CHAPTER 4

MODELING AND SIMULATION OF COMBUSTION AND NO\textsubscript{x} FORMATION IN DIESEL ENGINE

4.1 INTRODUCTION

The performance and emission of diesel engine depend on the effective burning of diesel in the combustion chamber which is highly complex heterogeneous exothermic chemical process. Modeling and simulation is an important avenue of research intended to understand the combustion and related process in the diesel engine. Computer simulation is the process of formulating a model of a physical system representing actual processes and analyzing the same. Usually, the model is a mathematical one representing the actual processes through a set of algebraic, differential or integral equations and the analysis is made using a computer (Ganesan 2000). The simulation and modeling is a cost effective process which eliminates number of experimental studies which are time consuming and costly (Stiesch 2003). However, the exact simulation of a real time process in a diesel engine is very difficult due to the complexity involved in the modeling.

Models of diesel engine combustion can be classified into two groups: thermodynamic models and multidimensional models (Ramos 1989). Thermodynamic models can be further classified into two subgroups: single and multizone or phenomenological models. In single zone models the cylinder charge is assumed to be uniform in both composition and temperature, and the first law of thermodynamics is used to calculate the
mixture energy accounting for the enthalpy flux due to fuel injection. This model is easy to handle and computationally very efficient. Phenomenological model is more complex than thermodynamic model, because the combustion chamber is divided into numerous zones that are characterized by different temperature and composition. Because of spatial resolution, important sub-process can be modeled and the prediction of heat release rate and exhaust emission as a function of characteristic engine parameters become possible. Computational Fluid Dynamics (CFD) model solves full set of differential equation for species mass, energy and momentum conservation on a relatively fine numerical mesh and also includes sub-models to account for the effect of turbulence. The computation time increases with the complexity of the model.

In the single zone model, the entire combustion chamber is considered as single zone. The fundamental assumptions for the model are:

- Cylinder charge is homogeneous gas mixture of fuel vapor and air
- Pressure and temperature inside the cylinder are uniform and vary with time
- Specific heats of the gaseous mixture are calculated as a function of temperature
- No chemical change in either fuel or air prior to combustion
- Effect of radiation neglected
- The charge is always in chemical equilibrium
4.2 ENGINE KINEMATICS

For a four stroke cycle diesel engine of diameter (b), stroke length (s) and compression ratio (r), as shown in Figure 4.1 the volume and surface area are calculated as follows.

Displacement volume or swept volume of the cylinder in m$^3$ is given by

$$V_d = \frac{\pi}{4} b^2 s \quad (4.1)$$

Volume of the cylinder when the piston is at BDC in m$^3$ is given by

$$V_b = V_d \left( \frac{r}{r-1} \right) \quad (4.2)$$

Volume of the cylinder when the piston is at TDC in m$^3$ is given by
Mean piston speed in m/s is given by

\[ S_p = \frac{2sN}{60} \]  \hspace{1cm} (4.4)

Change in cylinder volume with respect to crank angle is given by

\[ V_\theta = V_d \left[ \frac{r}{r-1} - \frac{1-\cos \theta}{2} + \frac{l}{s} - \frac{1}{2} \sqrt{\left(\frac{2l}{s}\right)^2 - \sin^2 \theta} \right] \]  \hspace{1cm} (4.5)

\[ \frac{dV}{d\theta} = \frac{V_d}{2} \left[ \frac{1}{2} \frac{\sin 2\theta}{\sqrt{(2l/s)^2 - \sin^2 \theta}} - \sin \theta \right] \]  \hspace{1cm} (4.6)

Combustion chamber surface area of the cylinder (m²) with respect to crank angle is given by

\[ A_s = A_{ch} + A_p + \frac{\pi bs}{2} \left[ \frac{2l}{s} + 1 - \cos \theta - \sqrt{\left(\frac{2l}{s}\right)^2 - \sin^2 \theta} \right]^{1/2} \]  \hspace{1cm} (4.7)

where \( A_{ch} \) is cylinder head surface area and \( A_p \) is the piston crown surface area.

