2 Phenomenology of Diesel Combustion and Modelling

Abstract Diesel is the most efficient combustion engine today and it plays an important role in transport of goods and passengers on road and on high seas. It is expected that the diesel engine will be active for another 100 years as increasingly economical sources are found with the increase in oil prices offering incentive to the explorers. The emissions must be controlled as demanded by the society without sacrificing the legendary fuel economy of the diesel engines. These important drivers caused innovations in diesel engineering like re-entrant combustion chambers in the piston, lower swirl support and high pressure injection, in turn reducing the ignition delay and hence the Nitric Oxides (NO_x). From 16 g/kWh in 1988, the limit on NO_x is reduced today to as low as 2.0 and PM limit is reduced from 0.8 g/kWh to 0.02. These limits are being continually reduced. Therefore, the required accuracy of the models to predict PM, NO_x and efficiency of the engines is high. The phenomenological combustion models are practical to describe diesel engine combustion and to carry out parametric studies. This is because the injection process, which can be relatively well predicted with the phenomenological approach, has the dominant effect on mixture formation and subsequent course of combustion. The need for improving these models was also established by incorporating developments happening in engine designs. A phenomenological model consisting of sub-models for combustion and emissions are proposed in detail in this chapter. With more and more "model based control programs" used in the ECU controlling the engines, phenomenological models are assuming importance now. The full CFD based models though give detailed insight into the combustion phenomena and guide the design engineer, they are too slow to be handled by the ECU's or for laying out the engine design. Therefore, phenomenological models have a bright future hand in hand with the sophisticated models. The diesel combustion is modelled by studying the structure of the spray, ignition delay, heat transfer, air-fuel mixing and heat release. These contribute to smoke, NO_x and engine performance.

The Phenomenological Combustion Models are very practical to describe diesel combustion and to carry out parametric studies. This is because the injection process. The models are improved by incorporating new developments in engine designs.

The combustion in modern DI diesel engines is mainly divided in two phases: (a) a small ignition delay event in which pre-flame activities take place followed by (b) main heat release event in which actual combustion happens. These events are modelled differently considering prominent role of chemical kinetics during ignition and physical mixing rate during heat release. This approach is described

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in detail in the following sections. This chapter summarizes different types of models along with description of popular models.

Combustion Model

The combustion starts almost at the onset of fuel injection because the ignition delay in modern DI diesel engines is very small with high compression ratio and highly retarded injection timing enabling substantial reduction in noise, NO_x and HC. The heat release estimated with this assumption predicts satisfactorily the important instantaneous parameters used by a designer e.g. heat transfer, fuel consumption, and the performance turbocharger and piston. On the same tenor, ignition delay cannot be neglected while estimating emissions however small it may be.

Ignition delay
In direct injection diesel engines, estimation of ignition delay is of great importance because of its effect on startability, noise and formation of NO_x. The ignition delay in a diesel engine is defined as the time interval between the start of injection and the start of combustion. This delay period consists of (a) physical delay, wherein atomisation, vaporization and mixing of air fuel occur and (b) chemical delay attributed to pre-combustion reactions. Both physical and chemical delays occur simultaneously. Early DI diesel engines operated at relatively low compression ratios and low injection pressures with very advanced injection timings in commensurate with the large ignition delay (Lakshminarayanan *et al.* 2002a). Reduction in ignition delay held the key to solving emission and noise problems. Higher temperature at the beginning of injection by increased compression-ratio reduces the delay period substantially.

Numerous ignition delay correlations have been proposed based on experiments carried out in constant volume bombs, steady state reactors, rapid compression machines and engines. Wolfer (1938) developed the earliest correlation for predicting ignition delay. The equation was in the form of an Arrehenius expression representing a single stage reaction. Kadota *et al.* (1976) related results of combustion bomb experiments to an Arrehenius type expression by introducing dependence of equivalence ratio. Lahiri *et al.* (1997) modified this equivalence ratio to fuel-oxygen ratio, attempting to make it suitable for oxygenated fuels. However, these correlations fail to predict the ignition delay under unsteady diesel engine conditions as they are based on experiments conducted in a constant volume bomb. On the other hand, a few correlations have been developed considering engine data (Hardenberg and Hase 1979, Watson *et al.* 1980). These correlations also were not successful in yields, satisfactory predictions under widely varying operating conditions as they have ignored the effect of mixture quality. Recently Assanis *et al.* (1999) have compared these correlations and found better predictability using the Watson correlation (1980). They improved the correlation by introducing the equivalence ratio and tuning the empirical constants. They postulated that the introduction of the dependency of ignition delay on overall equivalence ratio makes the correlation more dynamic.

