Development of a Comprehensive Two-zone Model for Combustion and Emissions Prediction in a Direct Injection (DI) Diesel Engine

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Abstract
A two zone model for the calculation of the closed cycle of a compression ignition direct injection (DI) diesel engine is developed. This model divides the cylinder contents into a non-burning zone of air surrounding the fuel spray jets issuing from injector nozzle holes and another homogenous zone in which fuel is supplied continuously from injector and burned with entrained air from the air zone. The growth of the fuel spray zone in the combustion chamber, consisting of a number of fuel-air conical jets equal to the injector nozzle holes, is carefully modeled by incorporating jet mixing and main relevant spray parameters. Application of the mass, energy and state equations in each one of the two zones yields local temperature and cylinder pressure histories. Furthermore, compression stroke, heat transfer, ignition delay period, rate of combustion, pollutants formation and expansion stroke are considered in this thermodynamic modeling. For the calculation of the constituents in exhaust gases, a chemical equilibrium scheme is adopted for the C-H-O-N system of 11 species considered. The precise amount of nitric oxide (NO) in exhaust gases is calculated by a chemical kinetics model. Also, the soot formation process is modeled by considering both the formation and oxidation processes in net soot formation. Eventually, the theoretical results are validated against experimental results and a multi-parametric study has been done to show the effects of various important parameters on emissions and in-cylinder pressure.
Key words: Direct Injection Diesel Engine, Emissions, Modeling, Performance, Simulation.

Introduction
Having offered suitable performance characteristics compared to SI engines such as higher fuel economy and thermal efficiency duo to their lean burn operation, higher compression ratio without knock constraints, good power density, and no part-load throttling losses problems, diesel engines are being used in a wide variety of applications, forming an important motive foundation for a modern society [1,2].
Mathematical models of combustion phenomenon in diesel engines can be classified from simple zero-dimensional thermodynamic models to sophisticated multi-dimensional models [3-5].
In the present work, to gain the advantage of relative simplicity and maintain the computer time cost within reasonable limits, a comprehensive two-zone model of diesel combustion is developed including the detailed modeling of the main various mechanisms involved in the cylinder through a comprehensive and validated phenomenological model. Plots of pressure, nitric oxide (NO) and soot densities have been presented as a function of crank angle for various injection timings and engine loads.

Engine model implementation
This section of the paper describes the engine modeling. The presented model involves the modeling of major mechanisms involved in the cylinder such as spray, ignition delay, combustion, heat transfer, and pollutants formation models in addition to the conservations and state equations all in the closed cycle operation of the engine in which both intake and exhaust valves are closed.

Spray Model
This section describes the total spray model encompassing spray penetration, break-up point, spray cone angle and rate of air entrainment into the spray.

Mathematical expressions for spray tip penetration and break-up point: Disintegration process and spray characterization of fuel jet issuing from the nozzle hole in diesel engine have been thoroughly analyzed by Arai and Hiroyasu [6,7]. According to their model, the spray tip penetration shows different relationships with time before and after break-up time, t_{br}:

$$x = C_D \left(\frac{2\Delta P}{\rho_l} \right)^{\frac{1}{2}} t \qquad 0 < t < t_{br} \qquad (1)$$

$$x = 2.95 \left(\frac{\Delta P}{\rho_a} \right)^{0.25} \sqrt{D_N} t^{\delta} \qquad t \geq t_{br} \qquad (2)$$

Where:

$$t_{br} = 4.351 \frac{\rho_l . D_N}{C_D{}^2 . \left(\rho_a . \overline{\Delta P} \right)^{\frac{1}{2}}} \qquad (3)$$

The above equations are generalized form of Arai model to include different discharge coefficients, C_D [4]. Also, the exponent δ was considered equal to 0.5 [8].

