

TWO ZONE THERMODYNAMIC MODEL FOR PREDICTION OF PARTICULATE MATTER EMISSION FROM DIRECT INJECTION DIESEL ENGINE

by

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In this work, two zone thermodynamic models have been developed for prediction of particulate matter (PM) from direct injection Diesel engine. Two key compositions of PM were considered in this simulation model developed, it consists of soot and soluble organic fraction (SOF). Soot formation model were developed initially and then coupled with SOF model to get overall PM formation rates. Primary soot formation rate was obtained by using Hirosysu model and Nagle and Strickland-Constable model was adopted to get soot oxidation rate. The oxidation and formation rate difference gives overall soot formation value. Unburned hydrocarbons were considered as key factor for SOF formation so the formation and oxidation rate of hydrocarbon was determined. Then the difference between these two gives overall SOF formation rate. At last soot formation and SOF model was integrated to get overall PM formation rate. Various submodels like ignition delay, heat release rate, and combustion model were involved in this study to predict PM formation rate. Validation of this simulation model developed were carried out on single cylinder, naturally aspirated water cooled direct injection Diesel engine. Simulation results matched well with the experimental results and it clearly shows that model developed is an accurate one. Results obtained shows that soot formation increases at higher loads and SOF formation rate increase at lower loads. Simulation model developed is very useful for understanding the PM formation mechanisms and also useful for control of PM formation.

Key words: *particulate matter, soot, soluble organic fraction, two zone, Diesel engine*

Introduction

Diesel engine is found to be used for many applications which include both commercial and industrial sectors. The major obstacle is that release of hazardous emissions into atmosphere which will cause serious health effects to both human beings and environment. Major pollutants emitted from Diesel engine include NO_x and PM. For the past few decades simulation model has been widely used for understanding mechanisms of both combustion and formation of pollutants. The PM modeling is found to be very complex in internal combustion engines. This is due to the composition of PM being very difficult to understand. The PM is defined as any substance excluding water that can be collected by filtering the exhaust gas [1, 2]. The PM

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composition mainly consists of two components soot and SOF [3]. Soot is formed from unburned fuel, which nucleates from vapour phase to solid phase in fuel rich regions at high temperature. Then on the surface of soot the HC and other liquid phase materials are absorbed, depending on surrounding conditions. Nearly 50% of PM is composed of soot. Soluble fraction present in particulates mainly consists of alkenes, aliphatic HC, aldehydes, polycyclic aromatic hydrocarbons (PAH) and its derivatives. Various other constituents like lubricating oil, partially oxidized fuel, and oil also contribute to SOF in PM [4].

Now a day's simulation approach of predicating Diesel engine behavior is used widely for combustion and emission analysis [5-7]. Simulation approach also found to be cost effective and is also more accurate one. For evaluation of exhaust pollutants from Diesel engine purposes the multi-dimensional and quasi-dimensional model found to be extensively used. Multi-dimensional model is an elaborated one, which includes flow aspects in cylinder and solves various governing equations for conservation of energy, momentum, and mass and their interactions. Detailed chemical kinetics reaction mechanisms and various species involved are also examined by using this model approach. The CFD simulation tool is found to be mostly used for this approach. Regardless of all merits involved in this model, the major drawback involves is that it increases computational time and memory. Regarding quasi-dimensional model composition based approach has been used to predict exhaust emissions and is found to be accurate one. In this approach cylinder has been divided into two or more zones each of the zone are treated as ideally mixed. Pressure and temperature histories in each zone are considered as function of exhaust gases composition. Another key factor is that this model requires very less computational time and memory space. In consideration of all previous mentioned advantages quasi-dimensional model is found to be used widely for modeling and simulation approach for internal combustion engine.

Although many quasi-dimensional models carried out earlier to predict PM emission it concentrates majorly on soot formation rate [8-10]. As mentioned earlier PM is combination of soot and SOF, for detailed prediction of PM, SOF content must also be determined. Some researchers also worked previously to predict both soot and SOF fraction but the model determined was not a detailed one. Various submodels involved for simulation were not elaborately discussed in those works. In the present work quasi-dimensional two zones model has been developed to evaluate PM. Soot primary formation rate is figured out initially and then the SOF model is developed. Finally, the integration of these models is carried out and that indicates the overall PM formation rate. For the validation of this model the experiments were conducted in single cylinder water cooled naturally aspirated Diesel engine

Two zone quasi-dimensional thermodynamic model

Simulation work proposed in this work is quite similar to a model developed by previous researchers [11-13] and also used by many researchers [14-17]. But in those models only pollutants formation model was discussed elaborately various other submodels involved was not discussed. In this work various submodels involved for computation of overall PM formation is also pointed out. The entire model was simulated in MATLAB platform, since it is user friendly and it requires very less computational time.

