Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression …
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

1131

DEVELOPMENT OF A SIMULATION MODEL FOR COMPRESSION IGNITION ENGINE RUNNING WITH IGNITION IMPROVED BLEND

by

Moranahalli Ponnusamy SUDESHKUMAR [a*]
and Gopalakrishnan DEVARADJANE [b]

[a] Department of Mechanical Engineering, Hindustan University, Chennai, Tamil Nadu, India
[b] Department of Automobile Engineering, Anna University, Chennai, Tamil Nadu, India

The present work describes the thermodynamic and heat transfer models used in a computer program which simulates the diesel fuel and ignition improver blend to predict the combustion and emission characteristics of a direct injection compression ignition engine fuelled with ignition improver blend using classical two zone approach. One zone consists of pure air called non-burning zone and other zone consist of fuel and combustion products called burning zone. First law of thermodynamics and state equations are applied in each of the two zones to yield cylinder temperatures and cylinder pressure histories. Using the two zone combustion model the combustion parameters and the chemical equilibrium composition were determined. To validate the model an experimental investigation has been conducted on a single cylinder direct injection Diesel engine fuelled with 12% by volume of 2-ethoxy ethanol blend with diesel fuel. addition of ignition improver blend to diesel fuel decreases the exhaust smoke and increases the thermal efficiency for the power outputs. It was observed that there is a good agreement between simulated and experimental results and the proposed model requires low computational time for a complete run.

Key words: *combustion model, Diesel engine, emissions, ignition improvers, performance*

Introduction

An intense research effort is ongoing in the engine combustion and pollutant emission of Diesel engines due to better fuel economy and widespread use in agricultural, transportation sectors. Compliance with the limited oil reserves and governmental regulations to meet emission standards, there has been an active research for alternate fuels. The prospective of improving the performance and minimizing the emissions seems to be quiet attractive in the case of ignition improvers which are considered as an alternative power source. Ignition improvers can be either synthetically prepared oxygenates or biomass products which can be produced from both fossil and renewable sources. 2-ethoxy ethanol has a high oxygen content and better intersolubility with diesel fuel at normal temperature and

---

1132

Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression ...
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

pressure; thus, it is regarded as a promising additive for Diesel engines. Although there are many experimental studies of ignition improvers, there is an obvious lack of thermodynamic models for analyzing their performance characteristics analytically. The thermodynamic models depend on the equations which are based on energy conservation laws from the first law of thermodynamics.
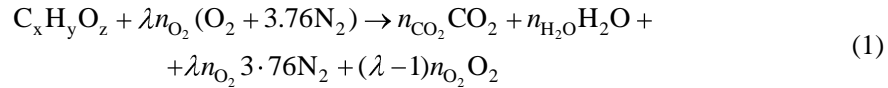
In the present work, a two zone thermodynamic model has been developed to study the combustion, performance and emission characteristics of the Diesel engine fuelled with ignition improver blend (12% 2-ethoxy ethanol). Using this model, pressure, temperature and other required properties are computed numerically for every crank angle step chosen. The heat transfer computations are also incorporated in the model using empirical equations. The ignition delay is also taken into account in the combustion model. The heat release calculations of the model are based on Whitehouse-ways method taking the premixed and diffusive combustions into account. The two zone thermodynamic simulation model developed is applied for a single cylinder four stroke direct injection Diesel engine. Initially the engine is operated with diesel fuel, subsequently ignition improver blend is used as fuel and then the results are compared and analyzed. The model has then been validated by an experimental analysis carried out at the author's institution.

Shroff *et al.* [1] developed mathematical models of Diesel engine to simulate and optimize the thermodynamic processes. Computer simulation [2] serves as a tool for a better understanding of the variables involved and also helps in optimizing the engine design for a particular application thereby reducing cost and time. Heywood [3] analyzed Heat release rate based on first law of thermodynamics and state equation. He proposed to use more sophisticated models for the gas properties before, during and after combustion with accurate heat transfer model. Annand [4] proposed an empirical formula to calculate the heat transfer in the cylinders of reciprocating internal combustion engines. Engine simulation and thermodynamic modeling [5] of various processes have been used along with experimental techniques to predict the performance and emission levels in Diesel engines. Ericson *et al.,* [6] used a quasi steady gas exchange model combined with a two zone combustion model to calculate NO_x and engine parameters. The model requires less computational effort than a computational fluid dynamics model which shows good agreement between measured and calculated emissions data. Because the detailed experiments on engines are difficult, thermodynamic models [7-11] have been setup to study the effect of engine operating variables on performance and emissions. The advances achieved by current automotive engines [12] would have been impossible without the simulation models providing quicker design insights. Ganapathy *et al.* [13] developed a thermodynamic model to compute the in-cylinder pressure and temperature histories in addition to various performance parameters of a Diesel engine fuelled with biodiesel derived from Jatropha oil. Low heat rejection diesel engine was analyzed comprehensively using two zone combustion models and different heat transfer models by Tamilporai *et al.* [14] to simulate the engine heat release, cylinder peak pressure and temperature and heat transfer details on zonal and cumulative basis.