### 4.3 COMBUSTION FUNDAMENTALS

Air contains nitrogen, but when the products are at low temperatures the nitrogen is not significantly affected by the reaction. For practical applications combustion air can be approximated as 21% oxygen and 79% atmospheric nitrogen by volume. For each mole of O₂ present in air,
there are \( \frac{0.79}{0.21} = 3.76 \) moles of \( N_2 \). In actual combustion fuel in the engine, the air sucked in may be less than or more than the stoichiometric requirement. The ratio of the actual fuel/air ratio to the stoichiometric ratio is a more informative parameter for defining mixture composition. The fuel-air equivalence ratio is given by

\[
\phi = \frac{(F/A)_{\text{actual}}}{(F/A)_{\text{stoichiometric}}}
\] (4.8)

Consider the combustion of a general hydrocarbon fuel of average molecular composition \( C_xH_y \) with air. The simplified combustion equation can be represented by (Turns, 1996)

\[
C_xH_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + cCO + dH_2O + eH_2 + fO_2 + 3.76aN_2
\] (4.9)

The CO and \( H_2 \) are products of incomplete combustion. The diesel engines operate significantly fuel lean conditions with typical value of \( \phi < 1 \), so there is no CO and \( H_2 \) in the exhaust gases and the coefficients \( c \) and \( e \) are zero because there is sufficient \( O_2 \) to have all fuel Carbon and Hydrogen react to form \( CO_2 \) and \( H_2O \) respectively. Then the equation 4.9 becomes

\[
C_xH_y + a(O_2 + 3.76N_2) \rightarrow bCO_2 + dH_2O + fO_2 + 3.76aN_2
\] (4.10)

where \( a, b, c, d, e, \) and \( f \) are coefficients given by

\[
\begin{align*}
    a &= (x + y/4)/\phi \\
    b &= x \\
    c &= 0 \\
    d &= \frac{y}{2} \\
    e &= 0 \\
    f &= (1 - \phi)a
\end{align*}
\]
The coefficients are used to balance the combustion equation for first law of thermodynamic analysis of the reacting combustion system. When water is added with diesel in the form of emulsion, the kilo moles of water present per kilo mole of diesel is computed by

\[
\frac{N_{\text{water}}}{N_{\text{diesel}}} = \frac{VF_{\text{water}}}{VF_{\text{diesel}}} \times \frac{\rho_{\text{water}}}{\rho_{\text{diesel}}} \times \frac{MW_{\text{diesel}}}{MW_{\text{water}}} \tag{4.11}
\]

where \(VF_{\text{water}}\) is volume fraction of water, \(VF_{\text{diesel}}\) is volume fraction of diesel, \(MW_{\text{water}}\) is molecular weight of water and \(MW_{\text{diesel}}\) is molecular weight of diesel.

For the combustion of diesel water emulsion with air, the combustion equation may be given as

\[
C_4H_y + a\left(O_2 + 3.76N_2\right) + gH_2O \rightarrow bCO_2 + dH_2O + fO_2 + 3.76aN_2
\tag{4.12}
\]

where \(g\) is the kilo moles of water per kilo moles of diesel present in the emulsion. The coefficients in the equation (4.12) are, now, given by

\[
\begin{align*}
      a &= (x + y/4)/\phi \\
b &= x \\
c &= 0 \\
d &= \frac{y}{2} + g \\
e &= 0 \\
f &= (1 - \phi)a
\end{align*}
\]

Kilo moles of air present in the cylinder at the beginning of compression stroke is given by

\[
N_a = \frac{P_1 \times V_h}{R_u \times T} - N_s
\tag{4.13}
\]

where \(N_s\) is kilo moles of residual gases present in the cylinder.
Chemically correct amount of oxygen required per mole of fuel

\[ Y_{cc} = N_{mc} + 0.25 N_{mH} - 0.5 N_{mO} \]  (4.14)

Minimum amount of oxygen required per mole of fuel

\[ Y_{min} = Y_{cc} - 0.5 N_{mc} \]  (4.15)

Actual amount of oxygen per mole of fuel for stoichiometric combustion

\[ Y = Y_{cc} \]  (4.16)

Air fuel ratio in kilo moles

\[ AFR = 4.76 Y \]  (4.17)

Kilo moles of air + fuel vapour in a mixture containing 1 kilo mole of fuel

\[ N_{mo} = 1 + 4.76 Y \]  (4.18)

Kilo moles of fuel vapour and air available in engine during compression stroke

\[ N_m = N_a + \frac{N_a}{AFR} \]  (4.19)

Kilo moles of gas species formed during combustion process in diesel engine \((\phi < 1)\) is computed by,
\[ N_{CO} = 0 \]
\[ N_{CO2} = N_{mc} \]
\[ N_{H2O} = \frac{N_{mH}}{2} + N_{water} \]
\[ N_{N2} = \frac{3.76}{\phi} \left( N_{mc} + \frac{N_{mH}}{4} \right) \]
\[ N_{O2} = \left( 1 - \frac{1}{\phi} \right) \left( N_{mc} + \frac{N_{mH}}{4} \right) \]

The simulated values of gas species formed in kilo moles at various equivalence ratios are given in Table 4.1.

