biodiesel in comparison with diesel fuel. But for the same blend ratio, the value of the maximum temperature increases with increasing the equivalence ratio because of increasing engine load.

Fig. 10 represents the variation of the value of combustion duration for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. From the figure we find that the value of combustion duration increases with increasing the diesel/biodiesel blend ratio for the same equivalence ratio. This is owed to the decrease of the maximum temperature in comparison with diesel fuel (D100B0) as shown in Fig. 9. But for the same blend ratio, the value of the combustion duration decreases with increasing the equivalence ratio because of the increase of maximum temperature as a result of increasing engine load.

The obtained result of the 10-zones model depicts a good agreement with the engine experimental data only for smooth engine operation. The multi-zone model was insufficient to predict the combustion behaviors in the case of the engine knocking condition.

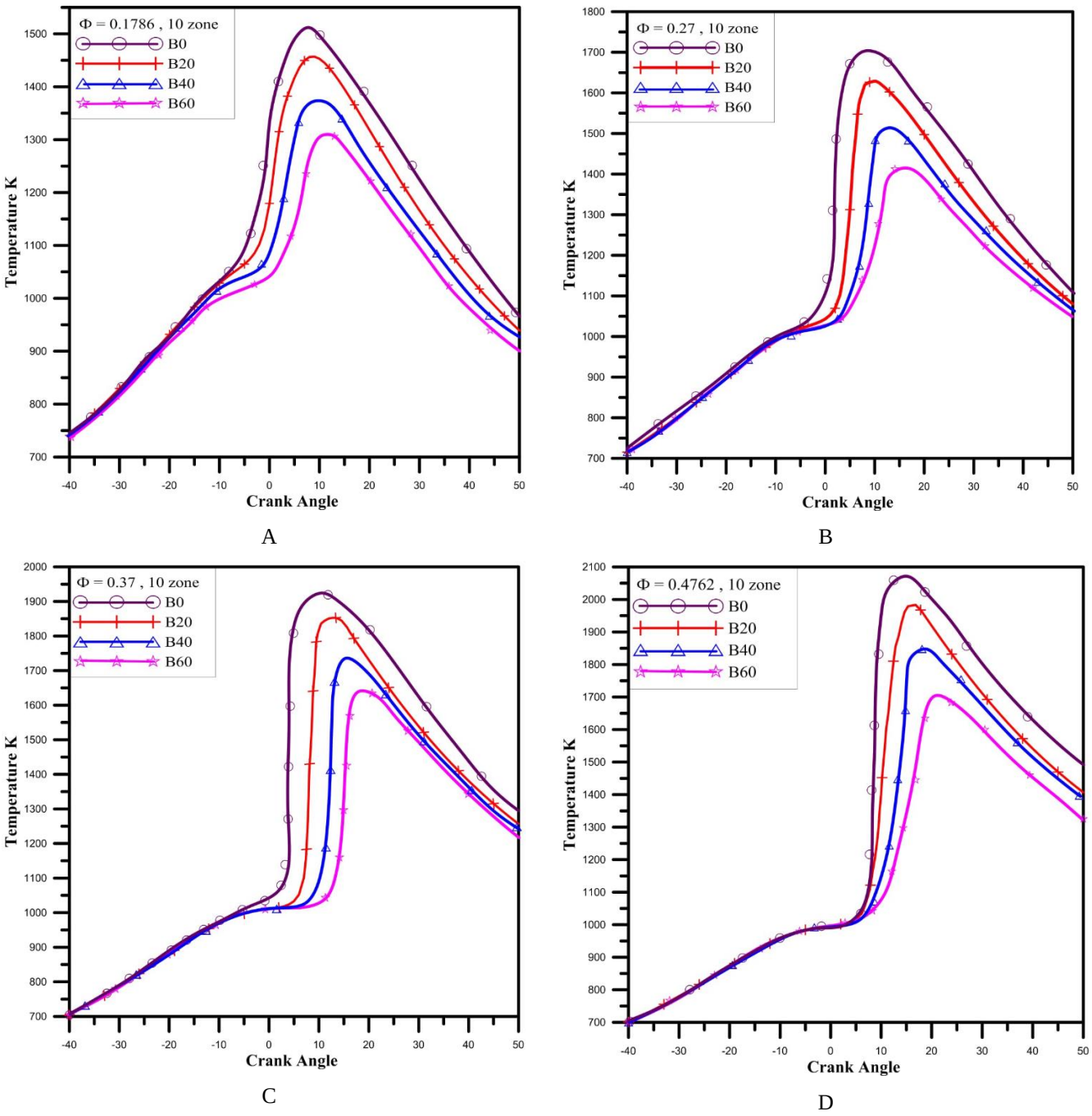

Fig. 6 Variation of the calculated Temperature for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. However, the temperature histories of each zone inside the engine have been used to validate the assumption of zone configuration. The average temperature of multi-zones model was numerically calculated by using the multi-zone model.

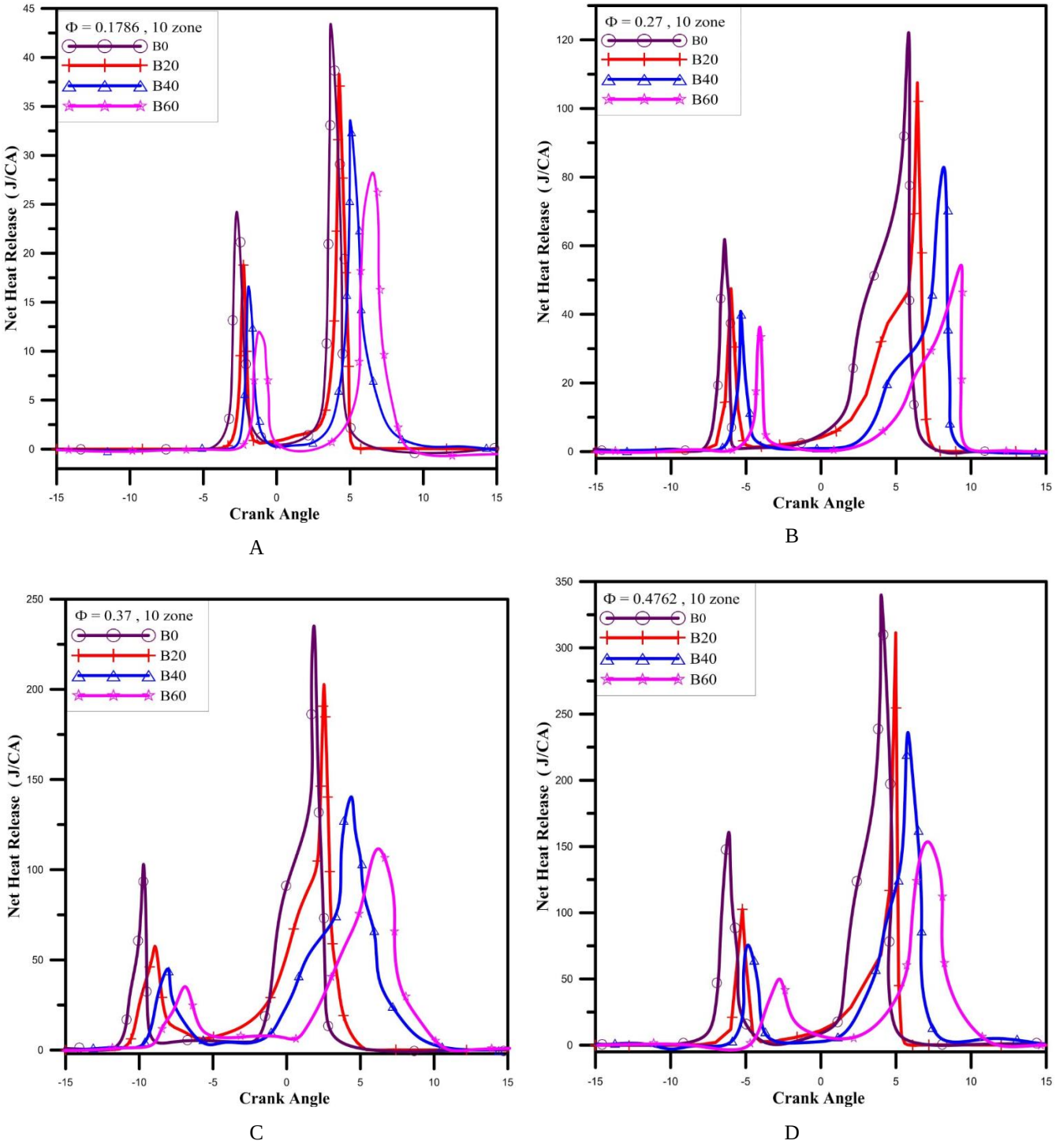

Fig. 7 Variation of the Net Heat Release for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3. However, the temperature histories of each zone inside the engine have been used to validate the assumption of zone configuration. The average temperature of multi-zones model was numerically calculated by using the multi-zone model.