Mathematical treatment

In simulation cycle calculations, state equation and first law of thermodynamics is applied. Two zones are considered inside the combustion chamber. During the start of compression the mole of different species that are considered to be present includes oxygen, nitrogen from intake and carbon dioxide, water (gaseous), nitrogen and oxygen from the

Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression ...
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

1133

residual gases. The reaction equilibrium is influenced the combustion of ignition improvers in the following way:

$$C_xH_yO_z + \lambda n_{O_2}(O_2 + 3.76N_2) \rightarrow n_{CO_2}CO_2 + n_{H_2O}H_2O +$$
$$+ \lambda n_{O_2} 3 \cdot 76N_2 + (\lambda - 1)n_{O_2}O_2 \tag{1}$$

For ignition improvers, a part of the oxygen needed for chemical reactions is already bound in fuel molecules.

Total moles of species of reactants for 2-ethoxy ethanol (2-EE) in the blend:

$$TMSR_1 = 1 + 4.773\lambda\left(i_1 + \frac{j_1}{4} - \frac{k}{2}\right) \tag{2}$$

Total moles of species of reactants for diesel in the blend:

$$TMSR_2 = 1 + 4.773\lambda\left(i_2 + \frac{j_2}{4}\right) \tag{3}$$

Total moles of species of reactants:

$$TMSR = TMSR_1 + TMSR_2 \tag{4}$$

Total moles of species of products for 2-EE in the blend:

$$TMSP_1 = i_1 + \frac{j_1}{2} + \left[3.773\lambda\left(i_1 + \frac{j_1}{4} - \frac{k_1}{2}\right)\right] + (\lambda - 1)\left(i_1 + \frac{j_1}{4}\right) - \lambda\frac{k_1}{2} \tag{5}$$

Total moles of species of products for Diesel in the blend:

$$TMSP_2 = i_2 + \frac{j_2}{2} + \left[3.773\lambda\left(i_2 + \frac{j_2}{4}\right)\right] + (\lambda - 1)\left(i_2 + \frac{j_2}{4}\right) \tag{6}$$

Total moles of species of products:

$$TMSP = TMSP_1 + TMSP_2 \tag{7}$$

For a closed system, the first law of thermodynamics states that:

$$dQ - dW = dE \tag{8}$$

where dQ is the heat loss to the chamber walls, dW – the network energy, and dE – the change in internal energy.

The state equation is applied for unburned zone consists of pure air:

$$PV = MR_{mol}T \tag{9}$$

where M is the number of kg-mol and V – the cylinder volume. The volume at each crank angle V_{ca} is calculated using the relation:

$$V_{ca} = V_{cyl} + \left(\frac{\pi d^2}{4}\right)r\left(1 + \frac{1}{\alpha} - \cos\varphi - \sqrt{\frac{1}{\alpha^2}\sin^2\varphi}\right) \tag{10}$$

where V_{cyl} is the cylinder clearance volume and α – the crank radius to piston rod length ratio.

For the surrounding air zone, which only loses mass (air) to the burning zone, the first law of thermodynamics for the unburned zone is written as:

$$\mathrm{d}E = \mathrm{d}Q - p\mathrm{d}V - h_\mathrm{a}\mathrm{d}m_\mathrm{a} \qquad (11)$$

The burning zone not only receives mass from the air zone, but also there is an enthalpy flow from the fuel which is ready to be burned in the time step. So, the first law of thermodynamics for the burning zone becomes:

$$\mathrm{d}E = \mathrm{d}Q - p\mathrm{d}V + h_\mathrm{a}\mathrm{d}m_\mathrm{a} + h_\mathrm{f}\mathrm{d}m_\mathrm{f} \qquad (12)$$

The total internal energy is calculated from the expression:

$$E(T) = M\Sigma[x_\mathrm{i}e_\mathrm{i}(T)] \qquad (13)$$

$$e_\mathrm{i}(T) = h_\mathrm{i}(T) - \mathrm{R}T \qquad (14)$$

where $h_\mathrm{i}(T)$ is the specific enthalpy of a gas of species.

The first law of thermodynamics for the combustion in time step $\mathrm{d}t$ is:

$$\mathrm{d}Q - \mathrm{d}W = E(T_2) - E(T_1) - \mathrm{d}m_\mathrm{f}\, Q_\mathrm{vs} \qquad (15)$$

$$E(T_2) = E(T_1) - \mathrm{d}Q + \mathrm{d}W + \mathrm{d}m_\mathrm{f}\, Q_\mathrm{vs} \qquad (16)$$

If $f(E)$ is greater than the accuracy required new value of T_2 is calculated using:

$$T_2 = T_2' - \frac{f(E)}{mC_\mathrm{v}T_2'} \qquad (17)$$

The unburned zone temperature is calculated using the equation:

$$T_\mathrm{u} = T_\mathrm{soc}\left(\frac{P}{PSOC}\right)^{\frac{\gamma-1}{\gamma}} \qquad (18)$$

Thermodynamic data for elements, combustion products and many pollutants are available in a compilation published by the National Bureau of Standards, called the Joint Army-Navy-Air Force (JANAF) tables (1971). For single component fuels the data presented in [15] is in the same format as that of JANAF tables.