The time taken for visible fire to appear in the pre-mixed zone of spray is a strong function of pressure and temperature of the ambient. In addition, the physical properties such as Cetane number, viscosity of fuel, nozzle-hole size, injected quantity and injection pressure contribute to the delay phenomenon in diesel engines (Chandorkar *et al*. 1988).

Heat release

The shaft work by a diesel engine is the sum of work on the piston by the pressure produced by the heat released by combustion and the losses due to pumping, heat transfer and friction. While the flow losses and friction work could be reasonably comprehended, the heat release is dependent on the complex turbulent mixing of fuel and air at high temperature after compression. The variety of combustion chambers and types of fuel injection equipments influence the heat release rate characteristically.

Models based on fluid dynamics

These types of models are often called as multidimensional models due to their inherent ability to provide detailed geometric information on the flow field based on the solution of the governing equations. In the numerical calculations of reacting flows, computer time and storage constraints severely restrict the complexity of the reaction mechanism that can be incorporated. They use simplified model for predicting combustion, which is mixing controlled and kinetically controlled. The choice between these two models is made by the ratio of the chemical reaction time to the turbulent mixing time. Several three-dimensional simulation models of injection, mixing and burning in diesel engines exist (Cartillieri and Johns 1983, Gosman *et al*. 1985) describing various phenomena in the engine and providing possibilities of understanding the inner mechanism of diesel sprays. However, the volume of computation in multi-dimensional models is too prohibitive to carry out many parametric studies. In addition, their sub-models require a thorough validation with detailed experiments before employing them confidently in engine design work.

Phenomenological models

In these types of models, details of different phenomenon happening during combustion are added to basic equation of energy conservation. In the simplest approach, Rife and Heywood (1974) assumed the growth and motion of the spray within the chamber and analysed it as a quasi-steady one-dimensional turbulent gaseous jet. Shahed *et al*. (1973), Dent and Mehta (1981), and Hiroyasu *et al*. (1983) found that the spray structure offered the clue to better heat release predictions. In these investigations, detailed two-dimensional axisymmetric spray calculations are attempted using the mixing of the injected fuel with the surrounding air entrained due to high shear velocity of the jet (Fig. 2.1). A criterion of stoichiometric burning of the fuel in ignitable elements has been used in these models by spray-mixing approach.

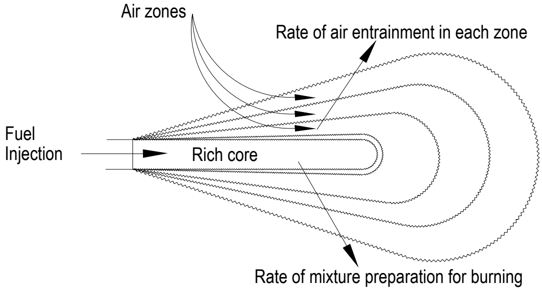

Fig. 2.1 Multi zone spray model

Zero-dimensional models

This type of models is more attractive due to their simplicity as they use simple algebraic equations to describe heat release rate. Lyn's work (Austen and Lyn 1960) is the earliest in identifying a strong relationship between fuel injection and heat release rates. The rate of injection diagram was subdivided into elemental fuel packets emanating as rectangular pulses, which results in exponentially decaying heat energy function. The convolution integral of the heat release from the individual packets summed neatly to the net heat release rate (Fig. 2.2). Due to the absence of universal decay constants for elemental heat-release rates in different types of engines and their operating conditions, the application of this elegant idea posed difficulty.