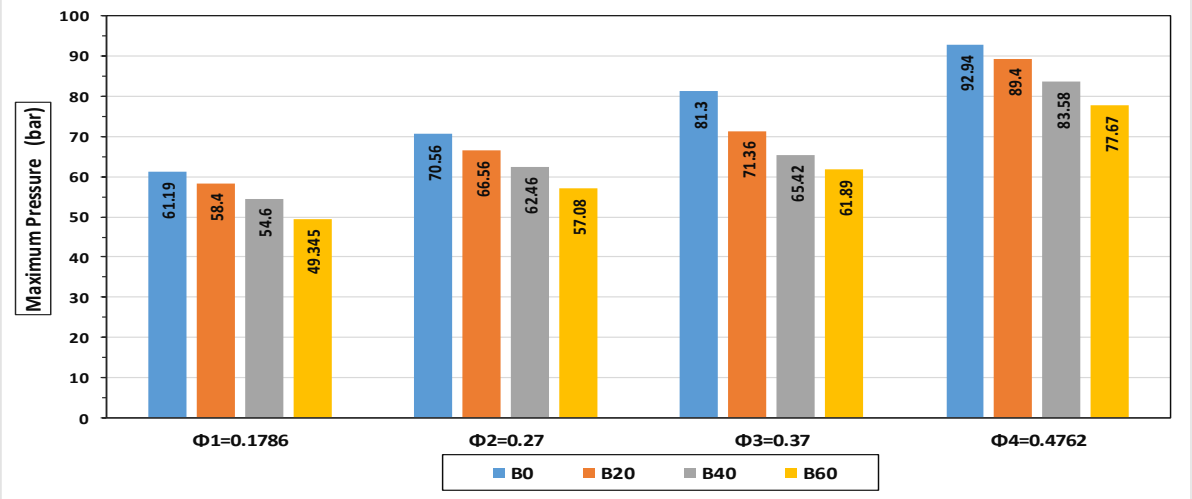

Fig. 8 Variation of the value of maximum pressure for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3