Fuel injection rate

The fluid in Diesel engine is generally heterogeneous. Considering the nozzle open area is constant during the injection period, mass of the fuel injected for each crank angle is calculated using the relation,

$$m_\mathrm{fi} = C_\mathrm{d}\frac{\pi}{4}d_\mathrm{n}^2\left(\frac{2\Delta P_\mathrm{n}}{\rho_\mathrm{f}}\right)^{0.5} \qquad (19)$$

Heat transfer

Due to the complexity of the flow patterns in the combustion chamber, estimating the heat transfer to the cylinder walls is very difficult. However various correlations have

been derived from measurements to predict the heat transfer coefficient. Heat transfer is calculated taking into account both convection and radiation. The heat transfer from cylinder to combustion chamber wall is calculated using the well proven Annand's correlation:

$$\frac{dQ}{dt} = A_h k \frac{Re^b}{D}(T_g - T_w) + C_h(T_g^4 - T_w^4) \tag{20}$$

A_h and b are constant for convective heat transfer. The factor C_h is calculated based on the injected fuel mass. The first term in the above equation shows that Prandtl number for the gases forming the cylinder contents will be approximately constant at a value 0.7, claims that Reynolds number is the major parameter affecting convection. The second term in eq. (20) is a straight forward radiation term assuming grey body radiation. The values for constants were chosen to the best fit between experimentally obtained and predicted results. T_g is the mean gas temperature and T_w is the cylinder wall temperature. The value of T_w is taken equal to 450 K.

Combustion model

Combustion is a chemical reaction between a fuel and oxygen, which is accompanied by the production of a considerable amount of heat. Combustion is modeled to describe the heat release rate and to predict the emissions. The heat release rate can be defined as the rate at which the chemical energy of the fuel is released by combustion. In a two-zone combustion model, the combustion chamber is divided into two zones namely premixed zone and diffusive zone. The two stage behavior of combustion heat release rate curves are commonly identified as premixed combustion and diffusive combustion. The current two zone model includes processes occurring during the closed cycle. The main calculation procedure is based on the integration of the first law of thermodynamics and the perfect gas state equation for each zone separately. White house-ways model [16] incorporating the rate of preparation of the fuel, surface area of fuel droplets and partial pressure of oxygen in the cylinder are used in the present work to calculate the heat release rate in these zones. In this method the rate of mixing was assumed to be dependant upon the total surface area of the droplets forming the fuel spray. The injected fuel in the burning zone mixes up with the air entrained from the air zone via a mixing and diffusion process, while the burning rate of the fuel is expressed by an Arrhenius-type expression. Premixed combustion rate is limited by the chemical reaction rate. Fuel injected after start of combustion is consumed by diffusive combustion and is controlled by the amount of locally available oxygen.

The preparation rate equation is given by:

$$P = k(m_i)^x (m_u)^y (P_{O_2})^m \tag{21}$$

The combustion constants are set to the values of $x = 0.33$, $y = 0.67$, and $m = 0.4$. Partial pressure of oxygen (P_{O_2}) in the eq. (21) allows for an effect of oxygen availability on mixing. The rate of preparation is proportional to the surface area of all the droplets having uniform diameter. Taking all droplets to be identical at any time then:

$$m_i = n\rho \left(\frac{1}{6}\right)\pi D_0^3 \tag{22}$$

$$m_u = n\rho \left(\frac{1}{6}\right)\pi D^3 \tag{23}$$

where ρ is the fuel droplet density, D_0 – the droplet initial diameter, D – the fuel droplet diameter at any instant, and n – the number of fuel droplets. Total surface area at any instant $n\pi D^2$. Assume the velocity of the gas molecules is proportional to the square root of the temperature, the density of oxygen is proportional to the partial pressure divided by the temperature, the unburnt fuel is given by $\int(P - R)\mathrm{d}\alpha$, where P is the rate of preparation and R is the rate of burning per degree crank angle. The delay period and reaction kinetics are time dependant phenomena so the formula includes N as a divisor to make the reaction rate formula crank angle dependant as required by the computer programme:

$$R = \frac{K'P_{O_2}}{N\sqrt{T}}\, \mathrm{e}^{\frac{-a}{T}} \int (P - R)\mathrm{d}\alpha \tag{24}$$

where K' is a constant in the reaction rate equation, and a – the index in the reaction rate equation.

Finally the combustion rate is given by the relations:

$$\frac{\mathrm{d}m_{\mathrm{f}}}{\mathrm{d}\varphi}\, P \quad \text{if} \quad R > P \quad \text{and} \quad \frac{\mathrm{d}m_{\mathrm{f}}}{\mathrm{d}\varphi} = R \quad \text{if} \quad R < P \tag{25}$$

At high temperatures corresponding to the main period of combustion, the time taken by the burning of the prepared fuel is negligible compared to the preparation time. Therefore, for most of the burning period the heat release can be taken as a measure of the preparation rate.

Ignition delay

The time delay between the start of injection and the start of combustion is defined as the ignition delay period. In the combustion model the ignition delay is also taken into account. The ignition delay period is calculated by integrating Wolfer's relation using trapezoidal rule.

Nitric oxide formation

Nitric oxide is generated in combustion processes under the influence of high gas temperatures and sufficient local oxygen. Diesel fuel contains only a very small amount of nitrogen, so NO formation occurs almost exclusively through the oxidation of atmospheric nitrogen. The NO formation stems from three principal sources:
– thermal NO which is formed due to the dissociation of the molecular air-nitrogen,
– prompt NO formed by the "attack" of hydrocarbon fragments on the air-nitrogen, and
– NO formed from nitrogen containing components in the fuel.

Fuel-NO formation can be neglected during the combustion process in internal combustion engines. Prompt NO formation can also be neglected since this process plays no dominant role in comparison to the thermal NO formation. In engines, the cylinder pressure rises during the combustion process, so earlier burnt gases are compressed to a higher temperature level as they have immediately after their combustion. Hence, the thermal NO formation in the burnt gases always dominates in comparison to the NO formed in the flame front and represents the main source of the NO in engines.