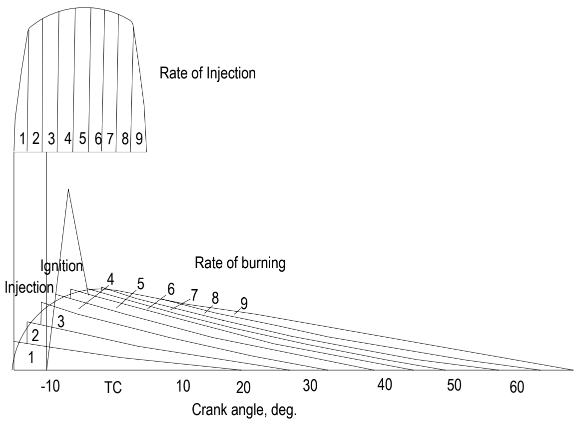

Fig. 2.2 Relation between rate of injection and rate of burning

In this regard, the global heat release rate function of Wiebe (1970) earned much wider acceptance in diesel engine simulation for several years now (Fig. 2.3). The Wiebe's function, however, requires two adjustable constants for a given engine type and even then fails to explain the effects of speed and load. In addition, this function does not reflect the effects of the shape of the combustion chamber and the fuel injection rate on the history of heat release as desired in current engine development.

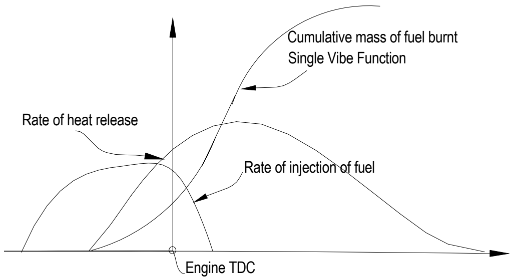

Fig. 2.3 Wiebe's model

The limitations of Wiebe's function to predict the rate of heat release during early premixed period was somewhat overcome by Watson *et al.* (1980) through the concept of double Wiebe function. This however, added more number of adjustable constants that are dependent on the engine type. While such algebraic functions are easy to compute, there are various other complex models (Table 2.1).

Table 2.1 Combustion models

Author (year)	Specialty of model	Remark
Austen and Lyn (1960)	Direct relation between fuel injection pump and heat release rate	Absence of universal constants
Wiebe (1970)	Exponential decay function with empirical constants	No effect of injection rate and combustion chamber
Shahed *et al.* (1973)	Detailed computation of two-dimensional axisymmetric spray	Engine dependant constant
Dent and Mehta (1981)		No effect of load and speed
Hiroyasu *et al.* (1983)		
Cartillieri and Johns (1983)	Three-dimensional finite volume technique	Large volume of calculation
Gosman *et al.* (1985)		
Chmela and Orthaber (1999)	Mixing controlled combustion	No effect of wall impingement

In a simpler approach, avoiding necessity of engine dependant tuning constants, Chmela and Orthaber (1999) proposed an innovative model on the premise that the fuel-air mixing, and hence the burning in diesel engines, is proportional to the average turbulent kinetic energy associated with the fuel injection rate. In addition, the turbulent energy decay in time is proportional to the total kinetic energy of the injected fuel itself. It is observed that this model predicts the trend of heat release quite closely if only there is no impingement of sprays on the piston.

A comparison of the predicted and the experimental results is not satisfactory in case of spray impinging on the wall. This situation arises in engines of capacities less than 2 L per cylinder operating at more than half load, where majority of diesel engines belongs. Therefore, an attempt has been made in this book to enhance this model by encompassing the phenomena at the wall and the instantaneous injection rate derived from the indicated performance of fuel injection equipment (Lakshminarayanan *et al.* 2002a).

Emission Models

DI diesel engines emit smoke, hydrocarbons, nitric oxides, carbon monoxide and particulate matter are mainly regulated. They are formed in different phases of combustion as described below.

Hydrocarbons
The fuel leaned beyond flammability limits (Greeves *et al.* 1977), bulk quenching during expansion, fuel effusing from nozzle sac after completion of injection (Yu *et al.* 1980) are the most important reasons for Hydrocarbon (HC) emissions. A semi-empirical phenomenological model was successfully made for HC emissions considering the fuel injected and mixed beyond the lean combustion limit during ignition delay and fuel effusing from the nozzle sac at low pressure (Lakshminarayanan *et al.* 2002b). Exhaust gas recirculation (EGR), a well-accepted method of NO_x reduction, alters ignition delay and HC emissions. The oxygen-enriched fuels that attract great attention worldwide owing to its excellent combustion characteristics, exhibit different behaviour especially in case of ignition delay and HC emissions.