In two zones thermodynamic model cylinder volume is divided into two zones burned and unburned zone. Various submodel used in this study comprises of ignition delay, heat release rate, combustion model, and finally PM emission model. Both soot formation and oxidation rate depends directly on pressure and temperature histories of mixture formed. Initial part of this work the pressure and temperature values for entire crank angle (CA) for one complete cy-

cle is calculated. Based upon the pressure and temperature histories the heat release rate model has been formulated. The mass of fuel injected is calculated by using the Ferguson model. After fuel injection begins the ignition delay model is figured out which will be mentioned in coming part. In order to find out the mass of burned gases composition combustion model was predicated. The difference between mass of fuel injected and mass of burned gases composition gives mass of unburned fuel vapour concentration. Finally, soot formation rate is calculated by using pressure, temperature, and combustion model input parameters obtained from previous mentioned models. Nagle and Strickland-Constable (NSC) model has been used to calculate soot oxidation rate. Finally, difference between these two models gives overall soot formation rate. Then the soot formation rate was coupled with the SOF model to get overall PM formation rate.

Assumptions considered

Mass of fuel injected in these two zones is assumed to be equal but the amount of fuel injected varies across each zones depends upon instantaneous fuel injection rate. Another consideration is that there is no mixing and interchange between these two zones. It is assumed that each zone has its own temperature, chemical composition and equivalence ratio scenarios. Regarding pressure, it varies uniformly in all zones with respect to time and also assumed to be uniform over entire cylinder volume. First law of thermodynamics and conservation of mass and momentum applications has been used to describe differential equations and state of each zone. The oxygen concentration, temperature, and pollutants have been calculated by solving those differential equations. The following flowchart gives overall brief description of the model developed in this work.

Various submodels developed

Pressure and heat release model

Pressure and temperature values are calculated for entire four strokes by adopting following algebraic equations which was developed previously [18].

Heat energy transferred between gas and the combustion chamber is called as engine heat transfer. The gross heat release rate is given by summation of heat transfer rate and net heat release rate:

$$Q_{\text{Gross}} = Q_{\text{net}} + Q_{\text{ht}} \quad (1)$$

Heat transfer between wall and gases is obtained by using Newton law of cooling for convective heat loss and it is heat loss and it is calculated using relations from previous work [19, 20]:

$$Q_{\text{ht}} = h_c A(\theta)(T_g - T_w) \quad (2)$$

Woschni conducted lot of tests in 4-stroke single cylinder water cooled engine and formulated a model for heat transfer coefficient (Woschni correlation):

$$h_c = CB^{m-1} p^m W^m T^{0.75-1.62m} \quad (3)$$

During intake, compression and exhaust, Woschni argued that the average gas velocity should be proportional to the mean piston speed. During combustion and expansion, it will vary with respect to change in density. Thus the term proportional to the pressure rise due to combustion was added. The average gas velocity is determined:

$$W = \left[C_1 S_p + C_2 \frac{V_d T_r}{P_r V_r} - (p - P_m) \right] \quad (4)$$

For the gas exchange period $C_1 = 6.18$ $C_2 = 0$; for the compression period $C_1 = 2.28$ $C_2 = 0$; for the combustion and expansion period $C_1 = 2.28$ $C_2 = 3.24 \cdot 10^{-3}$

Net heat release rate is calculated by using formula:

$$\frac{dQ_{ch}}{d\theta} = \frac{1}{\gamma - 1} V \frac{dp}{d\theta} + \frac{\gamma}{\gamma - 1} P \frac{dv}{d\theta} \quad (5)$$

If you substitute eds. (2) and (5) in eq. (1), overall gross heat release rate, will be obtained.

Fuel injection model

At the end of compression stroke fuel is injected into the combustion chamber at high pressure (around 200 bar). The rate of injection can be determined by using Ferguson model:

$$M_{fi} = \frac{M_{tot\omega}}{\varphi d \Gamma(n)} \left(\frac{\varphi - \varphi_s}{\varphi d} \right)^{n-1} \exp \left(\frac{\varphi_s - \varphi}{\varphi d} \right) \quad (6)$$

$$\Gamma(n) = n - 0.5 \ln n - n + 0.5 \ln 2\pi + \frac{1}{12n} - \frac{1}{360n^2} - \frac{1}{1260n^5} \quad (7)$$

