



Development of Three-Zone Transitional Model for Reciprocating Internal Combustion Engine Analysis Using Gasoline

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Authors' contributions

This work was carried out in collaboration between all authors. Authors AAD and OBO designed the study. Author OBO did the analysis, managed the literature searches and wrote the first draft of the manuscript. All three authors managed design strategy of the study and approved the final manuscript.

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ABSTRACT

A three-zone model based on the first law of thermodynamics has been developed for analysis of combustion in an Internal Combustion Engine. The three zones included an unburned zone, burned zone and transitory zone which is a mixture of burned and unburned gases. The model was used to analyse an SI engine operating with gasoline fuel. An arbitrary constant for each of fractional burnt zone (CC2) and fractional unburned zone (CC1) leakages was varied using 0.0005, 0.00025, 0.001, 0.002, 0.005, 0.1 and 0.5. The engine operating conditions were set at a speed of 2000 rpm, -35bTDC ignition time and burn duration at 60°. The obtained indicated mean effective pressure (IMEP), thermal efficiency (η), cylinder pressure and emission characteristics from the developed model and those of two zone analysis were both compared with literature values. Most favourable results were observed at CC1 and CC2 values of 0.00025 and 0.005 respectively. We can conclude the 3zone model predicts better the IMEP, η , and peak cylinder pressure. However, no significant change was observed in values of emission characteristics of the 2zone and 3zone models. It is worthy of note that the number of zones affects engine performance evaluation and the higher the computational zone the better the engine prediction.

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NOMENCLATURES

W : work (J)
 P : pressure (Pa)
 c_v : specific heat at constant volume (J/kg/K)
 c_p : specific heat at constant pressure (J/kg/K)
 h : enthalpy (J/kg)
 m : mass (kg)
 Q : heat transfer rate across the system boundary into the system (J)
 R : specific gas constant (J/kgK)
 T : temperature (K)
 u : internal energy of material in the system (J/kgK)
 v : volume (m^3)
 θ : crank angle ($^\circ CA$)
 m_x : mass fraction burned

SUBSCRIPTS

b : burned
 u : unburned
 un : unburned burned
 v_1 : volume of fuel A
 v_2 : volume of fuel B
 l : leakage/blowby
 $mx1$: mass burn rate for fuel A
 $mx2$: mass burn rate for fuel B

1. INTRODUCTION

Continuous efforts are being made to develop a model for internal combustion engines, to improve predictive capability for design purpose aimed at more efficient and environmentally friendly characteristics. If the mathematical model of an engine is proposed with realistic assumptions and this is arranged as a computer code, the engine cycle and performance can be predicted. For this reason, cycle simulation studies have had great interest to date. Zero-dimensional, Multi-zone modeling based on conservation of mass and energy equations is often employed if the objective is to evaluate a large range of conditions, perform parametric studies and/or predict optimum engine settings with reasonable accuracy and fast computation on a PC system [1]. Analyses bordering on the effect of engine properties on performance have been widely researched. Varieties of parametric studies bothering on spark timing, burn duration and equivalent ratio have been carried out using the multi-zone model. Such analysis is found in works of [2-7]. Employing step by step evaluation of engine geometrical and thermodynamic properties, it is assumed three prominent periods

are considered for the engine operations. The three periods are namely, compression, combustion and expansion. Consequently, earlier dimensional modeling consists of two major zones, consisting unburned mixture and burned products. The existing multi-zone model is two zone model in nature, [8-11], but sometimes the estimates obtained are less accurate. Moreover, engine model zoning methods have not been exhausted and additional research is required. This necessitated efforts to modify the existing multi-zone model to improve the emission and efficiency predictive capabilities. For instance, Jose et al. [12], in revising the Engine Heat Transfer calculation modified the conventional Woschni's equation by using a new set of constants to accommodate the swirl originating from combustion. Kapriellian et al. [13] tried to conceptualize the dual fuel engine by investigating a three-zone model which consists of a reacting zone at the wall with a lower assumed burning rate, a fresh gas zone and a core of reacting zone. Stewart and Clarke [14] reported a three-zone model consisting of air only or air and gaseous fuel and the third zone of combustion products. Other attempts have been made to investigating combustion chamber model by dividing the burned zone into subzones [15-17].