**Table 4.1  Kilo moles of species formed during combustion**

<table>
<thead>
<tr>
<th>Equivalence ratio</th>
<th>Gas species</th>
<th>CO</th>
<th>CO₂</th>
<th>H₂O</th>
<th>N₂</th>
<th>O₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \phi = 0.9 )</td>
<td>0% H₂O</td>
<td>0</td>
<td>10</td>
<td>11.000</td>
<td>64.756</td>
<td>1.7222</td>
</tr>
<tr>
<td></td>
<td>10% H₂O</td>
<td>0</td>
<td>10</td>
<td>12.056</td>
<td>64.756</td>
<td>1.7222</td>
</tr>
<tr>
<td></td>
<td>20% H₂O</td>
<td>0</td>
<td>10</td>
<td>13.376</td>
<td>64.756</td>
<td>1.7222</td>
</tr>
<tr>
<td></td>
<td>30% H₂O</td>
<td>0</td>
<td>10</td>
<td>15.073</td>
<td>64.756</td>
<td>1.7222</td>
</tr>
<tr>
<td>( \phi = 0.8 )</td>
<td>0% H₂O</td>
<td>0</td>
<td>10</td>
<td>11.000</td>
<td>72.85</td>
<td>3.875</td>
</tr>
<tr>
<td></td>
<td>10% H₂O</td>
<td>0</td>
<td>10</td>
<td>12.056</td>
<td>72.85</td>
<td>3.875</td>
</tr>
<tr>
<td></td>
<td>20% H₂O</td>
<td>0</td>
<td>10</td>
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<td>30% H₂O</td>
<td>0</td>
<td>10</td>
<td>15.073</td>
<td>72.85</td>
<td>3.875</td>
</tr>
<tr>
<td>( \phi = 0.7 )</td>
<td>0% H₂O</td>
<td>0</td>
<td>10</td>
<td>11.000</td>
<td>83.257</td>
<td>6.642</td>
</tr>
<tr>
<td></td>
<td>10% H₂O</td>
<td>0</td>
<td>10</td>
<td>12.056</td>
<td>83.257</td>
<td>6.642</td>
</tr>
<tr>
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<td>83.257</td>
<td>6.642</td>
</tr>
</tbody>
</table>

Kilo moles of products formed during combustion is calculated by

\[ N_{po} = N_{CO} + N_{CO2} + N_{H2O} + N_{N2} + N_{O2} \]  (4.20)
Kilo moles of products formed from the combustion of 
\( N_a + N_f + N_x \)

\[ N_p = N_{po} C_m \]

where 
\[ C_m = \frac{N_m}{N_{mo}} + \frac{N_x}{N_{po}} \]

Specific heat of air (kJ/kmol K) at initial temperature \( T_1 \),

\[ C_{pa} = 27.5 + 0.0057 T_1 \quad (4.21) \]

Specific heat of different products of combustion (kJ/kmol K) at constant pressure at temperature \( T \) is computed by

\[ \frac{C_{pi}}{R_u} = a_{i1} + a_{i2} T + a_{i3} T^2 + a_{i4} T^3 + a_{i5} T^4 \quad (4.22) \]

The coefficients \( a_{ij} \) for the products of combustion are taken from JANAF table given in Heywood (1988).

Specific heat of reactants (kJ/kmol K) at constant pressure is given by

\[ C_{pr} = N_a C_{pa} + \sum C_{p,i} \quad (4.23) \]

Specific heat ratio of reactants is given by

\[ k_r = \frac{C_{pr}}{C_{pr} - R_u} \quad (4.24) \]
Specific heat of reactants (kJ/kmol K) at constant volume is computed by

\[ C_{vr} = C_{pr} - R_u \]  (4.25)

Specific heat ratio of products is given by

\[ k_p = \frac{C_{pp}}{C_{pp} - R_u} \]  (4.26)

### 4.4 ADIABATIC FLAME TEMPERATURE

Adiabatic flame temperature is the maximum temperature obtainable in the combustion system where the combustion is complete and the system is adiabatic (Ganesan 2000). Consider an adiabatic, constant pressure process during which all the reactants are completely converted to products. If the kinetic energy is small compared with the enthalpy and there is no shaft work, the energy equation can be written as

Enthalpy of reactants (\(H_r\)) = Enthalpy of products (\(H_p\))

The enthalpy of gas species is computed by

\[ \frac{h_i}{R_i T} = a_{i1} + \frac{a_{i2}}{2} T + \frac{a_{i3}}{3} T^2 + \frac{a_{i4}}{4} T^3 + \frac{a_{i5}}{5} T^4 + \frac{a_{i6}}{6} T^5 \]  (4.27)

The coefficients \(a_{ij}\) for the products of combustion are taken from JANAF table given in Heywood (1988).