Ignition delay model

Both physical and chemical processes must take place before a significant fraction of chemical energy of the injected liquid fuel is released. The physical processes are: the atomization of liquid fuel jet; the vaporization of the fuel droplets; the mixing of fuel vapour with air. The chemical processes are the pre combustion reaction of fuel, air, residual gas mixture which leads to auto ignition. This will be affected by different operating parameters. Since both chemical and physical delay is overlapped it is quite difficult to distinguish between both delay periods separately:

$$\tau_{id}(CA) = (0.36 + 0.22SP) \exp \left[EA \left(\frac{1}{RT} - \frac{1}{17190} \right) \left(\frac{21.2}{P - 12.4} \right)^{0.63} \right] \quad (8)$$

$$EA = \frac{618840}{CN + 25} \quad (9)$$

Combustion model

Combustion model is predicated to find out mass of burned gas composition. Although many combustion model available Lyn's model is found to be most suitable one for single cylinder Diesel engine. In this model the description of compression ignition combustion a rapid premixed burning phase followed by a slower mixing controlled burning phase. The amount of the fuel injected that burns in each of these phases is empirically linked to the duration of the ignition delay. An algebraic function is formulated which is used to describe the premixed heat release rate and second function to describe the mixing controlled heat release phase. Phase proportionality factor, β , is used to rate these both the phases and it depends majorly on ignition delay and is given by:

$$\frac{m_{f,b}(t)}{m_{f,0}} = \beta f_1 + (1 - \beta) f_2 \quad (10)$$

where $m_{f,b}$ is the mass of fuel burned, $m_{f,0}$ – the total fuel mass injected per cycle per cylinder and t – the time from ignition non-dimensionalized by total time allowed for combustion $[(t - t_{ign})/\Delta t_{comb}]$. The premixed burning mixed controlled function is given:

$$f_1 = 1 - (1 - t^{k_1})^{k_2} \quad (11)$$

$$f_2 = 1 - \exp(-K_3 t^{k_4}) \quad (12)$$

The proportional factor, β , is given:

$$\beta = 1 - \frac{a\phi^b}{\tau_{id}} \quad (13)$$

where ϕ is over all fuel/air equivalence ratio and a , b , and c are empirical constants:

$$K_1 = 2 + 1.25 \cdot 10^{-8} (\tau_{id} N)^{2.4}$$

$$K_2 = 5000$$

$$K_3 = \frac{14.2}{\phi^{0.644}}$$

$$K_4 = 0.79 K_3^{0.25}$$

The PM emission model

The PM as mentioned already in earlier part is a combination of soot and SOF. Initially soot formation rate is determined by using Hiroyasu *et al.* model [11] which is considered as most widely used model to predict soot formation. Then the soot oxidation rate is determined by using NSC model [23]. The corresponding difference between these two indicates over all soot formation rate. Corresponding SOF emission model is also determined, finally integration between these soot and SOF model shows the overall PM formation rate given by:

$$\frac{d[\text{PM}]}{dt} = \frac{d[\text{Soot}]}{dt} + \frac{d[\text{SOF}]}{dt} \quad (14)$$

Emission model for soot formation

Soot formation model is divided into two parts soot primary formation and oxidation model [11, 12, 16, 21, 22]. Major dependence of soot primary formation rate is based on concentrations of fuel fragments and rate of collisions at molecular level. In this way two small active radical nuclei collide with each other to form large size nuclei. Similar case also exists for soot oxidation process, where major molecules involve in collision are carbon and oxygen.

Oxygen or OH radicals on internal burning and penetrate into the particle which leads to reduction in particle diameter, another parameters in addition to temperature, local fuel vapour concentration and oxygen concentration plays a dominant role for soot formation and oxidation rate. Other parameters like gas temperature inside the cylinder and equivalence ratio has more influence on soot thresholds. Soot formation rate increases generally when temperature of gas is high and when there is deficiency of oxygen concentration inside the engine cylinder. Hiroyasu model is used in this work to get formation rate of soot and is expressed:

$$\frac{d[\text{soot}_f]}{dt} = A_f [\text{fuel}] P^{0.5} \exp\left(-\frac{E_f}{RT}\right) \quad (15)$$