In the present study, a three-zone model was developed for performance analysis which had unburned mixture consisting of the fresh charge, burned gas consisting of combustion product and mixture of burned and unburned gases assumed to consist of infiltration from both unburned and burned zones.

2. METHODOLOGY

2.1 Mathematical Model

A 3-zone thermodynamic model being developed for this study consisting of burned, unburned and transitory zones is as shown in Fig. 1. The transitory zone is presumed to have been formed by infiltration from the unburned and burned zones. Fig. 1 shows the volume of unburned charge, V_u , volume of burned product, V_b and volume of mixture constituting of unburned burned gases(transitory zone), V_{un} . V_{un} is the addition of volume of unburned gases in unburned burned zone, V_{ub} and volume of burned gases in unburned burned zone, V_{bu} that is, $v_{un} = v_{ub} + v_{bu}$

v_{ub} = mass infiltration from the unburned zone into the transition zone

v_{bu} = mass infiltration from the burned zone into the transition zone

The model equations are developed using the same concept by Ferguson and Allan [18] by applying the first law of thermodynamics to each zone as detailed below.

The rate of change of mass within an open system is the net flux of mass across the system boundaries, i.e.

$$m = \sum_k \dot{m}_k \quad (1)$$

The mass flux in the combustion chamber at any instant can be expressed as

$$m = m_u + m_b + m_{un} \quad (2)$$

where m_u is mass of unburned mixture, m_b is mass of burned gas and m_{un} is mass of mixture of burned and unburned gases, addressed as transitory zone.

Based on the application of the first law of thermodynamics to an open system, the energy equation is written as,

$$\dot{E} = \dot{Q} - \dot{W} + \sum \dot{m}h \quad (3)$$

where, E, Q and W are internal energy of the cylinder mixture, heat exchange of content with cylinder wall and work done on piston by cylinder charge respectively. Equation (3) is thus applied to each of compression, expansion and combustion phases of the internal combustion engines as follows:

(i) Compression and expansion processes

For the compression and expansion phases, equation (3) is transformed to

$$\frac{d(mu)}{d\theta} = \frac{dQ}{d\theta} - p \frac{dv}{d\theta} + h \frac{dm}{d\theta} \quad (4)$$

Now

$$\frac{d(mu)}{d\theta} = \frac{mdu}{d\theta} + \frac{udm}{d\theta} = m \left(\frac{du}{d\theta} \cdot \frac{d\theta}{d\theta} \right) + \frac{udm}{d\theta} \quad (5)$$