NO is formed during the post flame combustion process in a high temperature region. The reaction mechanism can be expressed in terms of the extended Zeldovich mechanism:

$$N_2 + O \rightarrow NO + N \tag{26}$$

$$N + O_2 \rightarrow NO + O \tag{27}$$

$$N + OH \rightarrow NO + H \tag{28}$$

The initial NO formation rate is given as:

$$\frac{d(NO)}{dt} = \frac{6 \cdot 10^6}{\sqrt{T}} \exp\left(\frac{-69090}{T}\right)[O_2]_e^{0.5}[N_2]_e \tag{29}$$

NO formation is strong dependant on temperature and oxygen concentration during the combustion phase. The equilibrium oxygen and nitrogen concentration in the burned zone are given by:

$$[O_2]_e = f_{O_2}(P,T) \quad [N_2]_e = f_{N_2}(P,T) \tag{30}$$

Smoke formation

With Diesel engines, the maximum power is limited by the appearance of solid carbon (smoke) in the exhaust even though the engine is running lean [17]. Smoke forms because the combustion is heterogeneous. Smoke formation process is governed by a complex radical mechanism. In high temperature zones aromatic molecules are reactivated by hydrogen atoms and large dehydrogenated particles absorb at their surface hydrocarbon species from the gas mixture, which leads to the fast smoke growth. Smoke formation rate is calculated using a semi-empirical model that has been widely tested. The formation rate is calculated by assuming a first order reaction of vaporized fuel, m_f, as:

$$\frac{dm_{sf}}{dt} = A_f m_f P^{0.5} \exp\left(\frac{-E_{sf}}{R_{mol}T}\right) \tag{31}$$

The soot oxidation is predicted by assuming a second order reaction between soot, m_b, and oxygen:

$$\frac{dm_b}{dt} = A_b m_b \left(\frac{P_{O_2}}{P}\right) P^2 \exp\left(\frac{-E_b}{R_{mol}T}\right) \tag{32}$$

where P_{O_2} is the partial pressure of oxygen. Activation energies are set to the values of $E_{sf} = 1.25 \cdot 10^4$ kcal/kmol, $E_b = 1.40 \cdot 10^4$ kcal/kmol. A_f and A_b are constants that are determined by matching the calculated smoke with the measured smoke in the exhaust gas.

Net smoke formation is expressed as:

$$\frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_b}{dt} \tag{33}$$

Having applied the above equations smoke mass is calculated.

Computational procedure

The simulation of compression ignition engine fuelled with ignition improver blend was developed using Mathworks Matlab software and the various equations of the thermodynamic model are solved numerically. The fuel parameters such as number of moles of carbon, hydrogen, and oxygen, heating value, molecular weight of the fuel, cut off ratio and the various constants used in the model are defined in the data subroutine. Bore, stroke length, connecting rod length, compression ratio, relative air fuel ratio, engine speed, inlet conditions, and atmospheric conditions are given as input parameters. The number of moles of exhaust gas constituents are calculated from the air fuel ratio and molecular formula of the fuel employed. During the cycle, the program concerning the simulation model predicts the heat release rate, composition of burned and unburned zones, temperature of burned and unburned zones, cylinder pressure, heat loss by radiation and convection, workdone, concentration of pollutants emitted, and engine performance. The results and graphs were generated by Matlab software as outputs to the program for given inputs.

Experimental description

The engine used in the present study was a Kirloskar single cylinder direct injection Diesel engine with the specifications given in tab. 1. The engine was coupled to an electrical dynamometer and all the experiments were carried out at a constant engine speed of 1500 rpm. The single cylinder engine used in this study does not include any auxiliary systems. The ignition improver (2-EE) is blended with diesel fuel in proportions of 12% by volume. The engine is started and allowed to warm up for about 20 minutes. The time taken for 20 cm^3 of fuel consumption was measured. The pressure readings are taken from the signal obtained from piezoelectric transducer (Kistler) through the data acquisition system. For crank angle measurement, a Kistler crank angle encoder is used. The encoder gives a digital pulse for every one degree with an accuracy of 0.1°. The angle encoder flange also has a top dead center (TDC) position mark which represents TDC position of the engine. Self calibrating type Krypton 290 EN2 gas analyzer is used to measure the oxides of nitrogen. Smoke readings are obtained from diesel tune smoke meter interfaced with computer. The smoke meter is of self calibration type and can show smoke readings in fuel smoke number (Bosch units) to a scale of 1 to 10 with an accuracy of 0.01 units. To ensure accuracy five readings are taken at each stage and average is calculated. This procedure is repeated at the same

Table 1. Engine specifications

Type of engine	Four stroke single cylinder DI Diesel engine
Bore	102 mm
Stroke	118 mm
Compression ratio	17.5:1
Rated speed	1500 rpm
Injection pressure	200 bar
Injection timing	26° CA bTDC
Maximum power	10 hp

Figure 1. Experimental set-up

Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression …
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

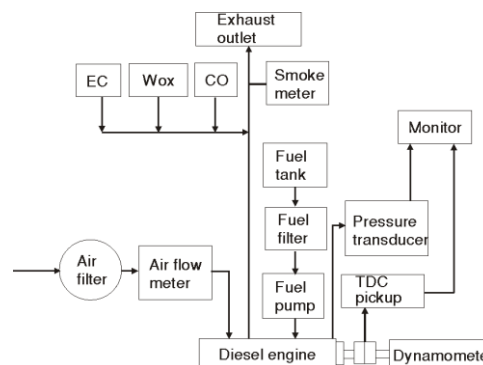1139

operating condition by changing the loads from no load to full load. The result obtained using 2-EE blend with diesel fuel is compared with the simulated values for validation of the simulation code. Figure 1 shows the experimental set-up.