The corresponding oxidation rate of soot is determined by adopting NSC [23] oxidation model and is given:

$$\frac{d[\text{soot}]_o}{dt} = \frac{6M_c}{\rho_s D_s} [\text{soot}] R_{ox} \quad (16)$$

where [soot] is the net soot mass and R_{ox} is the surface oxidation rate and is given:

$$R_{ox} = \left(\frac{K_A P_{O_2}}{1 + K_Z P_{O_2}} \right) x_A + K_A P_{O_2} (1 - x_A) \quad (17)$$

where x_A is given by:

$$x_A = \frac{P_{O_2}}{P_{O_2} + \left(\frac{K_T}{K_B} \right)} \quad (18)$$

where P_{O_2} refers to partial pressure of oxygen and the rate constants in the NSC oxidation model are:

$$K_A = 20 \exp\left(-\frac{15100}{T}\right) \quad (19)$$

$$K_B = 4.46 \cdot 10^{-3} \left(-\frac{7640}{T}\right) \quad (20)$$

$$K_T = 1.51 \cdot 10^5 \left(-\frac{48800}{T}\right) \quad (21)$$

$$K_Z = 21.3 \exp\left(\frac{2060}{T}\right) \quad (22)$$

Ultimately overall soot formation rate is given:

$$\frac{d[\text{soot}]}{dt} = \frac{d[\text{soot}]_f}{dt} - \frac{d[\text{soot}]_o}{dt} \quad (23)$$

Emission model for SOF

The unburned HC are considered as main cause which contributes more to SOF content of PM. At low temperature this HC has great tendency to condense or adsorb on to solid soot. Remaining little HC content gets condensed into the filter independently. This clearly shows that this HC emission becomes SOF in PM finally. The HC emission is mainly caused by the following reasons [1, 2]. Over rich mixture, over lean mixture, and quenching or misfiring.

Over rich mixture

The main cause for over rich mixture occurs due to fuel which is under mixed. There are two important reasons this under mixing of fuel will occur. First one is during over fueling conditions excess fuel enters in to the cylinder. Another reason is that fuel enters into the engine cylinder through the injector nozzles at low velocity conditions often occurs late in combustion process. Second source contributes more to over rich mixture at nominal operating conditions. A small amount of liquid fuel will be trapped on the tip of the nozzle. This very small volume of fuel is called sac volume, and depends majorly on nozzle design.

This sac volume of liquid fuel evaporates very slowly because it is surrounded by a fuel-rich environment and, once the injector nozzle closes, there is no pressure pushing it into the cylinder. Little amount of this fuel does not evaporate until combustion has stopped, and this results in added HC particles in the exhaust. The HC emission caused by over rich mixture is caused by following one:

$$\frac{d[\text{HC}_{um}]}{dt} = V_{sac} \frac{dx_{sac}}{dt} \rho_f \quad (24)$$

Over lean mixture

Over lean mixture occurs mainly due to over mixing of fuel in the combustion chamber. Fuel air equivalence ratio distribution across the fuel spray develops as soon as fuel injection into the cylinder begins. It is noted that rapid increase in lean combustion limit with time, when the amount of fuel is mixed leaner. In fuel lean zones combustion is limited these leads to improper burning of fuel. In these over mixing conditions there is a mixing of some fuel particles with gases burned already this will lead to incomplete combustion.

The amount of fuel injected during ignition delay quantifies the unburned HC content for these over lean regions. Ignition delay length directly influences the HC emission value; it rises when delay period increases. A unique correlative expression has been used in this work which will determine ignition delay under both steady and transient operation [24]:

$$\tau = 2.4 p^{-1.02} \alpha^{-0.2} \exp\left(\frac{2100}{T}\right) \quad (25)$$

The quantity of fuel injected during ignition delay can be calculated by using the following expression:

$$Q_{ID} = \int_0^{\tau} \frac{dq_f}{dt} dt = \tau C_d A_n \sqrt{2\Delta p_n \rho_f} \quad (26)$$

Finally the previous expression can be expressed as fraction of the fuel injected during ignition delay it is given by:

$$\frac{d[HC_{ol}]}{dt} = A_{HC} X_{HC} X_{O_2} \exp\left(-\frac{18375}{T}\right) \left(\frac{P}{RT}\right) K_{ol} Q_{ID} \quad (27)$$

where K_{ol} denotes the fraction of the HC emission derived from the over lean fuel to the fuel injected during the ignition delay period.