In the above equations, the parameters ΔP and $\overline{\Delta P}$ are instantaneous and mean pressure drop in the nozzle hole. The amount of fuel to be injected in the

cycle, m_{ftot}, can be calculated as follows, provided that both the total amount of air intaked in the cylinder until IVC, m_{atot}, and AFR is known:

$$m_{ftot} = \frac{m_{atot}}{AFR} \tag{4}$$

Then, the average rate of fuel injection from nozzle in a cycle $(kg/^\circ CA)$ can be obtained:

$$\overline{\dot{m}}_{f_{inj}} = m_{f_{tot}} / \Delta\phi_{inj} \tag{5}$$

Regarding the fact that each nozzle may contain a number of nozzle holes, represented by z in this work, the average rate of fuel injection from each nozzle holes in a cycle $(kg/^\circ CA)$ is:

$$\overline{\dot{m}}_{f_{inj_j}} = m_{f_{tot}} / (z.\Delta\phi_{inj}) \tag{6}$$

The subscript j refers to each one of the z sprays and $\Delta\phi_{inj}$ $(^\circ CA)$ is the width of the injection pulse. The average velocity of fuel issuing from each of nozzle holes can be calculated as:

$$\overline{u}_{inj_j} = \overline{\dot{m}}_{f_{inj_j}} \, 6N / (\rho_l.A_N) \tag{7}$$

Where A_N is the nozzle hole cross section area. Eventually, the mean pressure drop in each nozzle hole (Pa) is:

$$\overline{\Delta p}_j = 0.5\rho_l \left(\frac{\overline{u}_{inj}}{C_D} \right)^2 \tag{8}$$

Also, the parameter ΔP can be determined in each crank angle (ϕ) with the use of injection data. The cumulative mass of fuel injected in the cylinder up to each crank angle, m_{finj} (kg), can be calculated by integrating the fuel injection rate, $dm_{f_{inj}}/d\phi$ $(kg/^\circ CA)$ or $\dot{m}_{f_{inj}}$ $(kg/\sec)$:

$$m_{f_{inj}} = \int_{\phi_{soi}}^{\phi} \frac{dm_{f_{inj}}}{d\phi} d\phi \tag{9}$$

So, the cumulative mass of fuel injected and fuel injection rate from each nozzle hole at each crank angle are:

$$m_{f_{inj_j}} = m_{f_{inj}} / z \tag{10}$$

$$\dot{m}_{f_{inj_j}} = \dot{m}_{f_{inj}} / z \tag{11}$$

Finally, the spray tip velocity and pressure drop across nozzle holes are:

$$u_{inj_j} = \dot{m}_{f_{inj_j}} \, 6N / (\rho_l \cdot A_N) \tag{12}$$

$$\Delta p_j = 0.5\rho_l (u_{inj}/C_D)^2 \tag{13}$$

Spray cone angle: The fuel injected into the combustion chamber is broken up to the droplets and a cone shaped spray formed. The model of Reitz and Bracco [9] is used for spray cone angle which has a formulation as:

$$\tan\left(\frac{\theta}{2}\right) = \frac{1}{A''} 4\pi \sqrt{\frac{\rho_a}{\rho_l}} \frac{\sqrt{3}}{6} \tag{14}$$

$$A'' = 3 + 0.28(L_N/D_N) \tag{15}$$

Where A'' is an empirical factor.

Air entrainment in the spray: As the spray penetrates in the combustion chamber, the surrounding air entrains in it and the mixing of fuel vapor and air occurs. The following relations have been used for a conical shaped spray under the assumptions that both the volume taken by the fuel and the paraboloid part at the base of the cone are negligible against that of the air and that of the pure cone, respectively. The cumulative mass of air entrained in the spray up to the present crank angle is determined with respect to the time [8]:

$$t_{br} \langle t \leq \frac{\Delta\phi_{inj}}{6N} + t_{br} \tag{16}$$

$$m_{a_j} = \frac{\pi}{3} \left(\tan\frac{\theta}{2} \right)^2 \cdot \rho_a \cdot (x - x_{br})^3$$

Where x_{br} and t_{br} are break-up length and the corresponding time. The break up length is:

$$x_{br} = t_{br} \cdot \overline{u}_{inj_j} \tag{17}$$

And

$$t \rangle \frac{\Delta\phi_{inj}}{6N} + t_{br} \tag{18}$$

$$m_{a_j} = \frac{\pi}{3} \cdot \rho_a \cdot \left(\tan\frac{\theta}{2} \right)^2 (x - x_{br})^3 - \frac{\pi}{3} \cdot \rho_a \cdot \left(\tan\frac{\theta_t}{2} \right)^2 (x_t - x_{br})^3$$