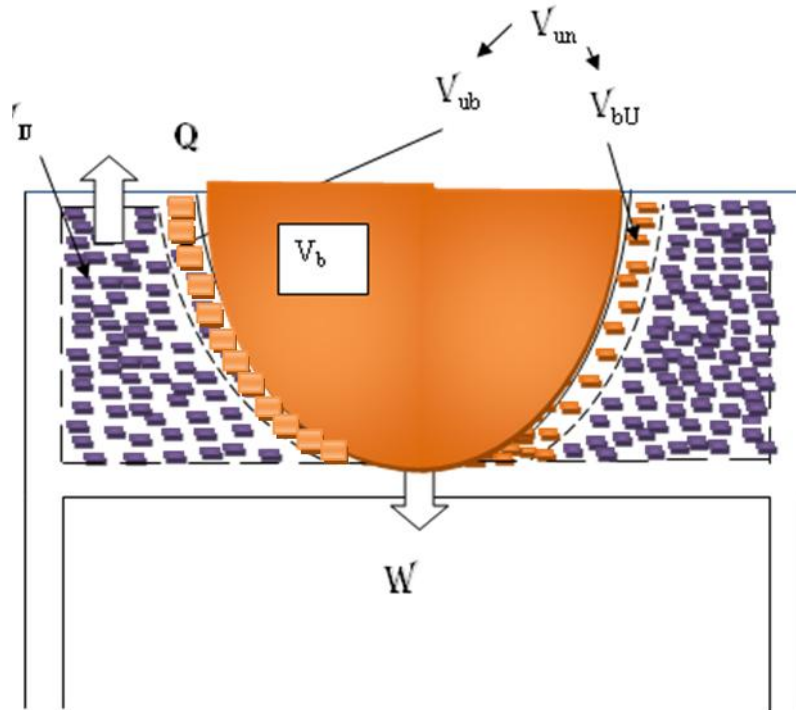


Fig. 1. Geometry representing the three zones (Burned, Unburned and Burned Unburned Zone) In Combustion Chamber

Thus by suitable manipulation

$$\frac{dT}{d\theta} = \frac{I}{mCv} \left[\frac{dQ}{d\theta} - p \frac{dv}{d\theta} + \frac{dm}{d\theta} RT \right] \quad (6)$$

By employing the ideal gas equation, $PV = mRT$, then

$$\frac{vdp}{d\theta} + p \frac{dv}{d\theta} = RT \frac{dm}{d\theta} + mT \frac{dR}{d\theta} + mR \frac{dT}{d\theta} \quad (7)$$

The cylinder composition is assumed frozen during compression and expansion processes i.e. $\frac{dR}{d\theta} \cong 0$

$$\frac{dp}{d\theta} = \frac{1}{v} \left[\frac{dm}{d\theta} RT + mR \frac{dT}{d\theta} - p \frac{dv}{d\theta} \right] \quad (8)$$

Combustion Process: During the combustion process, there will be three zones namely unburned, transitory and burned zones in the cylinder. The energy equation (Eqn. 3) is applied to each separately as detailed below

(a) Unburned zone

The energy equation for this zone is given as

$$\frac{d(m_u U_u)}{d\theta} = -\frac{dQ_u}{d\theta} - p \frac{dV_u}{d\theta} - h_u \frac{dm_x}{d\theta} - \frac{h_u dm_{lu}}{d\theta} - \frac{h_u dm_{ub}}{d\theta} \quad (9)$$

$\frac{dm_x}{d\theta}$ – mass burning rate (MBR)

m_u - mass unburned

m_{ub} – mass infiltration from the unburned zone to the transitory zone

m_{lu} – mass leakage from unburned zone to the crankcase

Eqn.(9) can be re-expressed as

$$\frac{d(m_u U_u)}{d\theta} = m_u \frac{dU_u}{d\theta} + U_u \frac{dm_u}{d\theta} = m_u \left[\frac{dU_u}{d\theta} \cdot \frac{dT_u}{d\theta} \right] + \frac{U_u dm_u}{d\theta} \quad (10)$$

By noting that

$$\frac{dm_u}{d\theta} = -\frac{dm_x}{d\theta} - \frac{dm_{lu}}{d\theta} - \frac{dm_{ub}}{d\theta} \quad (11)$$

Eqn.(10) becomes

$$m_u C_{v,u} \frac{dT_u}{d\theta} = -\frac{dQ_u}{d\theta} - p \frac{dV_u}{d\theta} - R_u T_u \frac{dm_x}{d\theta} - R_u T_u \frac{dm_{lu}}{d\theta} - R_u T_u \frac{dm_{ub}}{d\theta} \quad (12)$$

From the ideal gas equation, the following expression can be written

$$p \frac{dV_u}{d\theta} + \frac{V_u dP}{d\theta} = R_u T_u \frac{dm_u}{d\theta} + m_u R_u \frac{dT_u}{d\theta} \quad (13)$$

By substituting eqn, (13) in eqn. (12) yields

$$\frac{dT_u}{d\theta} = \frac{I}{m_u C_{p,u}} \left(-\frac{dQ_u}{d\theta} + V_u \frac{dP}{d\theta} \right) \quad (14)$$

(b) Transitory (obtained from infiltration of burned and unburned gases) zone.