Oxides of nitrogen
Considering the heterogeneous nature of fuel-air mixture in diesel engines, NO_x and particulate matter (PM) are important emissions. Continuous efforts are being made to minimize the quantities of these two pollutants from the diesel engine exhaust. Vioculescu and Borman (1978) carried out gas sampling from within the cylinder of a naturally aspirated direct injection (DI) diesel engine using a rapid acting sampling valve. This resulted in a plot showing time history of ratio of the average cylinder NO_x concentration in the exhaust during the combustion process. Similar modelling and gas sampling studies have been done with indirect injection (IDI) diesel engines, which suggest that prechamber is the prominent location for formation of nitrogen oxides (Mansouri *et al.* 1982). Duggal *et al.* (1978) plotted the NO concentrations and equivalence ratios as a function of crank angle using a rapid-acing sampling valve at different locations within the prechamber of a swirl chamber IDI engine. There are a number of potential mechanisms responsible for NO in combustion processes. The relative importance of these different mechanisms is strongly affected by the temperature, fuel-air equivalence ratio, pressure, flame

conditions, residence time and concentrations of key reacting species. Rapid NO_x formation begins after the start of heat release. Shortly after the end of heat release, the period of rapid NO_x formation ends because temperatures of the burned gas decrease due to mixing with cool bulk gas and expansion of the charge (Kitamura *et al.* 2005). Fuel-Air equivalence ratio is another important factor influencing NO_x formation. As the equivalence ratio becomes leaner, NO and NO_x decrease significantly as expected. NO_2 however shows an opposite trend to that of NO that causes the NO_2/NO_x ratio to increase at leaner conditions. The NO_2 peaks at an equivalence ratio near 0.25. Leaner equivalence ratio is indicative of lower loads and lower bulk gas temperatures that are conducive to the formation of NO_2 (Pipho *et al.* 1991).

Advancing injection timing or increasing injection pressure improves combustion efficiency raises combustion temperature. In general, higher combustion temperatures lead to higher NO_x formation (Henein and Patterson 1972). Addition of diluents to the engine intake air is considered as an effective mean to reduce the NO formation rate and hence the exhaust NO_x levels. The effect is primarily one of reducing the peak flame temperature, which is the driving factor for NO_x formation. Diluents such as N_2, CO_2 and exhaust gas were added to the intake air of direct injection (DI) engine to study their effect on NO_x reduction (Challen and Baranescu 1999). Similar studies done in indirect injection (IDI) engine showed similar trends (Yu and Shahed 1981). Plee *et al.* (1981, 1983) established a correlation showing the effect of changes in intake air composition and temperature on NO_x emissions.

NO_x emissions comprise of NO and NO_2. The NO_2 is formed via NO molecule. Therefore, the modelling of NO_x formation is most often reduced to studying the formation of NO. It is widely accepted that in diesel engines the major portion of NO is formed via thermal path (Ahmed and Plee 1983). Many multi-dimensional and multi-zone phenomenological models use extended Zeldovich mechanism (Heywood 1988). This mechanism was postulated by Zeldovich (1946) and improved by Lavoie *et al.* (1970). Khan *et al.* (1973) related FIE and engine operating conditions to NO formation and developed a method of calculation for emissions (Khan *et al.* 1973). They concluded that an increased rate of injection or increased air swirl reduces the amount of exhaust smoke and increases NO_x.

All these models utilize empirical heat transfer correlation, which are mass averaged. During combustion, the heat loss is caused partly by convection from burned gases at high temperature and partly by radiation from soot particles formed during the diffusion flame. Due to the short distance between the nozzle and the combustion chamber wall under typical operating conditions, diesel fuel impinges on the wall in the form of liquid followed by fuel vapour and flame after onset of auto-ignition. The peak radiant heat flux is always less than 20% total heat flux confirming the dominant role of spray and flame interaction with piston bowl (Arcoumenis *et al.* 1998).