Initially a value is assumed as adiabatic flame temperature (3000 K) and enthalpy and specific heat at constant pressure of the products are computed. The new value of adiabatic flame temperature is determined by iteration using the following relation:
where \( H_r \) is the heat of reactants given by

\[
T_{\text{new}} = T - \frac{H_p(T) - H_p(T_r) - H_r}{C_p(T)} \quad (4.28)
\]

Heat of reaction at constant pressure for diesel fuel \( \text{C}_{10}\text{H}_{22} \) is -6261300 kJ/kmol for gaseous \( \text{H}_2\text{O} \) in products. The adiabatic flame temperature decreases with the percentage of water in the emulsion as shown in Figure 4.2.

![Figure 4.2](image)

**Figure 4.2** Effect of water amount in the emulsion on AFT

### 4.5 COMPRESSION PROCESS

In a diesel engine, the compression process takes place rapidly with negligible heat transfer. The compression process is assumed as polytropic process. The pressure and temperature change during the compression process
are calculated using the following equations assuming the specific heat ratio of reactants is constant with temperature.

Pressure change during compression process is given by

\[ P_{\theta+1} = P_\theta \left( \frac{V_\theta}{V_{\theta+1}} \right)^{k_r} \]  \hspace{1cm} (4.30)

Temperature change during compression process is given by

\[ T_{\theta+1} = T_\theta \left( \frac{V_\theta}{V_{\theta+1}} \right)^{k_r - 1} \]  \hspace{1cm} (4.31)

4.6 IGNITION DELAY

The ignition delay in a diesel engine is defined as the time (or crank angle) interval between the start of injection and the start of combustion (Heywood 1988). The start of injection is usually taken as the time when the injector needle lifts off its seat which is measured with a strain gauge transducer. The start of combustion is determined from the engine pressure data obtained using a piezo-electric pressure transducer installed in the combustion chamber, the time or crank angle when the slope of the line changes. The ignition delay of a given fuel is very important in determining the engine performance such as thermal efficiency, smoothness of operation, misfiring, smoking, knocking of the engine and pollutant formation (Wong et al 1982).

Numerous steady state ignition delay correlations have been proposed using experimental data obtained from constant volume bomb test, steady flow test and engine test. Assanis et al (2003) proposed a correlation based on the engine test and is given by
where $E_a/R_u$ is a constant in the equation (4.32) and is taken as 2100 for all the three types of fuels (i.e.) DSL, DW10 and DW20. The ignition delay depends on the chemical reaction leading to the auto ignition of the diesel fuel. The chemical reaction between fuel and air depend on the equivalence ratio, pressure and temperature. So, the equivalence ratio term was introduced in the correlation. In the equation (4.32), the pressure and temperature are taken at TDC conditions (Heywood 1998). The simulated values of ignition delay are 0.988 ms for DSL, 1.01 ms for DW10 and 1.03 ms for DW20 fuels respectively as shown in Figure 4.3. From the simulation, it is found that ignition delay slightly increases with the percentage of water in the emulsion.

\[
\tau_{id} = \frac{2.4}{\phi^0.2 P^{1.02} \exp\left(\frac{E_a}{R_u T}\right)} \quad (4.32)
\]

Figure 4.3  Effect of water amount in the emulsion on ignition delay

4.7  COMBUSTION PROCESS

Combustion of diesel inside the engine cylinder is one of the processes that controls engine power, efficiency and emission. In the diesel engine, the fuel is injected into the cylinder into air already at a high pressure
and temperature, near the end of the compression stroke. The auto-ignition or self-ignition of portions of the developing mixture of already injected and vaporized fuel with this hot air starts the combustion process, which spreads rapidly. Burning then proceeds as fuel and air mix to the appropriate compositions for combustion to take place. Thus, fuel-air mixing plays a controlling role in the diesel engine combustion process. The combustion process is a fast exothermic gas-phase reaction. The diesel engine combustion process is predominantly an unsteady turbulent diffusion flame, and the fuel is initially in liquid phase (Heywood 1988).