In the same vein, the energy equation for the transitory zone is written as

$$\frac{d(m_{un} U_{un})}{d\theta} = \frac{dQ_{un}}{d\theta} - p \frac{dV_{un}}{d\theta} + \frac{h_u dm_{ub}}{d\theta} + \frac{h_b dm_{bu}}{d\theta} + \frac{h_{un} dm_{lu}}{d\theta} \quad (15)$$

mass in the transitory zone (m_{un})= mass infiltration from the unburned zone (m_{ub})+ mass infiltration from the burned zone (m_{bu})

With $\left[\frac{dm_{un}}{d\theta} = \frac{dm_{ub}}{d\theta} + \frac{dm_{bu}}{d\theta} - \frac{dm_{lu}}{d\theta} \right]$, where m_{lu} is mass leakage from the transitory zone to the crankcase, Eqn.(15) is re-expressed as

$$m_{un} C_{v,un} \frac{dT_{un}}{d\theta} = -\frac{dQ_{un}}{d\theta} - p \frac{dV_{un}}{d\theta} - U_{un} \frac{dm_{ub}}{d\theta} - U_{un} \frac{dm_{bu}}{d\theta} + h_u \frac{dm_{ub}}{d\theta} + h_b \frac{dm_{bu}}{d\theta} \quad (16)$$

The ideal gas equation for this zone is expressed as

$$p \frac{dV_{un}}{d\theta} + V_{un} \frac{dP}{d\theta} = R_{un} T_{un} \frac{dm_{un}}{d\theta} + m_{un} R_{un} \frac{dT_{un}}{d\theta} \quad (17)$$

Substituting eqn.(16) into eqn. (17) thus yields

$$\frac{dT_{un}}{d\theta} = \frac{I}{m_{un} C_{p,un}} \left(-\frac{dQ_{un}}{d\theta} + V_{un} \frac{dP}{d\theta} + (h_u - h_{un}) \frac{dm_{ub}}{d\theta} + (h_b - h_{un}) \frac{dm_{bu}}{d\theta} \right) \quad (18)$$

(ii) Conservation energy to burned gas zone

$$\frac{d(m_b U_b)}{d\theta} = \frac{dQ_b}{d\theta} - p \frac{dV_b}{d\theta} + h_u \frac{dm_x}{d\theta} - h_b \frac{dm_{lb}}{d\theta} - h_b \frac{dm_{bu}}{d\theta}$$

By using the same procedure adopted in the analysis of the other zone, the energy equation can be rearranged to obtain burned temperature derivative as below.

$$\frac{dT_b}{d\theta} = \frac{I}{m_b C_{p,b}} \left(-\frac{dQ_b}{d\theta} + \frac{V_b dP}{d\theta} + (h_u - h_b) \frac{dm_{x1}}{d\theta} \right) \quad (19)$$

When the overall energy equation is considered then the pressure derivative is obtained as

$$\frac{dP}{d\theta} = \left\{ \frac{V_u}{T_u} \frac{dT_u}{d\theta} + \frac{V_b}{T_b} \frac{dT_b}{d\theta} + \frac{V_{un}}{T_{un}} \frac{dT_{un}}{d\theta} + (v_b - v_u) \frac{dm_{x1}}{d\theta} + (v_{un} - v_u) \frac{dm_{ub}}{d\theta} + (v_{un} - v_b) \frac{dm_{bu}}{d\theta} - v_u \frac{dm_{lu}}{d\theta} - v_b \frac{dm_{lb}}{d\theta} - v_{un} \frac{dm_{lun}}{d\theta} - \frac{dV}{d\theta} \right\} \frac{V}{P} \quad (20)$$

2.2 Implementation of the Developed Model

The developed model was used to obtain the temperature and pressure history in a combustion chamber. Equations 4-14 were used during compression and expansion phases while equations 15-19 were used during the combustion phase. The model was applied to an internal combustion engine with operating and combustion parameters details as contained in Table 2. In the analysis, the mass infiltration into the transitory zone is such that:

$$m_{ub} = CC1 * m_u \text{ and } m_{bu} = CC2 * m_b$$

where CC1, fractional burnt leakage and CC2, fractional unburnt leakage are arbitrary constants

Table 1. Engine specifications for model evaluation

Parameter	Value
Number of cylinders	4
Bore	0.079
Stroke	0.086
Compression ratio	16
Displacement	1.7
Inlet Valve Close	136BTDC
Exhaust Valve Open	122ATDC
Engine speed	1500RPM

[19]

The performance parameters such as thermal efficiency and indicated mean effective pressure, as well as the emission obtained using the developed model, were compared with those of the standard two-zone model. Submodels including engine geometry, fuel data and air data inherent in the two-zone model as reported by [8] were used in analyzing the present three-zone model.