Results and discussion

The simulation model developed for performance and emission characteristics is based on the engine parameters and fuel specifications given as input. The time step used was 1° crank angle. To verify the accuracy of the two zone model over a wide range of operating conditions, engine performance was simulated and compared with experimental data for a range of loads from 20% to 100% at a speed of 1500 rpm. The model can be useful for both diesel and ignition improver blend analysis.

Figure 2 shows the comparison of predicted and experimental cylinder pressure variations as a function of engine crank angle for diesel and ignition improver blend at an engine speed of 1500 rpm and 80% load. The prediction shows that the peak pressure value is 67 bar for diesel at 6° CA and 69 bar for 2-EE blend at 5° CA aTDC. Under the same operating conditions the experimental peak pressure is 68 bar for diesel at 6° CA and 70 bar for 2-EE blend at 5° CA aTDC. It can be observed that the addition of ignition improver blend to diesel fuel increases the cylinder pressure during premixed combustion phase. This is due to reduced ignition delay of ignition improver blend because of oxygen in the fuel-air parcel. The energy released by the blended fuel would be lower in the diffusive combustion leads to lower the cylinder pressures. The trends of the predicted cylinder pressure curves for ignition improver blend and diesel fuel and experimental cylinder pressures are almost similar in nature. Therefore, both the magnitude and timing of occurrence of the peak pressure are precisely predicted by the model.
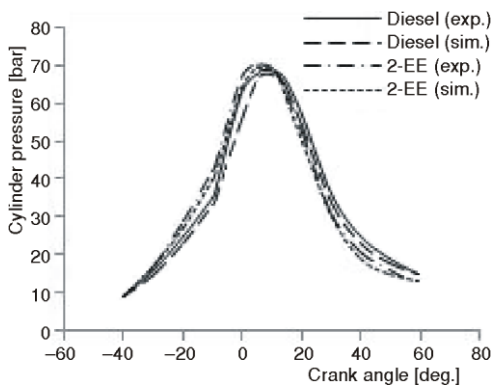

Figure 2. Comparison of cylinder pressure at 80% of power output
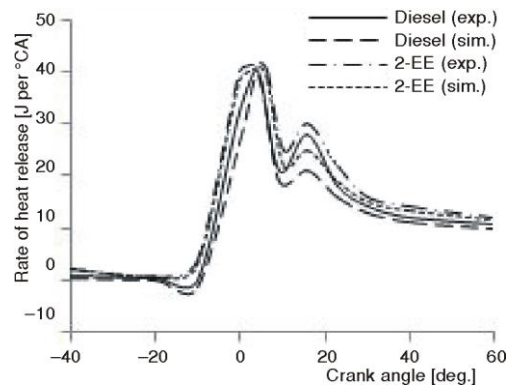
Figure 3. Comparison of rate of heat release at 80% of power output

Figure 3 shows the heat release rate predicted by the simulation model and the experimental one for ignition improver blend and Diesel fuel at an engine speed of 1500 rpm and 80% load with a compression ratio of 17.5 and an injection timing of 27 deg. crank angle bTDC. Figure 3 exhibits the double-peak shape that characterizes the direct injection diesel combustion. It was observed from the results that the addition of 12% 2-EE blend increases the heat release rate in both the premixed combustion and diffusive combustion phases compared to that of pure diesel fuel. Heat release rate is increased at higher load due to

decrease in delay period because of higher cetane number of the blended fuel compared to diesel fuel. Addition of blended fuel also prompts combustion, improves burning rate and combustion efficiency, makes heat release rate higher. The measured peak heat release rate for 2-EE blend with diesel fuel is 41.5 J/°CA and for pure diesel it is 40 J/°CA. The predicted peak heat release rate for the blended fuel is 40.7 J/°CA and for diesel fuel it is 39 J/°CA. The close analysis of the heat release rate at higher engine load showed proper utilization of the blended fuel inside the combustion chamber of the engines, resulting in a faster combustion rate.

Figure 4 shows the comparison of cumulative heat release for diesel and ignition improver blends. A slight advance in cumulative heat release is observed for 2-EE blend with diesel fuel as compared to diesel fuel for the predicted values which can be attributed to better ignition and improved burning characteristics of the blended fuel. The prediction shows that the increase in cumulative heat release is 2.93% compared to diesel fuel. 2-EE helps to accelerate the combustion process which improves engine thermal efficiency.
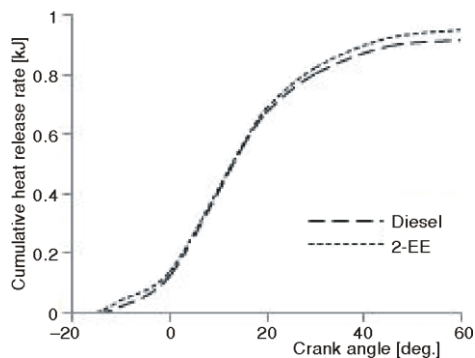

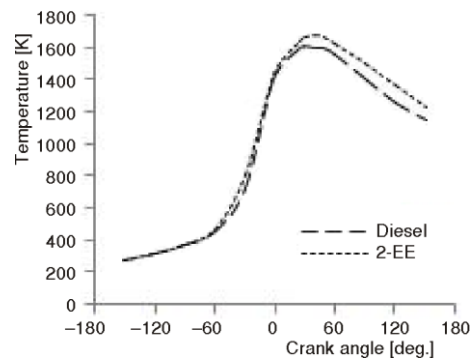**Figure 4. Comparison of cumulative heat release rate at 80% of power output**

Figure 5. Comparison of cylinder mean temperature at 80% of power output

Figure 5 shows the comparison of cylinder mean temperature for diesel and the blended fuel. From the results it was observed that there is an increase in cylinder temperature for 2-EE blend compared with diesel fuel. The addition of blended fuel with pure diesel increases the combustion rate leads to increase in the cylinder temperature. The cylinder temperature is higher due to higher cetane number of the blended fuel compared to diesel fuel. The maximum temperature for diesel is 1604 K whereas for 2-EE blend with diesel fuel the combustion temperature is 1680 K.