The model described in this section is thermodynamic single zone combustion model which is based on the first law of thermodynamics and mass balance only (Stiesch 2003). The entire combustion chamber of the engine is typically treated as a single, homogeneously mixed zone. The simplicity and modest computer time requirements make the single zone model useful for diesel cycle simulation and more complex engine system studies. Watson et al (1980) heat release model is used for modeling the combustion in direct injection diesel engine which is based on Lyn’s description of compression ignition combustion- a rapid premixed burning phase followed by a slower mixing controlled burning phase. The fraction of the injected fuel that burns in each of these phases is empirically linked to the duration of the ignition delay. One algebraic function is used to describe the premixed heat release phase and a second function to describe the mixing controlled heat release phase. These two functions are weighted with a phase proportionality factor, \( \beta \), which is largely a function of the ignition delay.

The premixed burning function

\[
 f_1 = 1 - (1 - X^{k_1})^{k_2} \tag{4.33}
\]

The mixing controlled function

\[
 f_2 = 1 - \exp(-k_3 X^{k_4}) \tag{4.34}
\]
where $X$ is the time from ignition, non-dimensionalized by total combustion duration given by

\[ X = \frac{\theta - \theta_{\text{ign}}}{\Delta \theta_c} \]

\[ k_1 = 2 + 1.25 \times 10^{-8} \left( \tau_{id} N \right)^{2.4} \]
\[ k_2 = 5000 \]
\[ k_3 = \frac{14.2}{\phi^{0.644}} \]
\[ k_4 = 0.79 k_3^{0.25} \]

The proportionality factor $\beta$ given by

\[ \beta = 1 - \frac{a \phi^b}{\tau_{id}^c} \]

where $a$, $b$, $c$ are constants

\[ 0.80 < a < 0.95; \]
\[ 0.25 < b < 0.45; \]
\[ 0.025 < c < 0.50 \]

The combustion duration is calculated by (Ganesan 2000)

\[ \Delta \theta_c = 40 + 5 \left( \frac{N}{600} - 1 \right) + 166 \left( \frac{Y_{\infty}}{Y} - 1.1 \right)^2 \]

The mass of fuel burned is given by

\[ \frac{m_{fb} X}{m_{fo}} = \beta f_1 + (1 - \beta) f_2 \]
Heat release by combustion of fuel is computed as

\[ \frac{dQ_c}{d\theta} = Q_{LHV} \times \frac{dm_{fb}}{d\theta} \times \eta_c \]  

(4.37)

where \( \eta_c \) is combustion efficiency.

Rate of heat transfer between the gases and cylinder wall is given by

\[ \frac{dQ_h}{d\theta} = hA_s(T - T_w) \]  

(4.38)

Rate of work done by gases is calculated by

\[ \frac{dW}{d\theta} = P \frac{dV}{d\theta} \]  

(4.39)

The energy equation for the closed cycle period can be written as

\[ m \frac{du}{d\theta} = \frac{dQ_c}{d\theta} - \frac{dQ_h}{d\theta} - \frac{dW}{d\theta} \]  

(4.40)

Substituting the equation (4.38) and (4.39) in (4.40) gives

\[ mC_v \frac{dT}{d\theta} = \frac{dQ_c}{d\theta} - hA_s(T - T_w) - P \frac{dV}{d\theta} \]

\[ \frac{dT}{d\theta} = \frac{1}{mC_v} \frac{dQ_c}{d\theta} - \frac{hA_s(T - T_w)}{mC_v} - \frac{P}{mC_v} \frac{dV}{d\theta} \]

\[ \frac{dT}{d\theta} = \frac{1}{mC_v} \frac{dQ_c}{d\theta} - \frac{hA_s(T - T_w)}{mC_v} - \frac{R_uT}{C_v} \frac{1}{V} \frac{dV}{d\theta} \]  

(4.41)

The equation is solved by fourth order Runge-Kutta method to determine the temperature at different crank angle during combustion.
(Ganesan 2000). Knowing the temperature at every crank angle, the pressure at each crank angle can also be determined by the relation

\[ P = \frac{mR_s T}{V} \]  

(4.42)

The net heat release rate then computed from the cylinder pressure data as

\[ \frac{dQ_n}{d\theta} = k_p \frac{P}{k_p - 1} \frac{dV}{d\theta} + \frac{1}{k_p - 1} V \frac{dP}{d\theta} \]  

(4.43)