Quenching or misfiring

Wall quenching and misfiring are the various other sources contributes to HC emissions. Quenching parameter depends greatly on degree of impingement by fuel spray on combustion chamber walls. In well-designed electronically controlled engine probability of misfiring occurrence is very less. So these two parameters may not take part in HC formation reaction that much and it can be neglected. Over mixing and under mixing of fuel considered as two major sources of HC emissions at normal operating conditions for direct injection Diesel engines. Finally, HC emission is divided into two parts HC primary formation and oxidation model. In HC primary formation model effects due to under mixing and over mixing of fuel discussed earlier was considered. Therefore the overall HC primary formation rate is determined by summing up eqs. (24) and (27) and is given by:

$$\frac{d[HC_f]}{dt} = \frac{d[HC_{ol}]}{dt} + \frac{d[HC_{um}]}{dt} \quad (28)$$

The escaped HC molecules from primary formation reactions go through oxidation reaction during expansion and exhaust process. Although many previous empirical correlations available to determine HC oxidation rates, the best suitable model was discussed in previous work which fit reasonably into experimental data:

$$\frac{d[HC_o]}{dt} = A_{HC} X_{HC} X_{O_2} \exp\left(-\frac{18375}{T}\right) \left(\frac{P}{RT}\right) \quad (29)$$

Finally over all HC formation rate is given by difference between HC primary formation rate and oxidation rate and is given by:

$$\frac{d[\text{HC}]}{dt} = \frac{d[\text{HC}_f]}{dt} - \frac{d[\text{HC}_o]}{dt} \quad (30)$$

The SOF is the heavier HC emission and its proportions vary with different engine types and its operating conditions and are given by:

$$\frac{d[\text{SOF}]}{dt} = K_{\text{SH}} \frac{d[\text{HC}]}{dt} \quad (31)$$

In order to determine coefficient K_{SH} the various parameters like torque, T_{tq} , speed, n , and empirical coefficient, M , for different types of engines are introduced. Final detailed expression for SOF emission:

$$\frac{d[\text{SOF}]}{dt} = MK_{\text{tq}}^{m_1} K_n^{m_2} \frac{d[\text{HC}]}{dt} \quad (32)$$

where K_{tq} denotes load coefficient given as $K_{\text{tq}} = T_{\text{tq}}/T_{\text{tqmax}}$, T_{tq} and T_{tqmax} are operating torque and maximum torque of the Diesel engine, respectively, K_n denotes load coefficient and is given by $K_n = n/n_{\text{rat}}$, n , and n_{rat} denotes speed at operating condition and rated speed of Diesel engines, respectively. Finally, over all PM formation rate is obtained by substituting the eqs. (23) and (32) in eq. (14)

Experimental validations

In order to validate the simulation model determined the experiments were conducted in single cylinder, water cooled naturally aspirated Diesel engine. The detailed specification of engine is given in the tab. 1. The inputs to acquire combustion parameters are obtained by using Kistler pressure transducer and CA encoder and it is analyzed by using LAB view software. The various other emissions are measured by using AVL direct injection gas analyzer and PM was measured by using filter paper technique.

Table 1. Engine specifications

Manufacturer	Kirloskar oil engines Ltd.
Cylinder bore	80 mm
Stroke	110 mm
Rated speed	1500 rpm
Compression ratio	17:1
Number of cylinders	1
Cubic capacity	552 cc
Injection pressure	200 bar
Injection angle	23 °bTDC
Rated power	3.7 kW

In filter paper technique initially in order to eliminate influence of interference of foreign substances in the filter paper, it is put in an oven (100 °C) and baked for several hours. Then the fiber glass filter paper is weighed using electronic balance and put it in dry glass tube. After the Diesel engine is made to operate sturdily for about seven minutes about one operating condition, fiber glass filter paper is taken out and exhaust PM is sampled. The PM emission from Diesel engine under five operating condition was separately obtained with the same method. Then the filter paper was heated in a constant temperature equipment (100 °C) to remove the moisture content present. For various load conditions for PM emission the graphs are plotted finally and it is compared with simulation model.

Results and discussion

The simulated and experimental graphs for in cylinder pressure, temperature, and heat transferrate is shown clearly in figs. 1-3, obtained reveals that both predicated and experiment

results are almost identical this confirmed that model developed is an accurate one. Regarding pressure CA diagram for suction stroke (0-220 °CA) the pressure nearly equals to atmospheric pressure, while piston moves from top dead center (TDC) to bottom dead center (BDC). After this compression stroke starts (220-337 °CA) while both the valves are closed at this moment, thus pressure increases and volume decreases. At 337 °CA drop in pressure is noted due to fuel injection soot formations initiates at this point. Then after ignition delay period premixed combustion start and pressure increased drastically. Over all combustion duration starts after ignition delay period and accounts for nearly 57 °CA premixed combustion duration accounts for 12 °CA and diffusion combustion lasts for another 45 °CA. Fuel injection also continues until diffusion combustion ends corresponding soot formation rate is also high during this period. During diffusion combustion due to lack of oxygen content soot formation rate is high during this period. Then the pressure got reduced because of blow down and expansion stroke prevails, soot formation rate also start decreases after this point. Regarding in cylinder temperature trend shows that for suction stroke the temperature is almost constant. Then the temperature increased during compression stroke due to molecular collisions and little drop is observed during fuel injection. After this, the combustion gets initiated and temperature increases drastically. Finally during expansion stroke temperature value reduces since heat energy transformed into work and it is further transformed into cylinder wall.