The contribution of convective mode of heat transfer is about 80% to total engine heat transfer (Heywood 1988, Stiesch 2003). However, it is known that in diesel engines radiative heat transfer may have a significant contribution in addition to convective heat transfer. The radiative heat transfer in diesel engines is caused by both radiation of hot gases and by radiation of soot particles within the diffusion flame. It is agreed in the literature that the latter has a significantly greater impact on the radiative heat flux, and thus most heat transfer models concentrate on the radiation of soot only. It should be noted though, that a general difficulty in the evaluation of soot radiation exists in that the prediction of the soot concentration itself is typically subject to significant uncertainties (Stiesch 2003). Therefore, the empirical heat transfer correlations focused mainly on convective mode.

The heat transfer coefficient has been derived by many researchers by assuming an analogy with a steady turbulent flow over a solid wall. The colour pyrometer and fast response thermocouples were employed for experimental investigations. Annand (1963) developed correlation for convective heat transfer but it was based on experiments conducted on only cylinder head. Probably, the most widely used approach in this category is the one suggested by Woschni (1967). Hohenberg (1979) improved the above correlation by using a length based on instantaneous cylinder volume and exponent of the temperature term. This approach gives an estimate of the surface-averaged heat transfer coefficient history in terms of the bulk gas temperature and a surface-averaged or total heat flux (Ikegami *et al.* 1986, Nishiwaki 1998). However, this approach cannot give the kind of information necessary to design modern engines. The empirical correlations underestimate to varying degrees the heat transfer during combustion. The investigations have revealed that during the combustion period the wall heat flux is substantial locally in space and time, due to the transient nature of the flame propagation. In particular, during combustion the heat flux increases rapidly after impingement on the wall (Kleemann *et al.* 2001). The characteristics of injected spray and its interaction with the swirling air and the wall of the combustion chamber determine the efficiency and the exhaust emissions. In Chapter 14, a phenomenological model for NO_x prediction is proposed based on spray combustion incorporating localised effect of heat transfer in wall spray and exhaust gas recirculation.

Smoke and particulate matter

The characterization of diesel smoke has remained a challenge in engine development and modeling work. Effect of different parameters of combustion chamber and injection on soot and NOx emissions were investigated by De Risi *et al.* (1999, 2005). Kurtz and Foster (2004) identified critical time for mixing in diesel engine and its effect on emissions. Based on in-situ laser diagnostics, a conceptual model of burning jet was developed (John Dec 1997). Khan et al (1973) first presented a model for the prediction of soot related to engine operating condition. Hiroyasu *et al.* (1976) proposed a two-step semi empirical model and applied it to the multi-packet combustion model. Later on, the model was extended up to a simple three-dimensional model (Nishida K, Hiroyasu H 1989). Fusco *et al.* (1994) proposed that either pyrolysis of fuel could result in soot precursor radicals or growth species with possibilities of oxidation at intermediate stages. There is a principal mathematical problem in the modeling of the engine-out soot emissions by using formation and oxidation methodology (Stiesch G 2003). Since the soot mass in the exhaust is the very small difference between two nearly equal large quantities i.e. between formation and oxidation, a significant error will result if only a small deviation in either the production or the formation rate. Magnussen *et al*. (1976) carried out experiments on steady state free diffusion flames and concluded that soot was formed and contained in the turbulent eddies within the flame. The burn up of the soot was related to the dissipation of turbulence. In this view, Dent's work (1980) was unique. The importance of turbulent energy dissipation rate on smoke in quiescent chamber diesel engines was identified quantitatively. Recently, Dec and Tree (2001a, 2001b) investigated interactions of combusting fuel jet free in air and at the wall using laser diagnostics. They found that soot deposition on the wall and blow-off are not the major contributors to engine-out soot emissions. In chapter 12, a model that clearly distinguishes the free jet and wall jet regimes of a diesel-engine spray and their turbulence structure is developed to explain the smoke.