4.8 ENGINE WALL HEAT TRANSFER

Heat transfer between the cylinder gases and the wall of the reciprocating engine is an unsteady phenomenon that changes periodically with the thermodynamic cycle of an engine, so the problem is complicated both from a theoretical and experimental standpoint. While the combustion is in progress, heat transfer is complex because of accompanying chemical reactions. Gaining knowledge about this complex phenomenon is of immense importance to a designer as well as to a researcher. Heat transfer affects engine performance, efficiency, and emissions. For a given mass of fuel within the cylinder, higher heat transfer to the combustion chamber walls will lower the average combustion gas temperature and pressure, and reduces the work per cycle transferred to the piston. Heat transfer from the gases to the wall of the combustion chamber consists of two types of heat transfer: convection and radiation.

From the investigations of various pioneers (LeFeuvre et al 1969, Dent et al 1977 and Sitkei et al 1972), it is learnt that heat transfer in the diesel engine depends on intake swirl, shape of the combustion chamber, mean gas temperature, average surface temperature, soot deposits on the
surface of combustion chamber, turbulence level in the combustion chamber, engine speed, equivalence ratio, and coolant temperature

The heat transfer from the gases in the diesel engine combustion chamber to the wall primarily depends on the flow conditions in the vicinity of the wall. The exact mathematical description of these conditions is extremely complicated and can only be solved in those few cases where defined peripheral conditions exist (Hohenberg 1979).

In this simulation, the correlation proposed by Hohenberg (1979) is used to determine the heat transfer coefficient $h_c$ (W/ m$^2$ K),

$$h_c = \frac{130 \rho^{0.8} (S_p + 1.4)^{0.8}}{V^{0.06} T^{0.4}}$$ (4.44)

### 4.9 ENGINE FRICTION

The friction work is defined as the difference between the work delivered to the piston while the working fluid is contained within the cylinder and the usable work delivered to the drive shaft. The friction work is determined by motoring test for both direct injection and indirect injection diesel engine. In this research work, the friction mean effective pressure in kPa is computed using the correlation (Heywood 1988) given as

$$FMEP = C_1 + 48 \left( \frac{N}{1000} \right) + 0.4S_p^2$$ (4.45)

where $C_1$ is 75 kPa for direct injection diesel engine and $S_p$ is mean piston speed in m/s.
4.10 EXPANSION PROCESS

The expansion process is assumed as polytropic process with constant value of specific heat ratio of the combustion products. The change in temperature and pressure during expansion process is calculated using the following equations.

Temperature change during expansion process is given by

\[ T_{i+1} = T_i \left( \frac{V_i}{V_{i+1}} \right)^{\frac{k_p}{k}} \]  \hspace{1cm} (4.46)

Pressure change during expansion process is given by

\[ P_{i+1} = P_i \left( \frac{T_{i+1}}{T_i} \right)^{\frac{k_p}{k-1}} \]  \hspace{1cm} (4.47)

4.11 GAS EXCHANGE PROCESS

The gas exchange process in a diesel engine includes exhaust and intake processes. The purpose of gas exchange process is to remove the burned gases at the end of the power stroke and admit the fresh charge for the next cycle. The diesel engine gas exchange process is characterized by the volumetric efficiency (Heywood 1988). The gas exchange process is influenced by

(i) Mixture temperature as influenced by heat transfer

(ii) Ratio of exhaust to inlet manifold pressure

(iii) Compression ratio

(iv) Engine speed
(v) Intake and exhaust manifold and port design

(vi) Intake and exhaust valve geometry, size, lift and timings

The pressure change during exhaust process is given by

$$\frac{dP}{d\theta} = k_p P \left( \frac{1}{M} \frac{dM}{d\theta} - \frac{1}{V} \frac{dV}{d\theta} \right)$$  \hspace{1cm} (4.48)

The pressure change during intake process is given by

$$\frac{dP}{d\theta} = k_r \left( \frac{R_u T_u}{V} \frac{dM}{d\theta} - \frac{P}{V} \frac{dV}{d\theta} \right)$$  \hspace{1cm} (4.49)

In the equations (4.48) and (4.49), \(dM/d\theta\) is the mass flow rates which are to be obtained from the principle of fluid mechanics. In diesel engine, based on the pressure and temperature in the flow of air and exhaust gases, the flow may be subsonic or supersonic (Ganesan 2000). The flow can be characterized as subsonic or supersonic flow based on the critical pressure ratio which is defined as

$$PR_{crit} = \left( \frac{k+1}{k} \right)^{\frac{k}{k-1}}$$  \hspace{1cm} (4.50)