The index t refers to the tail of the spray. In this case, the volume of a conical part at tail of the spray should be subtracted from that of the spray. The parameters x_t and θ_t are the length and angle of this conical part:

$$x_t = 2.95 \left(\frac{\Delta p}{\rho_a} \right)^{0.25} \sqrt{D_N} \left[t - \frac{\Delta\phi_{inj}}{6N} - t_{br} \right]^{\delta_t} \tag{19}$$

$$\theta_t = \theta \tag{20}$$

Ignition Delay Model

In general, ignition delay is a multivariable function of pressure, temperature, fuel ignition quality (fuel Cetane number) and mixture equivalence ratio [5]. In order to modeling the ignition delay, the Arrhenius type expression proposed by Watson [10] is used:

$$\tau = A' P^{-n} \exp(T_a/T) \tag{21}$$

The constants A', n and T_a are depend on the fuel used [5].

In view of the fact that the cylinder pressure and temperature are considerably varied during the ignition delay period, the following equation has been developed to account for these changing conditions [5,10]:

$$\int_{t_{soi}}^{t_{soc}} \frac{dt}{\tau} = 1 \tag{22}$$

The ignition delay time (t_{delay}) can be evaluated once the above relationship is satisfied:

$$t_{delay} = t_{soc} - t_{soi} \tag{23}$$

In the above equation, t_{soc} and t_{soi} are the start of combustion and injection time, respectively.

Combustion Model

In the present work, an empirical model proposed by Miamoto et al. [11] for the rate of combustion has been used. In this model, to consider the complex two-stage nature of diesel combustion, the rate of combustion, $dQ/d\phi$, described by using a double Wiebe's function including six parameters:

$$\tag{24}$$
$$6.9 \frac{Q_P}{\phi_P}\left(M_P + 1\right)\left(\frac{\phi}{\phi_P}\right)^{M_P} \exp\left[-6.9\left(\frac{\phi}{\phi_p}\right)^{M_P+1}\right] +$$
$$6.9 \frac{Q_d}{\phi_d}\left(M_d + 1\right)\left(\frac{\phi}{\phi_d}\right)^{M_d} \exp\left[-6.9\left(\frac{\phi}{\phi_d}\right)^{M_d+1}\right]$$
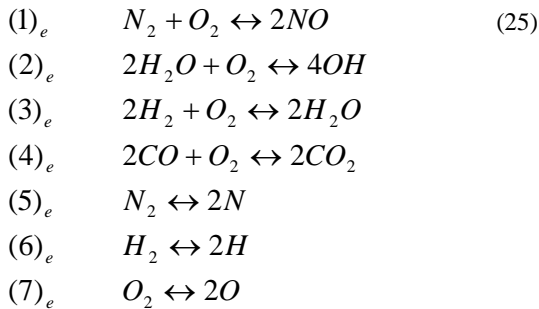
The subscripts p and d refer to the premixed and diffusive combustion parts, respectively. The parameter ϕ denotes the duration of energy release, Q and M are combustion parameters and shape factors [10].

Chemistry of combustion

Combustion products are defined by dissociation considerations. The complete chemical equilibrium scheme proposed by Way is used for the C-H-O-N system [12,13]. A generic fuel molecule composed by carbon, hydrogen, oxygen, and nitrogen atoms, $C_n H_m O_r N_s$, was used in the model, in order to open the range of application to fuels in which the nitrogen and oxygen content may not be negligible, such as many bio-fuels or residual fuels with interesting future perspective. The following 11 species are considered to be present in the exhaust gases:

(1) N_2 (2) O_2 (3) CO_2 (4) H_2O
(5) CO (6) H_2 (7) NO (8) OH
(9) N (10) H (11) O

The equilibrium distribution of these constituents can be fully described by the following seven chemical equilibrium reactions:

$(1)_e \qquad N_2 + O_2 \leftrightarrow 2NO \tag{25}$

$(2)_e \qquad 2H_2O + O_2 \leftrightarrow 4OH$

$(3)_e \qquad 2H_2 + O_2 \leftrightarrow 2H_2O$

$(4)_e \qquad 2CO + O_2 \leftrightarrow 2CO_2$

$(5)_e \qquad N_2 \leftrightarrow 2N$

$(6)_e \qquad H_2 \leftrightarrow 2H$

$(7)_e \qquad O_2 \leftrightarrow 2O$

Heat Transfer Model

Annand model of heat transfer in internal combustion engines, between in-cylinder trapped mass and surrounding walls, has been considered in the present work. This model has the general formulation as follows [14,15]:

$$\tag{26}$$
$$\dot{Q}_W = aA_{hex} \frac{\lambda_g}{D}\left(\mathrm{Re}\right)^b\left(T_W - T_g\right) + c\left(T_w^{\,4} - T_g^{\,4}\right)$$

In the above equation, $\dot{Q}_W(w)$ is the rate of heat transfer, T_W is the temperature of surrounding wall and T_g is the mean temperature of the in-cylinder charge varied in each crank angle. A_{hex} is the instantaneous heat exchange area in the cylinder. The parameter Re represents the Reynolds number of the in-cylinder charge, $\mathrm{Re} = \rho D u_{pis}/\mu_g$, which ρ, u_{pis} and μ_g are the density of in-cylinder trapped mass, mean piston velocity and dynamic viscosity of cylinder charge, respectively. The parameter u_{pis} can be simply calculated as $2NS/60$. The parameter λ_g is the thermal conductivity of the in-cylinder mass.

Pollutant Emissions

Nitric oxide formation: The rate kinetic model based on the theory developed by Lavoie [16] is used for NO formation. In this model, the governing equations for the mechanism of NO formation are:

$$N + NO \leftrightarrow N_2 + O \tag{27}$$
$$N + O_2 \leftrightarrow NO + O$$
$$N + OH \leftrightarrow NO + H$$
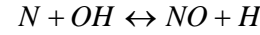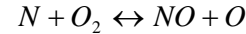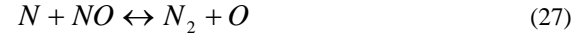
And the corresponding forward reaction rates of the above equations are $\left(m^3/kmol.\sec\right)$ [13-16]:

$$k_{1f} = 3.1 \times 10^{10} \exp\left(-160/T\right) \tag{28}$$
$$k_{2f} = 6.4 \times 10^6 T \exp\left(-3125/T\right)$$
$$k_{3f} = 4.2 \times 10^{10}$$

Finally, the rate equation for NO concentration is:

$$\frac{1}{V}\frac{d((NO)V)}{d\phi} = 2\left(1-\alpha^2\right)\frac{R_1}{1+\alpha R_1/(R_2+R_3)}\cdot\frac{1}{N'} \tag{29}$$

Where in the left hand side of the equation, V is the volume of burnt gasses and (NO) is the concentration of NO $\left(kmol/m^3\right)$, and in right hand side:

$$\alpha = (NO)/(NO)_e \tag{30}$$
$$R_1 = k_{1f}\left(N_e\right)(NO)_e$$
$$R_2 = k_{2f}\left(N\right)_e\left(O_2\right)_e$$
$$R_3 = k_{3f}\left(N\right)_e\left(OH\right)_e$$

Subscript e means equilibrium and N' is the engine angular velocity ($rad/\sec$).

Soot formation: In the present work, the total soot formation rate has been calculated by modified method of Lipkea [17] which is on the basis of the model primarily proposed by Hiroyasu and Kadota [5,9]:

$$\frac{dm_{st}}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{so}}{dt} \qquad (31)$$

$$\frac{dm_{sf}}{dt} = c_{sf} dm_f^{0.8} P^{0.5} \exp\left(-E'_{sf}/(R_{mol}T)\right)$$

$$\frac{dm_{so}}{dt} = c_{so} m_{st}\left(P_{O_2}/P\right)P^{1.8} \exp\left(-E'_{so}/(R_{mol}T)\right)$$

The parameters P and P_{O_2} are the cylinder pressure (bar) and partial pressure of oxygen in the burning zone. The subscripts st, sf and so denote total soot, soot formed and soot oxidized. dm_f is the mass of fuel vapor ready to be burned in the step obtained from combustion model. Also, E'_{sf} and E'_{so} are activation energies $(kJ/kmol)$. Both of the constants, c_{sf} and c_{so}, should be determined so as to match the computed soot with the experimental results.