Figure 4 shows the overall PM formation rate at different load conditions. These PM rates were predicted by solving the corresponding eqs. (14), (23), and (32). The curves of PM reveals clearly that soot and SOF content varies almost same at all operating conditions. Initially the trend shows that during early stage of combustion, it is observed that there is rapid increase in primary soot formation rate. This phenomenon occurs because at early combustion stage during premixed duration more amount of fuel gets injected. Since fuel contains large number of carbon particles and less oxygen content at this stage will enhance primary soot formation rate greatly.

Then after reaching peak value soot formation rate decrease quickly, on the other hand soot oxidation rate increases drastically. This scenario occurs since at diffusion combustion more amount of oxygen is present, at one point even the soot

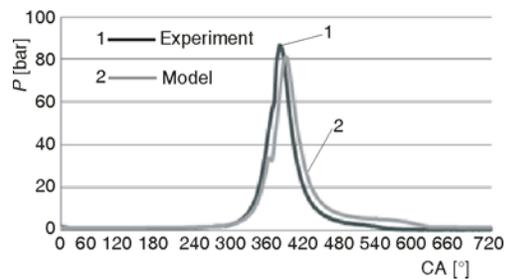


Figure 1. Experimental and predicted cylinder pressure at 100% load

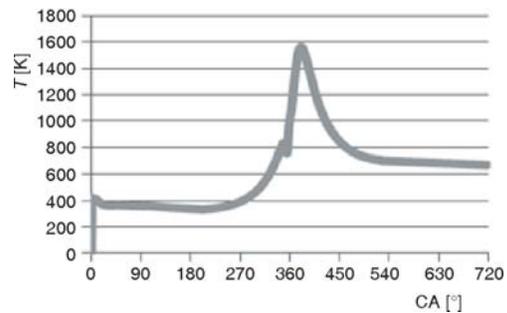


Figure 2. Predicted in cylinder temperature at 100% load

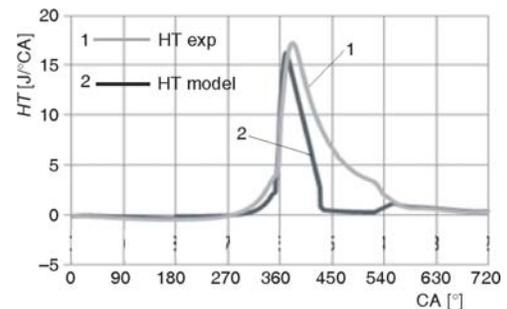


Figure 3. Heat transfer rate at 100% load

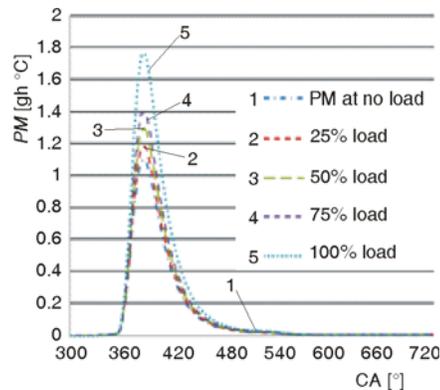


Figure 4. Simulated PM at various load conditions

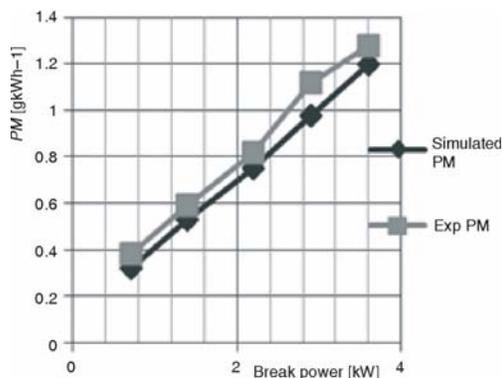


Figure 5. Experimental and simulated PM at various load conditions

low load conditions SOF content majorly influences PM formation rate, at high load conditions soot formation plays a crucial role in whole PM formation process.