Total heat transfer is the sum of convective and radiative heat transfer. Figure 6 shows the variation of total heat transfer for diesel and ignition improver blend with diesel fuel. It was observed that the total heat transfer for 2-EE blend is reduced by about 16.5% than that of diesel at 80% of rated power output. The reduced total heat transfer is due to the reduction of surface area for heat transfer. The increase in the density of blended fuel with diesel increases the swirl velocity and thereby reducing the surface area for heat transfer. The constants in the Annand formulae have been adjusted to give reasonable accuracy between simulated and experimental values of total heat transfer.

Compression ratio and cylinder temperature influence the net work done. Figure 7 shows the variation of cumulative work done for diesel and ignition improver blend with diesel fuel. The predicted value of work done of 2-EE blend with diesel fuel is slightly increased compared to diesel fuel. The increase in the cumulative work done of the blended fuel is due to increase in the heat release rate and peak pressure.
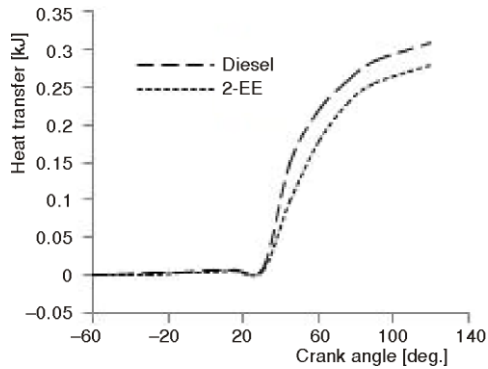
Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression …
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

1141

Figure 6. Comparison of total heat transfer at 80% of power output
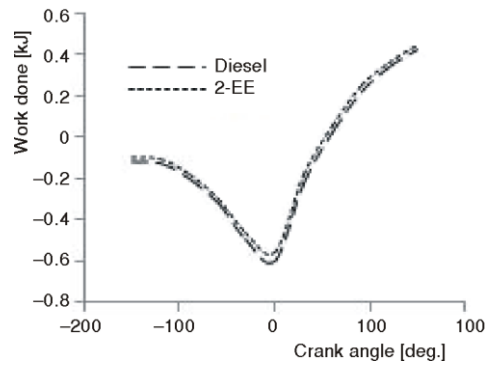

Figure 7. Comparison of cumulative work done at 80% of power output

Figure 8 shows the comparison of brake specific fuel consumption predicted by the simulation model and the experimental one for diesel fuel and ignition improver blend at varying brake loads. It was observed from the figures that the specific fuel consumptions of diesel and ignition improver blend were decreased with increasing load from 1 kW to 4 kW and tended to increase with further increase in brake power. The blended fuel has brake specific fuel consumption (BSFC) very close to that of diesel fuel. The predicted BSFC values for the blended fuel is 0.77 kg/kWh at 1 kW and 0.25 kg/kWh at 4 kW, respectively, and it is 0.75 kg/kWh at 1 kW and 0.22 kg/kWh at 4 kW for diesel fuel. Under the same operating condi-

Figure 8. Comparison of experimental and predicted values of BSFC

tions the experimental BSFC values for blended fuel is 0.78 kg/kWh at 1 kW and 0.28 kg/kWh at 4 kW, respectively, and for diesel fuel it is 0.76 kg/kWh at 1 kW and 0.25 kg/kWh at 4 kW. The combined effects of higher fuel density and lower heating value of the blended fuel slightly increases the BSFC. Table 2 shows the properties of disel, 2-EE, and blended fuels. The coincidence between the predicted and measured values is good.
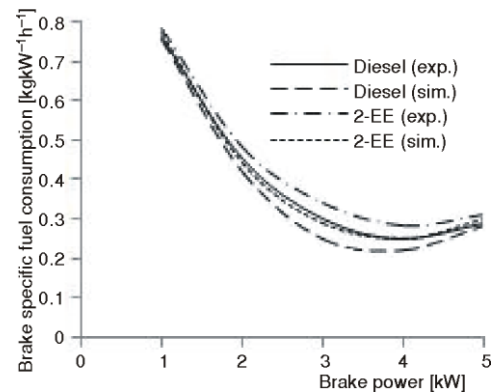
Table 2. Fuel properties

Properties	Diesel	2-EE	Blended fuel
Oxygen content	–	35.5	4.45
Cetane number	45	58	49.5
Density [gcm^{-3}]	0.86	0.93	0.88
Boiling point [°C]	320	135	230
Heat of combustion [MJkg^{-1}]	42	22	38.5
Viscosity at 40 °C	2.61	2.25	2.4
Flash point [°C]	55.5	54	52.3