Conservation and state equations
During the compression, only one zone of pure air exists in the cylinder having no mass exchange; therefore, the first law of thermodynamics for a closed system is applied together with the perfect gas state equation [5,9]:

$$dQ = dE + PdV \qquad (32)$$

$$P.V = m_{ch}(R_{mol}/M_{ch})T \qquad (33)$$

Where dQ is the total heat between cylinder charge and combustion chamber walls, dE is the change in the internal energy of mixture, and P, V, T, and m_{ch} are the cylinder pressure, volume, temperature, and cylinder charge mass, respectively. The parameter M_{ch} is the cylinder charge molecular weight. The cylinder volume can be calculated by the following equation [9]:

$$(34)$$

$$V = V_{cl}\left\{1 + \frac{1}{2}(R_c - 1)\left[R + 1 - \cos\phi - (R^2 - \sin^2\phi)^{\frac{1}{2}}\right]\right\}$$

Where V_{cl}, R, and R_c are cylinder clearance volume, connecting rod to crank radius ratio, and cylinder compression ratio, respectively.
During the combustion, both burning and non-burning zones should be taken into account. Since there is mass transfer between these two zones, the first law of thermodynamics for an open system should be applied for them both, in addition to the perfect gas state equation.
For the air zone, which only losses mass (air) to the burning zone, the first law is written as [5,9,14]:

$$dQ_{uz} = dE_{uz} + PdV_{uz} + h_a dm_a \qquad (35)$$

$$PV_{uz} = N_{mol,uz} R_{mol} T_{uz} \qquad (36)$$

The subscript uz denotes the unburned zone. The terms h_a and dm_a are the specific enthalpy and mass of lost air.

The corresponded equations for the burning zone which gains the mass from the air (non-burning zone) and also an enthalpic flow from the fuel ready to be burned in the time step, are [5,9,14]:

$$dQ_{bz} = dE_{bz} + PdV_{bz} - h_a dm_a - h_f dm_f \qquad (37)$$

$$PV_{bz} = N_{mol,bz} R_{mol} T_{bz} \qquad (38)$$

The subscript bz refers to the burning zone. The terms h_f and dm_f are the specific enthalpy and mass of enthalpic flow of fuel.

Simulation results
In this section, results of simulation on the basis of the proposed relations are investigated. The results are shown for a specified reference operating state. This state refers to the start of injection at 20 Deg. BTDC, duration of injection equal to 35 CA, the value of 42 for AFR, the engine speed of 2500 rpm, cylinder wall temperature equal to 450 K, and 80% full load. The selected fuel is n-Dodecane ($C_{12}H_{26}$), representing a common fuel for commercial diesel engines. The design characteristics of a single cylinder, water cooled, naturally aspirated, Ricardo-Cussons Hydra direct injection (DI) diesel engine have been considered as input data for the corresponding computer program. Also, the simulated and validated pressure diagram of this engine obtained from the work of Rakopoulos et al [8] has been used to validate the present simulation. The engine basic specifications are listed in table1.

Table 1. Engine specifications	
Bore (m)	0.08026
Stroke (m)	0.08890
Displacement volume (m^3)	0.4501e-3
Intake valve closing (IVC)	42 Deg. ABDC
Exhaust valve opening (EVO)	60 Deg. BBDC
Compression ratio	19.81
Diameter of nozzle hole mm)	0.25
Number of nozzle holes	4