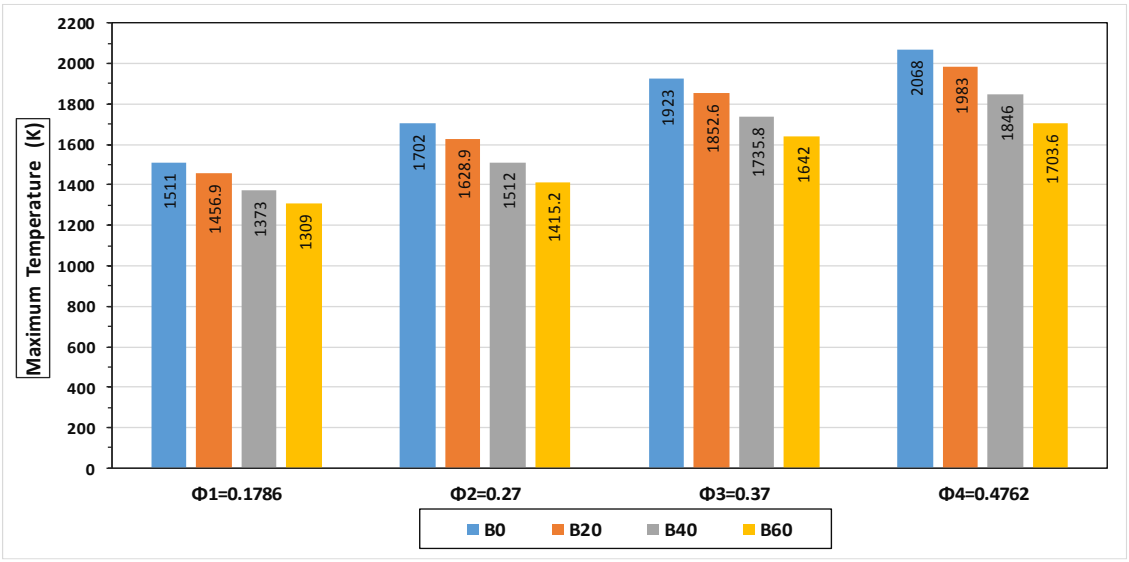

Fig. 9 Variation of the value of maximum temperature for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3

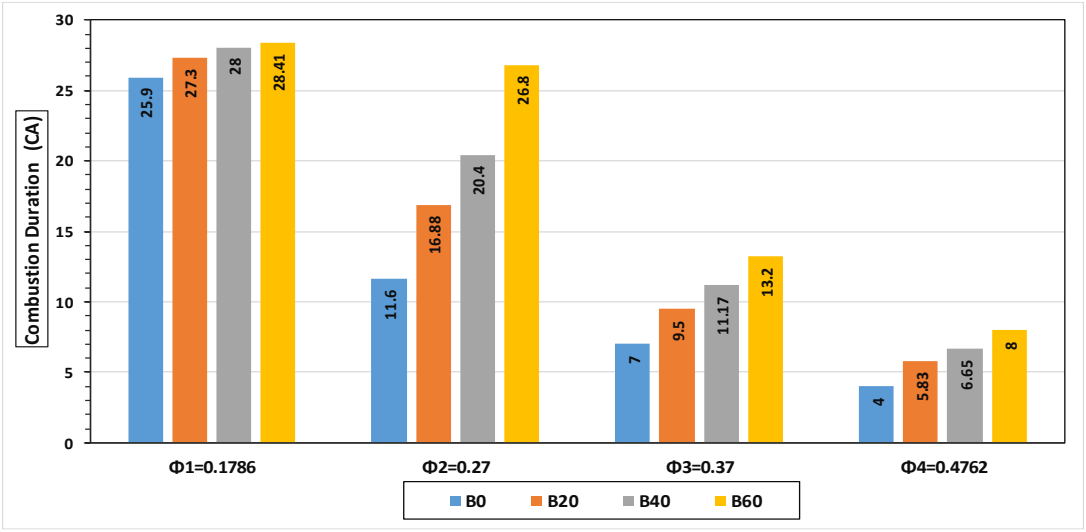

Fig. 10 Variation of the value of combustion duration for 10-zones model at different dose of Diesel/Biodiesel blends at different engine load, Cases of equivalence ratio represented in Table 3

V. CONCLUSIONS

All these features contribute in making the proposed multi-zone model a useful predictive tool to investigate combustion chemistry in homogeneous compression ignition engines. a new multi zone model is developed for HCCI engines simulation. Model contains four different types of zones, which are core, boundary layer, zones between them, and crevice zone. Heat and mass transfer are considered between all of zones. Semi detailed chemical kinetics mechanisms of fuels are used for their combustion simulation. A new heat transfer model is used for calculating convective heat transfer, which enhanced the model ability in prediction of combustion and performance characteristics of engine accurately. Model results are in good agreement with experimental data in prediction of in-cylinder pressure, temperature and net heat release.

VI. NOMENCLATURE

HCCI	Homogenous Charge Compression Ignition Engine
TDC	Top Dead Center
NO_x	Nitrogen oxide
PM	Particulate Matter
SI	Spark Ignition Engine
CIDI	Compression Ignition Direct Injection
CI	Compression Ignition
RPM	Revolution Per Minute
UHC	Unburned Hydro Carbon
CO	Carbon Oxide
CO_2	Carbon Dioxide
BTE	Brake Thermal Efficiency
HC	Hydrocarbon
BTDC	Before Top Dead Center
LTO	Low Temperature Oxidation
HTO	High Temperature Oxidation
NTC	Negative Temperature Coefficient
HR	Heat Release
NHR	Net Heat Release
SOC	Start of Combustion
CD	Combustion Duration
CA	Crank Angle

Subscripts

av	Average.

Greek symbols

Φ	Equivalence ratio.

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