The model was run at constant value of CC2 of 0.001 while CC1 takes on values of 0.0005, 0.00025, 0.001, 0.005, 0.1, 0.5 in turn. Thereafter the model was again run with constant CC1 of 0.001 while CC2 takes on values of 0.0005, 0.00025, 0.001, 0.005, 0.1, 0.5 in turn.

Results from the developed three-zone model was compared to the results from the existing two-zone model and both were compared to a

simulation result with detailed chemical kinetics as rendered in figures 2-19, The indicated mean effective pressure (IMEP), thermal efficiency (η), pressure (Pe) and emission characteristics were used in the comparison as shown in Tables 2-4.

Table 2. Engine specifications for 2Zone model

Parameter	Value
Number of cylinders	4
Bore	0.1
Stroke	0.08
Compression ratio	10
Equivalence ratio	0.8
Burn duration angle	60
Start of burning	-35
Engine speed	1500RPM

[8]

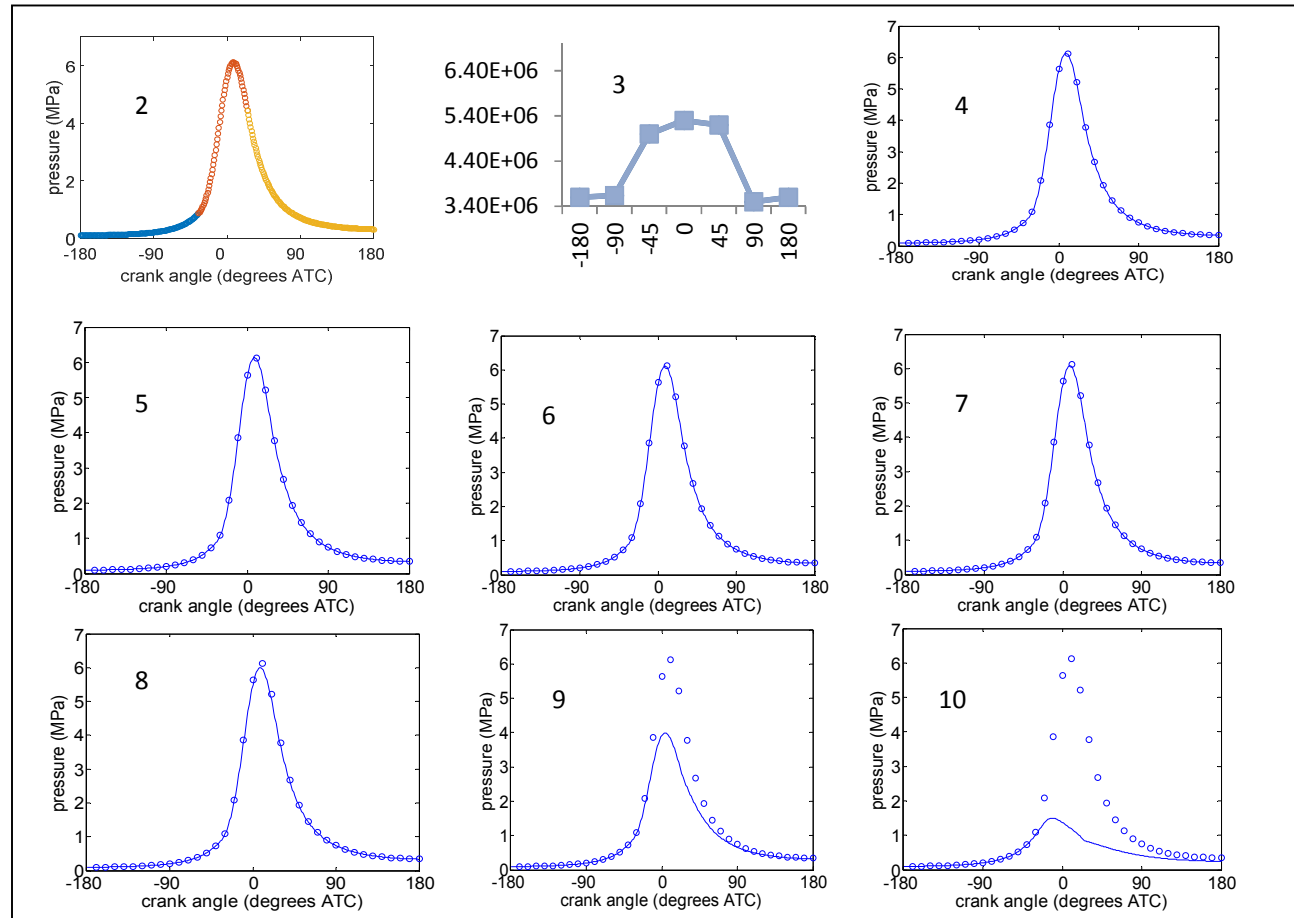
3. RESULTS AND DISCUSSION

Fig. 2 is the 2-zone pressure distribution originally written by Ferguson, now in MATLAB by [8] while the CFD results obtained by [19] is shown in Fig. 3. Figs. 4-10 are pressure history obtained using the developed model. When CC1 was assigned values more than 0.005, the peak pressure values were appreciably decreased (see Figs. 9 and 10).

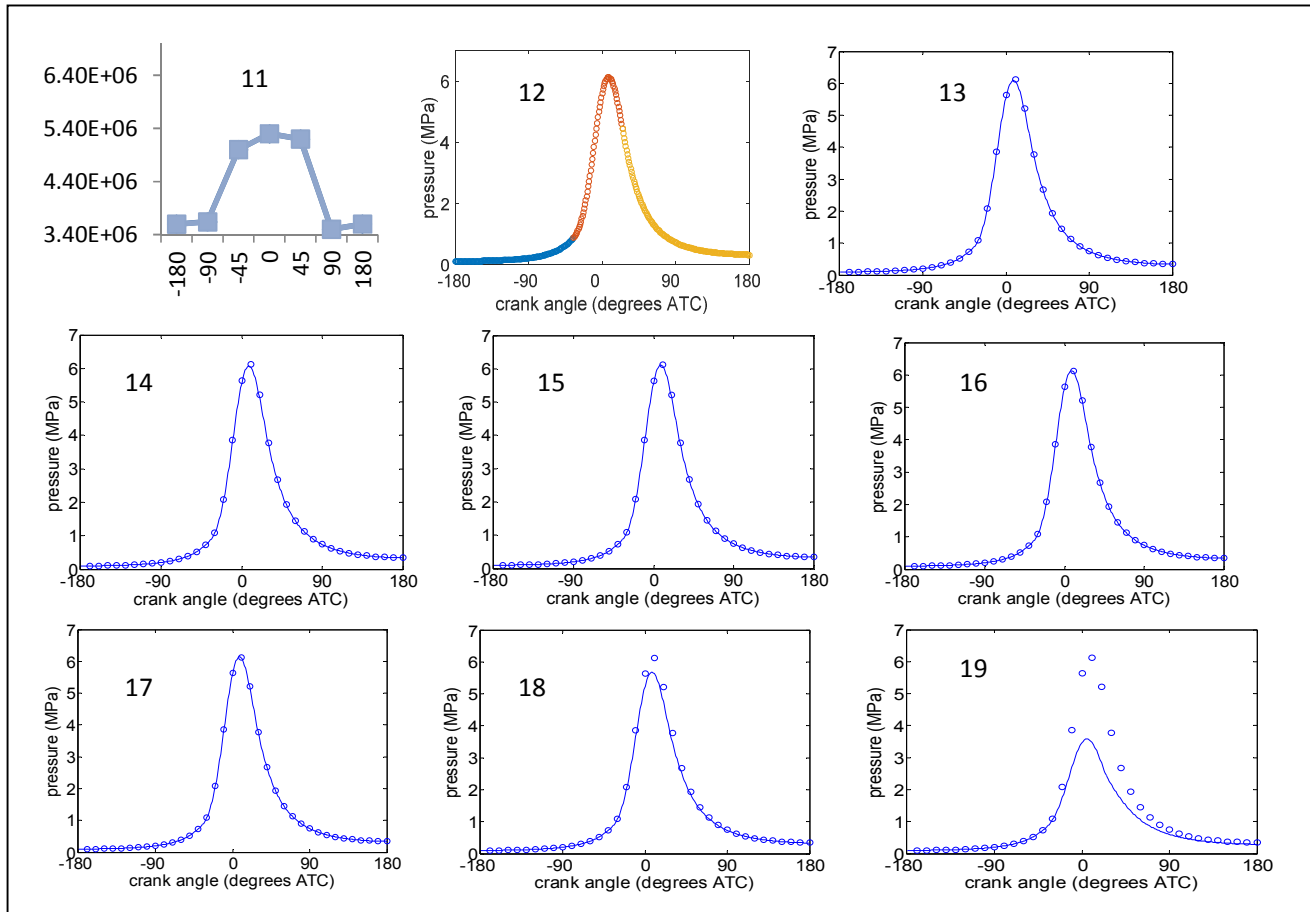
Fig. 3 is the 2zone pressure distribution originally written by Ferguson, now written in MATLAB by [8]. Fig. 2 represents the simulated values for pressure by [19].