Figure 1 presents the theoretical pressure diagram obtained from simulation at the mentioned reference state. Also, this simulated diagram is compared with the experimental one related to the mentioned engine at the same operating condition. This figure shows a good coincidence between these two diagrams.
Figure 2 illustrates the calculated kinetic nitric oxide (NO) concentration histories at three different injection timings. As expected, at more advanced injection timings the amount of nitric oxide is increased because earlier injection timings lead to higher temperatures in the cylinder and this fact affects directly the temperature sensitive process of kinetic nitric oxide formation. In other words, the higher the temperature is, the higher the rate of formation and the amount of NO will be.
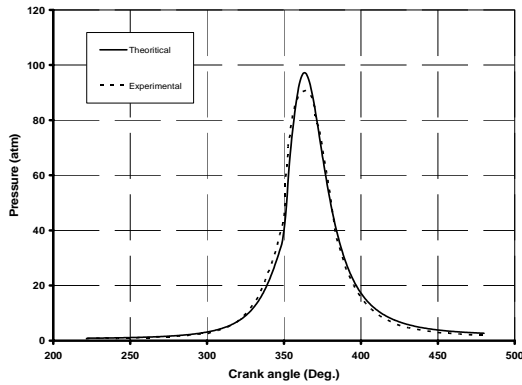
Figure1-Theoritical and experimental pressure diagrams versus crank angle.
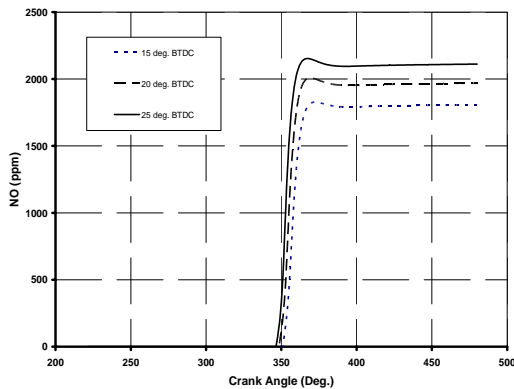

Figure 2- Calculated kinetic concentration of nitric oxide versus crank angle at three different injection timings.

Figure 3 depicts the amount of NO at three different engine loads. According to the figure, the NO concentration increases with increasing load. This is expected because NO formation mechanism is favoured for high temperature condition, which is approached by higher loads in a diesel engine. Besides, more inlet air which produces more oxygen and nitrogen is another reason for increased amount of NO concentration in higher loads.

Figure 4 shows the calculated soot density histories at three different injection timings. As shown in this figure, advanced injection timing leads to decrease in the soot concentration at the end of cycle. It is presumably due to the fact that advanced injection provides more enough time for soot oxidation, which causes the amount of net soot formed to be less.

The effect of load on the soot emissions is illustrated in figure 5. It is obvious in the figure that the higher the amount of load is, the more concentration of soot in exhaust gases will be. This is predicted because at higher loads combustion occurs at richer conditions and higher temperatures, which both of these facts increase the soot content in exhaust gases.
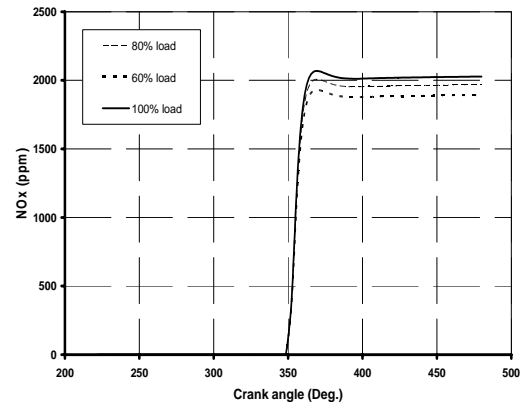

Figure 3- Calculated nitric oxide concentrations versus crank angle for three different loads.
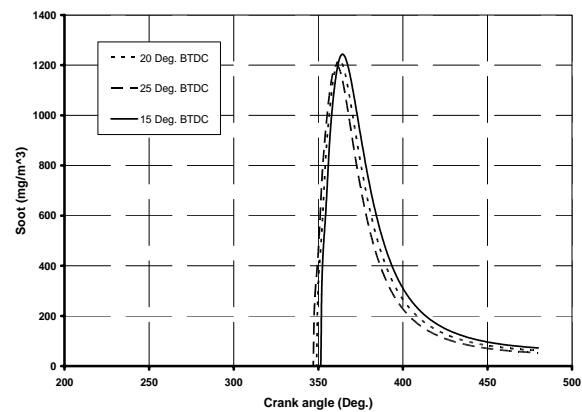

Figure 4- Calculated soot density histories versus crank angle at three different injection timings.
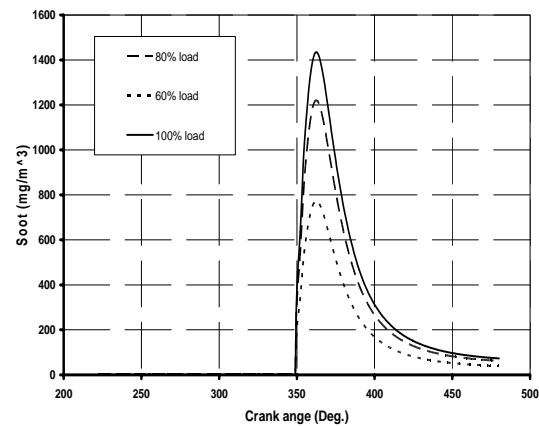

Figure 5- Calculated soot density histories in exhaust gases versus crank angle for three different loads.