When \(P/P_o\) is less than \(PR_{crit}\), the flow is sonic and the mass flow rate is given by

$$\frac{dM}{d\theta} = AP_{o} \sqrt{\frac{2k}{R_u T(k-1)}} \left( \frac{P}{P_o} \right)^{\frac{k-1}{k}} \left[ \left( \frac{P}{P_o} \right)^{\frac{k-1}{k}} - 1 \right]$$  \hspace{1cm} (4.51)

When \(P/P_o\) is greater than \(PR_{crit}\), the flow is sonic, then
\[
\frac{dM}{d\theta} = AP \sqrt{k \frac{2}{k+1}} \left( \frac{2}{k+1} \right)^{k-1} \tag{4.52}
\]

On the exhaust stroke, \( P \) is the cylinder pressure and \( P_o \) is the exhaust manifold pressure. On the intake stroke, \( P \) is the intake manifold pressure and \( P_o \) is the cylinder pressure.

In the gas exchange process, the crucial parameter is effective valve opening area (A) which is a complex function of valve and valve seat dimensions. The most convenient reference area in practice (Heywood 1988) is given by

\[A = C_d \pi D_v L_v\]  \(\text{(4.53)}\)

where \( C_d \) is coefficient of discharge (0.62), \( D_v \) is valve head diameter and \( L_v \) is the valve lift. The equation is linear with valve lift and easy to determine. The valve lift is calculated by curve fitting to the measured valve lift at different crank angles from the valve opening to closing in actual engine and is given by

\[L_v = -0.0008 \theta^2 + 0.1679 \theta + 0.7273\]  \(\text{(4.54)}\)

where \( \theta \) is the crank angle from valve opening to closing.

\section*{4.12 NITRIC OXIDE MODELING}

The thermal NO formed during the combustion process given by extended Zeldovich mechanism is modeled in this section. The initial rate of NO formation in the flame front region is given by (Heywood 1988)

\[
\frac{d[NO]}{dt} = \frac{6 \times 10^{16}}{T^{0.5}} \exp\left(-\frac{69090}{T}\right) \left[N_2\right]^0 \left[O_2\right]^{0.5} \text{kmol/m}^3\text{s} \tag{4.55}
\]
where \([N_2]_e\) and \([O_2]_e\) are the equilibrium species concentration in kmol/m\(^3\) and the temperature (T) in K. The equilibrium concentration of \(N_2\) and \(O_2\) are given by

\[
\begin{align*}
[N_2]_e &= \chi_{N_2} \frac{P}{R_u T} \\
[O_2]_e &= \chi_{O_2} \frac{P}{R_u T}
\end{align*}
\]  

(4.56) (4.57)

The NO formation per crank angle is calculated by multiplying the equation (4.55) by 1/6N, where N is the speed of the engine in rpm.

\[
\frac{\Delta[NO]}{\Delta CAD} = \frac{d[NO]}{dt} \frac{1}{6N} \quad \text{kmol/m}^3 \text{ deg}
\]  

(4.58)

where \(\Delta CAD\) is the crank angle increment used in the calculation.

Substituting the equation (4.55) in (4.58),

\[
\frac{\Delta[NO]}{\Delta CAD} = \frac{6 \times 10^{16}}{T^{0.5}} \exp\left(-\frac{69090}{T}\right) [N_2]_e [O_2]_e^{15} \times \frac{1}{6N}
\]  

(4.59)

The temperature of the gas calculated during combustion duration is given as input in the equation (4.59) to estimate the NO formation during the combustion period. The volume associated with the current increment of NO formation in the model is the incremental volume \(\Delta V_b\) which is related to the increment of mass of fuel burned during angular interval using ideal gas law (Timoney et al 2005).

\[
\Delta V_b = \frac{R_u T}{P} \left(1 + \frac{1}{SFAR}\right) \frac{\Delta FMB}{MWF} \quad \text{m}^3
\]  

(4.60)
where $\Delta FMB$ is the fuel mass burned at every crank angle, calculated from the zero dimensional model. The NO formed at each crank angle increment is therefore given by

$$\frac{\Delta [NO]}{\Delta CAD} = \frac{\Delta [NO]}{\Delta CAD} \Delta V_b \text{ kmol/deg} \quad (4.61)$$