Conclusions

In this work a two zone combustion model has been developed to simulate PM emission. The Two zone model developed is based upon two main composition of PM the soot and SOF. Various other submodels like heat release rate, ignition delay, and combustion models was developed initially in this work. Regarding pollution model to begin with, initially primary soot formation and oxidation model has been established. The difference between these two models gives overall soot formation rate. Hiroyasu soot formation model is used to determine soot primary formation rate and for soot oxidation NSC is followed. The SOF emission model is based upon HC emission model and is given by difference between HC primary formation model and HC oxidation model. Finally, these two models are coupled to give single PM emission model. Regarding validation of simulated PM model, experiments were carried out in a single cylinder, naturally aspirated water cooled direct injection Diesel engine. Final results shows that simulated PM and experimental PM are almost identical this show the model is a valid one.

formation rate becomes less than zero, it clearly reveals that oxidation rate exceeds formation rate. On the other hand, the corresponding difference between primary formation rate and oxidation rate attains its maximum value. Finally, oxidation rate decreases during after burning period and formation rate of PM increases slowly. Also the trend shows that soot plays a crucial role in PM formation process at high loads. The SOF content has great influence on whole PM formation at low loads (0%, 25%, and 50% conditions). This phenomenon occurs since at lower and middle load conditions fuel air equivalence ratio is lower and ignition delay is longer. On the surface of soot this SOF content readily absorbs, since the oxidation rate is slow and temperature in the cylinder is lower at this load conditions. During high load conditions (75% and 100%) the ignition delay gets reduced and corresponding in cylinder temperature gets increased. This leads to reduction of SOF formation rate, but soot formation rate increases at this condition.

Figure 5 shows the simulated and experimental PM were plotted at various load conditions. In this PM formation rate is plotted against brake power by giving loads using eddy current dynamometer. The trend shows that the simulated and experimental PM is almost identical and it finally reveals that PM model developed is a valid one. The PM gets increased at high load conditions this is because during high load conditions more amount of fuel gets injected and also premixed combustion duration get reduced.

Therefore, finally conclusion says that at

Both the simulation and experimental results clearly reveals that at lower loads SOF formation dominates the PM formation rate, whereas soot formation contributes more to whole PM formation rate at higher loads. The PM model developed is found to be very useful for researchers working in controlling of PM emission.

Nomenclature

A_f	– empirical constant for soot formation	S_p	– mean piston speed, [ms^{-1}]
A_{HC}	– empirical constant	T	– temperature, [K]
A_n	– flow area of nozzle holes, [m^2]	T_g	– gas temperature, [K]
C_d	– flow coefficient	T_{tq}	– torque, [Nm]
CA	– crank angle, [$^\circ$]	T_w	– cylinder wall temperature, [K]
D_s	– soot diameter ($3 \cdot 10^{-3} \text{ m}^3$)	t	– time for injection
dq_f/dt	– instantaneous injection rate	Δt_{comb}	– combustion duration, [$^\circ\text{CA}$]
dQ_f/dt	– instantaneous injection rate	V_d	– displacement volume, [m^3]
E_f	– activation energy	V_{sac}	– sac volume
[fuel]	– mass of unburned fuel vapour, [kgCA^{-1}]	X_{HC} and X_{O_2}	– the mole fractions of HC and O_2
h_c	– convective heat transfer coefficient, [$\text{Wm}^{-2}\text{K}^{-1}$]	x_{sac}	– fraction of fuel evaporated from sac volume
M_c	– carbon molecular weight (12 gmol^{-1})	Greek symbols	
M_{fb}	– mass of fuel burned, [kgCA^{-1}]	α	– fuel air equivalence ratio
m_i	– mass of fuel injected per crank angle, [kgCA^{-1}]	τ	– ignition delay, [$^\circ\text{CA}$]
$m_{f,0}$	– total fuel mass injected per cycle per cylinder, [kgCA^{-1}]	γ	– specific heat ratio in [$\text{Jkg}^{-1}\text{K}^{-1}$]
P	– cylinder pressure, [bar]	φ	– angle between vertical axis and connecting rod in degree, [rad]
p_m	– motored cylinder pressure, [bar]	ρ_s	– soot density (2000 kgm^{-3})
Δp_n	– difference between the pressures before the nozzle holes, [bar]	ρ_f	– density of fuel, [kgm^{-3}]
R	– universal gas constant, [$\text{Jkg}^{-1}\text{K}^{-1}$]	ω	– angular velocity in rad [s^{-1}]