Figs. 13-19 are pressure distribution at varying CC2 with the value of CC1 kept constant at 0.001. When CC2 has values more than 0.005, the peak pressure values exhibited sharp deviation from the 2zone model results (see Figs. 18 and 19).

From Table 3, it was observed that values of Pe, IMEP and η were highest at CC1= 0.00025, while the same observed parameters had the highest value when CC2 = 0.005 in Table 4. The results suggest that the infiltration from the burnt zone should be appreciably higher than that from the unburnt zone for the model to give a very good estimate. However, it is also established that beyond a certain infiltration level, the model exhibited a decrease in performance. Figure 20 is the pressure history for a 3 zone model with CC1 =0.00025 and CC2 =0.005. The peak pressure was appreciably higher than any of the previous cases.



Figs. 2-10. Pressure distribution for; 2) 2zone model 3) 3zone experimental model 4) 3zone Case1 model when $CC1=0.0005$, 5) 3zone model when $CC1=0.00025$, 6) 3zone model when $CC1=0.001$, 7) 3zone model when $CC1=0.002$, 8) 3zone model when $CC1=0.005$, 9) 3zone model when $CC1=0.1$, 10) 3zone model when $CC1=0.5$, respectively at a constant value of $CC2=0.001$



Figs. 11-19. Pressure distribution for; 11) 3zone CFD model 12) 2zone model 13) 3zone model when $CC2=0.0005$, 14) 3zone model when $CC2=0.00025$, 15) 3zone model when $CC2=0.001$, 16) 3zone model when $CC2=0.002$, 17) 3zone model when $CC2=0.005$, 18) 3zone model when $CC2=0.1$, 19) 3zone model when $CC2=0.5$, respectively at a constant value of $CC1=0.001$

Table 3. Three zone model values for the fractional burnt region using CC2=0.001

Emission characteristics species fraction													
CC1	Pressure (MPa)	IMEP (MPa)	η	CO2	H2O	N2	O2	CO	H2	H	O	OH	NO
0.0005	4.4613e+06	9.4659e+05	0.3864	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.00025	4.4684e+06	9.4770e+05	0.3869	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.001	4.4494e+06	9.4464e+05	0.3856	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.002	4.4270e+06	9.4093e+05	0.3841	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.005	4.3606e+06	9.2977e+05	0.3795	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.1	2.7077e+06	6.1817e+05	0.2523	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.5	8.4418e+05	1.2037e+05	0.0491	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001