Figure 9 shows the comparison of break thermal efficiency with respect to the loads predicted by the simulation model and the experimental one for diesel fuel and ignition improver blend. From the results it was observed that initially with increasing loads the brake thermal efficiencies of diesel fuel and 2-EE blend with diesel fuel is increased and the maximum thermal efficiency is obtained at 4 kW and then tended to decrease with further increase in brake power. Addition of 2-EE blend increases the thermal efficiency compared to diesel fuel at all loads. The increase in thermal efficiency is due to complete combustion, lower viscosity and the presence of oxygen in the ignition improver blend with diesel fuel. For the ignition improver blend, the brake thermal efficiency is 13.5, 21.5, 30.5, 35, and 33% at 1, 2, 3, 4, and 5 kW, respectively, and for diesel it is 12.8, 20.4, 28, 33, and 31% predicted by the simulation model. Under identical conditions the experimental values for blended fuel is 13.6, 22, 30.7, 36, and 34% at 1, 2, 3, 4, and 5 kW, respectively, and for diesel it is 13, 21, 29, 34, and 31.5%. The coincidence of simulation and experimental values are found to be in good agreement.
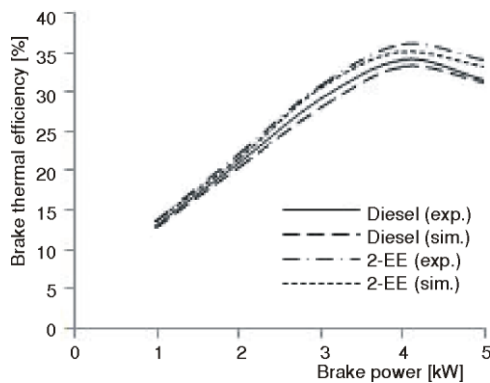

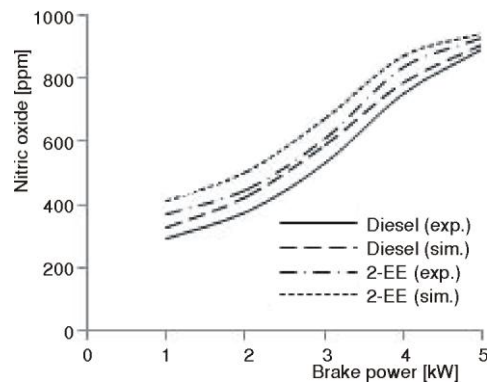**Figure 9. Comparison of experimental and predicted brake thermal efficiency**

Figure 10. Comparison of experimental and predicted NO

Figure 10 shows the comparison of simulated and experimental NO concentration with respect to the loads for ignition improver blend and diesel fuel. NO emissions were continuously increased as engine load increases. Increase of engine load causes increase of fuel burning and prevalence of higher flame temperature which favors increased NO formation. This is expected, since nitrogen oxide formation is favoured for near stoichiometric conditions towards the lean side, which are approached by the higher loads in a Diesel engine. Addition of 2-EE blend increases the NO emission at all loads. NO emission for blended fuel is increased compared to diesel fuel due to faster combustion and increase in average temperature reached in the combustion cycle. The oxygen in the cylinder might have attained the atomic status and so also nitrogen causes increase in NO emission. NO emission is 890 ppm at full load with diesel and it is increased to 930 ppm with the addition of 2-EE blend with diesel fuel at full load predicted by the experiments. The coincidence of simulation and experimental values are found to be good agreement.

The smoke in the engine exhaust is the net result of soot formation and the subsequent oxidation during the combustion process. Soot consists of carbon and hydrogen in the core and with toxic components like metals, acids and organics absorbed on the surface area [18]. Figure 11 shows the comparison of smoke intensity with respect to load predicted by the

Sudeshkumar, M. P., *et al.*: Development of a Simulation Model for Compression …
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

1143

simulation model and the experimental one for diesel fuel and ignition improver blend. The formation of smoke is strongly dependent on the engine load. As the load increases more fuel is injected and this increases the formation of the smoke. The results clearly showed that the addition of 2-EE blend decreases the smoke level at all load operations. The oxygen content in the fuel and the lower viscosity of ignition improver blend is responsible for lower smoke emissions and therefore the smoke content in the exhaust is reduced. The smoke intensity is reduced by 20% with the blended fuel

Figure 11. Measured and simulated smoke

compared to diesel fuel. The coincidence between predicted and measured smoke intensity is good for all the load operations.

Conclusions
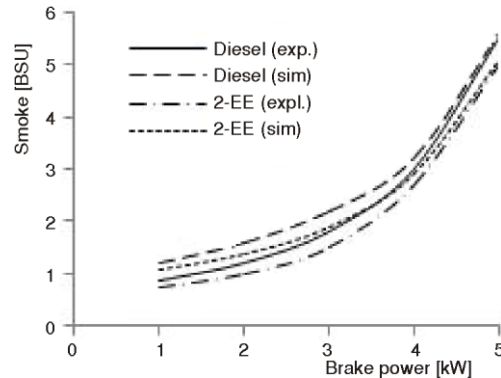
In the present work a two zone simulation model for ignition improver blend with diesel fuel and pure diesel fuel has been developed to predict the combustion, performance characteristics and engine-out emissions in direct injection compression ignition engines.

Results were validated and compared with the experimental data for single cylinder direct injection Diesel engine for mean cylinder pressure, rate of heat release, and exhaust emission. The same values of the set of calibration constants were used throughout for all conditions examined, performance and emission-wise. A good agreement between the predicted and experimental values ensures the accuracy of the numerical predictions with the present work. The simulation model developed successfully captures the single cylinder compression ignition engine operating characteristics.