Diesel particulates consist principally of carbonaceous material (soot from smoke) generated by combustion on which some organic compounds have become absorbed. Most of the particulate material results from incomplete combustion of fuel hydrocarbons; some is contributed by the lubricating oil (Heywood 1988). Diesel particulate matter is therefore a complex mixture of organic and inorganic compounds in solid and liquid phases (Johnson *et al.* 1994). The basic measurement of particulate matter is by its mass and it can be described as any exhaust components other than uncombined water that collects on a filter in a dilution tunnel at a temperature less than 53°C. In the standard procedure of measurement of mass emission, dilution tunnels are used to simulate the physical and chemical processes the particulate emissions undergo in the atmosphere. In the dilution tunnel, the raw exhaust gases are diluted with the ambient air to a temperature of 53°C or less and the sample stream from the diluted exhaust is filtered to remove the particulate matter. The mathematical modelling of particulate matter is always concentrated around soot because of its complex nature. Different studies have been carried out to establish contributions of soot, unburnt HC from fuel and lubricating oil (Cartillieri and Trittari 1984, Cartillieri and Wachter 1987, Cartillieri and Herzog 1988). Most of the PM correlations consider only soot to estimate particulate matter. Recently one phenomenological model is proposed for PM based on soot and unburnt HC from fuel (Tan *et al.* 2007). However, this model requires tuning of engine and load dependent constants. It does not account for SOF from lubricating oil and IOF from sulphates.

Theme of the Book

The literature survey highlighted some of the limitations of present phenomenological models for application to modern engines. The available models require many engine-dependent empirical constants and consideration is given to neither spray-wall interaction nor the effect of oxygenated fuels. The book presents the results of the research work based on comprehensive experimental work undertaken for improving phenomenological modelling of combustion in modern engines.

The highlights of the phenomenology of diesel combustion considered in the following chapters are as follows.

- Analysis of modern in-cylinder emission control technologies
- Turbulence structure for engine sprays
- Spray-wall interaction and its effect
- Mixing controlled combustion
- Localized heat transfer
- Quasi one-dimensional approach to the heat release in DI engines
- Consideration to fuel bound oxygen
- Avoid engine dependent constants
- Sub-model for prediction of combustion
- Sub-models for important exhaust emissions

About 50 modern engines (Table 3.2) from 21 different engine families with widely varying features like bore-sizes, aspiration and cooling system are selected for experimental work. These engines meet current emission norms and are capable of upgrading to next stage with minor changes. Observations pertaining to fuel injection, emissions and engine performance were collected simultaneously using experimental set up specially developed. Additional experiments were also carried out to study the effect of oxygenated fuels and exhaust gas recirculation on a few engines. The new models are thoroughly validated by using a large number of data collected from many experimental data. In addition, the results of new models are compared with 1-D engine cycle simulation tools like 'AVL Boost (2005) which are being extensively used for engine development. The objectives of research work are:

- To improve understanding of ignition delay and mixing controlled combustion
- Develop turbulence structure for engine spray
- Estimation of combustion cavity – spray interaction
- Wall impingement of sprays causing loss of kinetic energy and intense heat transfer
- Effect of exhaust gas recirculation, EGR on combustion
- Effect of fuel bound oxygen on combustion and emission
- Effect of injection characteristics and nozzle features

To meet above objectives, a research scheme was developed as shown schematically in the Fig. 2.4.

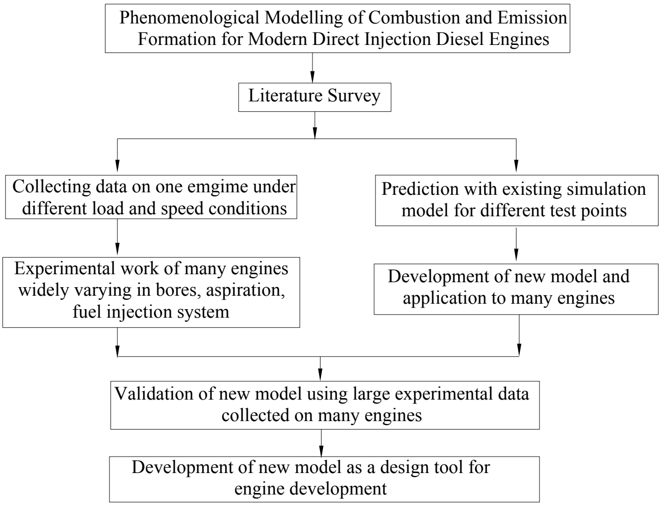

Fig. 2.4 Book scheme

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