The effect of variation in the global air-fuel ratio (AFR) on in-cylinder pressure has been depicted in figure 6. As it can be concluded from the figure, with an increasing amount of AFR, the pressure will be decreased. This is attributed to the fact that increased amount of AFR causes less amount of fuel to be injected in the cylinder per a cycle.
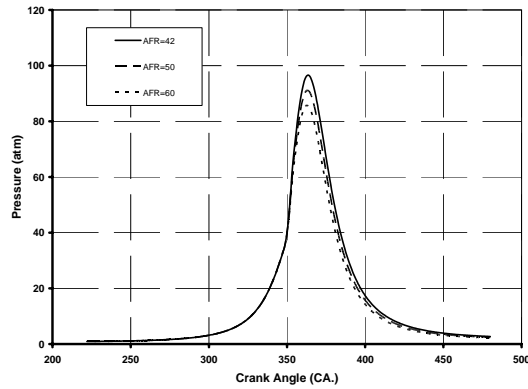
Figure 6- Calculated cylinder pressure versus crank angle for three different amounts of global air-fuel ratios (AFR).

Conclusions

A comprehensive, two-zone, thermodynamic, crank-angle resolution model of a direct injection diesel engine has been developed. Emphasis is given to including most of the processes taking place in the cylinder during the closed cycle and to describing as many as possible of these processes by correct and detailed modeling of physical laws. A parametric study has been done to analyze the sensitivity of the proposed model to variations in the values of some considered parameters and to investigate the effects of some important parameters such as the start of injection and the amount of engine load on the in-cylinder pressure and engine-out emissions. The presented model has shown results with favorable agreement with experimental data.

Nomenclature:

A_N	Nozzle hole cross section area (m^2)
AFR	Global air-fuel ratio (by mass)
C_D	Discharge coefficient of nozzle holes
D_N	Nozzle hole diameter (m)
E	Internal Energy (J)
h	Specific enthalpy (J/kg)
L_N	Length of nozzle hole (m)
m	Mass (kg)
M	Molecular weight $(kg/kmol)$
N	Engine rotational speed (rpm)
N_{mol}	Number of mole $(kmol)$
P	Cylinder pressure (Pa)
Q	Heat (J)
R	Connecting rod length to crank radius ratio
R_c	Cylinder compression ratio
R_{mol}	Universal gas constant $(J/kmol.K)$
t	Time $(\sec)$
T	Absolute temperature (K)
u	Speed $(m/\sec)$

V	Volume (m^3)
V_{cl}	Clearance volume of the cylinder (m^3)
V_d	Displacement volume (m^3)
x	Spray penetration (m)
z	Number of nozzle holes

Greek letters

ΔP	Pressure drop in the nozzle hole (Pa)
$\Delta\phi_{inj}$	Injection pulse width $(^\circ CA)$
ϕ	Crank angle (rad)
μ	Dynamic viscosity of cylinder charge $(kg/m.\sec)$
λ	Thermal conductivity of cylinder charge $(w/m.K)$
θ	Spray cone angle (rad)
ρ	Density (kg/m^3)
τ	Ignition delay time $(m\sec)$

Subscripts

a	Air
br	Break-up of fuel spray
bz	Burning zone
ch	Cylinder charge
e	Chemical equilibrium
f	Fuel
g	In-cylinder gas
inj	Injection
j	Spray number
l	Liquid fuel
t	Tail of spray
uz	Unburned zone

Superscripts

.	First time derivative
-	Mean value

Abbreviations

ABDC	After bottom dead center
BBDC	Before bottom dead center
BTDC	Before top dead center
CA	Crank angle
DI	Direct injection
EVO	Exhaust valve opening
IVC	Intake valve closing
rpm	Revolution per minute

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