The operational range of the model is wide and computational run time is short, thus making the simulation model suitable for use with thermodynamically based cycle simulations in compression ignition engines running with ignition improver blend and diesel fuel. Due to its simplicity, the model can be used for wide range of alternate fuels to optimize the design.

Nomenclature

Af, Ah – preexponential constants
C_d – coefficient of discharge, [–]
C_v – heat of reaction at constant volume, [kJkg^{-1}]
dm_a – mass of air in each step, [kg]
dm_f – mass of fuel in each step, [kg]
d_n – diameter of the nozzle, [m]
D – cylinder bore, [m]
dQ – heat transfer in each step, [kJ]
E – total energy, [J]
h_a – specific enthalpy of air, [Jkg^{-1}]
h_f – specific enthalpy of fuel, [Jkg^{-1}]
m_b – mass of fuel burnt, [kg]

m_{fi} – mass of the fuel injected, [kg]
m_i – initial mas of the fuel, [kg]
m_u – unprepared mass of the fuel, [kg]
N – engine speed, [revmin^{-1}]
P – pressure, [Nm^{-2}]
P_1 – pressure after entrainment, [Nm^{-2}]
P_2 – final pressure, [Nm^{-2}]
P_{soc} – pressure during start of combustion, [Nm^{-2}]
ΔP – pressure drop, [Nm^{-2}]
Q_{vs} – lover heat of reaction, [kJ]
R_{mol} – universal gas constant, [Jmole^{-1}K^{-1}]
Re – Reynolds number, $(= UD/\nu)$, [–]

1144

Sudeshkumar, M. P., *et al*.: Development of a Simulation Model for Compression …
THERMAL SCIENCE, Year 2011, Vol. 15, No. 4, pp. 1131-1144

r	– compression ratio, [–]		ρ	– density, [kgm^{-3}]
T	– absolute temperature, [K]		φ	– crank angle, [deg.]
T_{soc}	– temperature during the start of combustion, [K]		*Subscripts*	
T_u	– unburned zone temperature, [K]		a	– air
V	– volume, [m^3]		f	– fuel
V_{cyl}	– cylinder displacement, [m^3]		g	– gas conditions
x_i	– mole fraction of individual species		sf	– smoke formation

Greek symbols

λ – excess air, [–]

References

[1] Shroff, H. D., Hodgetts, D., Simulation and Optimization of Thermodynamic Processes of Diesel Engine, SAE paper 740194, 1974

[2] Ganesan, V., Computer Simulation of Compression-Ignition Engine Processes, University Press Ltd., Hyderabad, India, 2000

[3] Heywood, J. B., International Combustion Engine Fundamentals, McGraw Hill Book Company, New York, USA, 1988

[4] Annand, W. J. D., Heat Transfer in the Cylinders of Reciprocating Internal Combustion Engines, *Proceedings Instn Mech Engrs., 177* (1963), 36, pp. 973-996

[5] Chow, A., Wyszynski, M. L., Thermodynamic Modeling of Complete Engine Systems – a Review, *Proceedings Instn Mech Engrs., 213* (1999), 4, pp. 403-415

[6] Ericson, C., *et al.,* Modeling Diesel Engine Combustion and NOx Formation for Model Based Control and Simulation of Engine and Exhaust after Treatment Systems, SAE paper 2006-01-0687, 2006

[7] Rakopoulos, 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

[8] Merker, G. P., Hohlbaum, B., Rauscher, M., Two-Zone Model for Calculation of Nitrogen Oxide Formation in Direct-Injection Diesel Engines, SAE paper 932454, 1993

[9] Hountalas, D. T., Papagiannakis, R. G., Development of a Simulation Model for Direct Injection Dual Fuel Diesel-Natural Gas Engines, SAE paper 2000-01-0286, 2000

[10] Ishida, M., *et al.,* Combustion Analysis by Two-Zone Model in a Diesel Engine, 3rd International Symposium COMODIA, Yokohama, Japan, 1994

[11] Ramachandran, S., Rapid Thermodynamic Simulation Model of an Internal Combustion Engine on Alternate Fuels, *Proceedings,* International Multiconference of Engineers and Computer Scientists, Hong Kong, 2009

[12] McCartan C. D., *et al.,* Computer Simulation of the Performance of a 1.9 Litre Direct Injection Diesel Engine, SAE paper 2002-01-0070, 2002

[13] Ganapathy, T., *et al.,* An Analytical and Experimental Study of Performance on Jatropha Biodiesel Engine, *Thermal Science, 13* (2009), 3, pp. 69-82

[14] Tamilporai, P., *et al*., Simulation and Analysis of Combustion and Heat Transfer in Low Heat Rejection Diesel Engine using Two Zone Combustion Model and Different Heat Transfer Models, SAE paper 2003-01-1067, 2003

[15] Stull, D. R. Westrum, E. F., Jr., Sinke, G. C., The Hemical Thermodinamics of Organic Compounds, 2nd ed., John Wiley and Sons, New York, USA, 1969

[16] Whitehouse, N. D., Benson, R. S., Internal Combustion Engines, Pergamon Press, London, 1979

[17] Ferguson., C. R. Internal Combustion Engines, Applied Thermo Sciences, John Wiley & Sons, Inc., New York, USA, 1986

[18] Boussouara, K., Kadja, M., Empirical Soot Formation and Oxidation Model, *Thermal Science, 13* (2009), 3, pp. 35-46