References

- [1] Colin, R. F., Allen, T. K., *Internal Combustion Engine*, John Wiley and Sons, New York, USA, 2001
- [2] Heywood, J. B., *Internal Combustion Engine Fundamentals*, McGraw-Hill, New York, USA, 1988
- [3] Tan, P. Q., *et al.*, Analysis of Particulate Matter Composition from a Heavy-Duty Diesel Engine, Proc Inst Mech Eng, Part D, *J. Automobile Engg.*, 218 (2004), 11, pp. 1325-1331
- [4] Williams, P. T., The Role of Lubricating Oil in Diesel Particulate and Particulate PAH Emissions, SAE technical paper 87084, 1987
- [5] Kennedy, I. M., Models of Soot Formation and Oxidation, *Prog. Energy Combust.sci.*, 23 (1997), 2, pp 95-132
- [6] Taskinen, P., *et al.*, Simulation of Combustion, Soot and NO_x -Emissions in a Large Medium Speed Diesel Engine, SAE paper 981449, 1998
- [7] Cheng, X., *et al.*, Study on Soot Formation Characteristics in the Diesel Combustion Process Based on an Improved Detailed Soot Model, *Energy Conversion and Management*, 75 (2013), Nov., pp. 1-10
- [8] Kunpen, Qi., *et al.*, Simulation of Quasi-Dimensional Combustion Model for Predicting Diesel Engine Performance, *Applied Mathematical Modelling*, 35 (2011), 2, pp. 930-940
- [9] Lipkea, W. H., Dejoode, A. D., Direct Injection Diesel Engines Soot Modeling: Formulation and Results, SAE paper 940670, 1994
- [10] Suneel, K., *et al.*, Numerical Modelling of Compression Ignition Engine: A Review, *Renewable and Sustainable Energy Reviews*, 19 (2013), Mar., pp. 517-530
- [11] Hiroyasu, H., *et al.*, Development and Use of a Spray Combustion Modelling to Predict Diesel Engine Efficiency and Pollutant Emissions, Part 1: Combustion Modelling, *Bull JSME*, 26 (1983), 214, pp. 569-575
- [12] Hiroyasu, H., *et al.*, Fuel Spray Characterization in Diesel Engine, *Proceedings*, Symposium on Combustion Modelling in Reciprocating Engines, Plenum Press; New York, USA, 1980, pp. 369-408

- [13] Rakopolous, C. D., *et al.*, Validation and Sensitivity Analysis of a Two Zone Diesel Engine Model for Combustion and Emissions Prediction, *Energy Conversion and Management*, 45 (2004), 9-10, pp. 1471-1495
- [14] Gao, Z., Schreiber, W., A Multizone Analysis of Soot and NO_x Emission in a D.I. Diesel Engine as a Function of Engine Load, Wall Temperature, and Intake Air O₂ Content, ASME paper 2000-ICE-314, 2000
- [15] Kouremenos, D. A., *et al.*, Multi-Zone Combustion Modelling for the Prediction of Pollutants Emissions and Performance of DI Diesel Engines, SAE paper 970635, 1997
- [16] Stiesch, G., Merker, G. P., A Phenomenological Model for Accurate and Time Efficient Prediction of Heat Release and Exhaust Emissions in Direct Injection Diesel Engines, SAE paper 1999-01-1535, 1999
- [17] Welch, S., Moss, J. B., Zonal Modelling of Diesel Engine Smoke Emission, IMechE Paper C499/027/96, 1996
- [18] Jose, P., *et al.*, Algebraic Modelling for Thermodynamic Study of the Compression-Ignition Engine, SAE paper 2005-01-4143, 2005
- [19] Whitehouse, N. D., A Simple Method for the Calculation of Heat Release Rates in Diesel Engine, SAE paper 710134, 1971
- [20] Rezaei, R., Zero Dimensional Modelling of Combustion and Heat Release Rate in Diesel Engine, SAE paper 2012-01-1065, 2012
- [21] De Risi, A., *et al.*, A Theoretical Investigation on the Effects of Combustion Chamber Geometry and Engine Speed on Soot and NO_x Emissions, ASME paper 1999-ICE-207, 1999
- [22] Micklow, G. J., Gong, W., Combustion Modelling for Direct Injection Diesel Engines, *Proc. Inst. Mech. Eng, Part D, J. Automobile Eng*, 2015 (2001), 5, pp. 651-663
- [23] Nagle, J., Strickland-Constable, R. F., Oxidation of Carbon Between 1000-2000 °C, *Proceedings*, 5th Conference on Carbon, Pergamon Press; London, 1962, pp. 154-164
- [24] Assanis, D. N., *et al.*, A Predictive Ignition Delay Correlation Under Steady-State and Transient Operation of a Direct Injection Diesel Engine, *J. Eng Gas Turb Power*, 125 (2003), 2, pp. 450-457