Substituting the equations (4.59) and (4.60) in (4.61) gives

$$\frac{\Delta [NO]}{\Delta CAD} = \kappa \frac{T^{0.5} \Delta FMB}{NP} \exp\left(-\frac{69090}{T^{0.5}}\right) \left[N_2\right] \left[O_2\right]^{0.5} \text{ kmol/deg} \quad (4.62)$$

where \(\kappa = \frac{R_u}{MWF} \left(1 + \frac{1}{SFAR}\right) \times 10^{16}\)

The estimated total NO formed during the entire combustion process is then computed as

$$E_{NO} = \sum_{CAD=SOC}^{EOC} \frac{\Delta NO}{\Delta CAD} \Delta CAD \text{ kmol} \quad (4.63)$$

The estimated NO formed in ppm is given by

$$E_{NO, ppm} = \frac{MW_{NO} E_{NO}}{M_f} \times 10^6 \text{ ppm} \quad (4.64)$$

From the estimated NO, the NO$_x$ formed during combustion is predicted by multiplying the above equation by the calibration factor 1.533 which is the ratio of molecular weight of NO$_2$ to NO as per the approach developed by Yuan et al (2007).

$$E_{NO_x, ppm} = 1.533 \times E_{NO, ppm} \quad (4.65)$$
4.13 WORK OUTPUT AND EFFICIENCIES

Work done during compression process is given by

\[ W_{COMP} = (N_d + N_x) \ C_v r \ (T_{ICB} - T_1) \]  \hspace{1cm} (4.66)

Work done during combustion process, between the pressure at the beginning of combustion (PICB) and pressure at the end of combustion (PICE), is calculated by

\[ W_{COMB} = \sum \left( P + \frac{\Delta P}{2} \right) \Delta V \]  \hspace{1cm} (4.67)

Work done during expansion process is given by

\[ W_{EXP} = UPT_{ICE} - UPT_{EE} \]  \hspace{1cm} (4.68)

Work done during the intake and exhaust processes (EVO to IVC) is calculated by

\[ W_{LOOP} = \sum \left( P + \frac{\Delta P}{2} \right) \Delta V \]  \hspace{1cm} (4.69)

Net work done during the diesel cycle is computed as

\[ W_{NET} = W_{COMB} + W_{EXP} - W_{COMP} - W_{LOOP} \]  \hspace{1cm} (4.70)

Indicated mean effective pressure is given by

\[ IMEP = \frac{W_{NET}}{100V_d} \ \text{bar} \]  \hspace{1cm} (4.71)

Indicated power of the engine is computed as

\[ IP = \frac{W_{NET} \times N}{120} \ \text{kW} \]  \hspace{1cm} (4.72)
Indicated thermal efficiency is calculated as

\[ ITEFF = \frac{IP}{M_f \times Q_{LHV}} \times 100 \]  
(4.73)

Brake mean effective pressure is given as

\[ BMEP = IMEP - FMEP \]  
(4.74)

Brake power available at the crankshaft of the engine is computed as

\[ BP = \frac{100 \times BMEP \times V_a \times N}{120} \text{ kW} \]  
(4.75)

Mechanical efficiency of the engine is

\[ MEFF = \frac{BMEP}{IMEP} \times 100 \]  
(4.76)

Brake thermal efficiency of the engine is given by

\[ BTEFF = ITEFF \times MEFF \]  
(4.77)

Brake specific fuel consumption of the engine is calculated as

\[ BSFC = \frac{M_f}{BP} \]  
(4.78)

### 4.14 COMPUTER PROGRAM

Based on the modeling scheme given above, a computer program was written in C language to compute the engine performance parameters, cylinder pressure and NO\textsubscript{x} formation during combustion. The main input and
output parameters of the simulation program are given below. The detailed computer codes are given in Appendix 4.

<table>
<thead>
<tr>
<th><strong>Input parameters</strong></th>
<th><strong>Output parameters</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder diameter</td>
<td>Cylinder pressure</td>
</tr>
<tr>
<td>Stroke length</td>
<td>Indicated power</td>
</tr>
<tr>
<td>Length of connecting rod</td>
<td>Brake power</td>
</tr>
<tr>
<td>Engine speed</td>
<td>Mechanical efficiency</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>Indicated thermal efficiency</td>
</tr>
<tr>
<td>Properties of diesel</td>
<td>Brake thermal efficiency</td>
</tr>
<tr>
<td>Properties of air</td>
<td>Specific fuel consumption</td>
</tr>
<tr>
<td>Water percentage in the emulsion</td>
<td>NO\textsubscript{x} generation during combustion</td>
</tr>
<tr>
<td>Mass of fuel supplied</td>
<td></td>
</tr>
</tbody>
</table>