(IMEP= Indicated Mean Effective Pressure (MPa), η =Thermal efficiency)**Table 4. Three zone model values for the fractional unburnt region using CC1=0.001**

Emission characteristics species fraction													
CC2	Pressure (MPa)	IMEP (MPa)	η	CO2	H2O	N2	O2	CO	H2	H	O	OH	NO
0.0005	4.4350e+06	9.4221e+05	0.3846	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.00025	4.4203e+06	9.3968e+05	0.3836	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.001	4.4494e+06	9.4464e+05	0.3856	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.002	4.4612e+06	9.4654e+05	0.3864	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.005	4.4674e+06	9.4726e+05	0.3867	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.1	4.0931e+06	8.8177e+05	0.3599	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
0.5	2.4322e+06	5.3169e+05	0.2170	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001

(IMEP= Indicated Mean Effective Pressure (MPa), η =Thermal efficiency)**Table 5. Comparison of results from 2zone model, 3zone model and experimental values**

	2zone model	Experimental results	3zone model with C1=0.00025 and C2= 0.001	3zone model at 0.005	3zone model for optimal values of C1 at 0.00025 and C2 at 0.005
Pressure (MPa)	4.4358e+06	5.30E+06	4.4684e+06	4.4674e+06	4.4657e+06
IMEP	9.1635e+05	-	9.4770e+05	9.4726e+05	9.4688e+05
H	0.3741	-	0.3869	0.3867	0.3865

(IMEP= Indicated Mean Effective Pressure (MPa), η =Thermal efficiency)

Table 6. Comparative Values of the Performance Indices for the 2-zone and 3-zone models

	Emission characteristics species fraction												
	Pressure	IMEP	η	CO ₂	H ₂ O	N ₂	O ₂	CO	H ₂	H	O	OH	NO
3zone using CC1= 0.00025 and CC2=0.005	4.4657e+06	9.4688e+05	0.3865	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
2zone model	4.4358e+06	9.1635e+05	0.3741	0.0983	0.1194	0.7428	0.0395	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001

(IMEP= Indicated Mean Effective Pressure (MPa), η =Thermal efficiency)

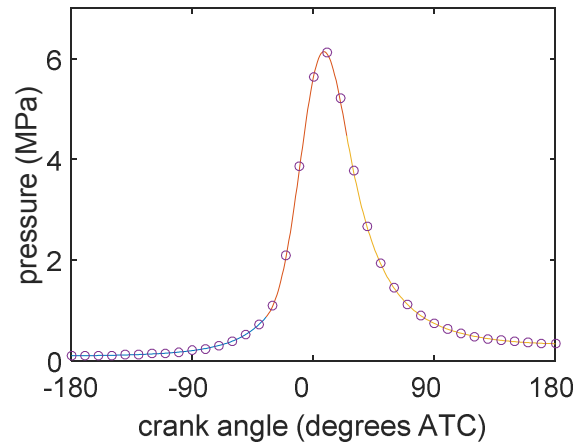


Fig. 20. Pressure Distribution for 3zone model at greatest pressure values of CC1 and CC2

A comparison of the experimental, 2zone and 3zone models results is presented in Table 5. Higher peak pressure values were observed for 3zone model which was 15% closer to the experimental value as compared to the 2zone model which was 16.4% closer. This could imply an improved engine work estimate using the 3zone model. Thermal efficiency values were observed appreciably higher for the 3zone model as compared with the 2-zone model.

A comparison of the emission characteristics using the 2zone and 3 zone models results is presented in Table 5. There were no significant changes in the estimate values for the emissions obtained using the 2zone and 3zone models, see Table 6. However since the 3zone model predicts better the engine performance, it is considered to be better.

4. CONCLUSION

A 3-zone model for the prediction of performance of an internal combustion engine has been developed. The results obtained established that by incorporating a third zone comprising of mixture of unburned and burnt gases at a determined optimal range, the 3-zone model gave a better estimate of an internal combustion engine performance characteristics.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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