

Mechanical Engineering Series

P. A. Lakshminarayanan  
Yogesh V. Aghav

# Modelling Diesel Combustion

*Second Edition*

 Springer

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P. A. Lakshminarayanan · Yogesh V. Aghav

# Modelling Diesel Combustion

Second Edition

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# Preface

## Phenomenology of Diesel Combustion and Modelling

Diesel is the most efficient combustion engine today, and it plays an important role in the transport of goods and passengers on land and on high seas. The emissions must be controlled as stipulated by society without sacrificing the legendary fuel economy of 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. The limits on emissions are being continually reduced. Therefore, the required accuracy of the models to predict the emissions and efficiency of the engines is high. The phenomenological combustion models based on the physical and chemical description of the processes in the engine 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, has the dominant effect on mixture formation and subsequent course of combustion. The need for improving these models by incorporating new developments in engine designs is explained in Chap. 2. With “model-based control programs” used in the electronic control units (ECUs) of the engines, phenomenological models are assuming importance now because the detailed CFD-based models are too slow to be handled by the ECU.

Experimental work is necessary to develop a basic understanding of the processes. Chapter 3 describes the experimental set-up of the bomb for interferometry and real engine studies for validation of the phenomenological models. This chapter also includes the details of the measurement techniques for obtaining the experimental data needed for validating the phenomenology. Empirical relations have been obtained in Chap. 4 to describe the axial and radial variations of fuel concentration in the vaporizing and burning sprays, and to evaluate penetration and air entrainment of the free and wall jet regions. The movement of the “tail” of the spray in the post-injection period has been studied. These equations form the basis for building the phenomenological models of ignition delay, emissions, and heat release rate in subsequent chapters.

The norms for  $\text{NO}_x$  and HC emissions are so tight that the prediction of ignition delay has become necessary. In Chap. 5, phenomenological calculations of the cooling of spray surface have shown that the physical parameters and fuel type influence the temperature of the mixture of air and the fuel vapour throughout its life up to the end of ignition delay. A model is proposed in Chap. 6 to predict rapid convective heat transfer between spray and wall by extending the analogy by Woschni.

The rate of heat release in an indirect injection engine is modelled on the lines of its observed rate in a direct injection engine. The diffusion combustion is modelled as proportional to the available fuel and rate of air entrainment in Chap. 7. Chapter 8 introduces the concept of air useful for combustion. The ratio of momentum of the useful air to the total momentum of injected fuel near TDC at the end of the ignition delay period is found to bear a universal relationship with the indicated efficiency and dry soot emissions in the case of combustion chambers supported by air swirl. In Chap. 9, the combustion rate is precisely described using the concept developed in Chap. 7 by relating the fuel–air mixing rate to the turbulent energy created at the exit of the nozzle as a function of the injection velocity and by considering the dissipation of energy in free air and along the wall. The absence of adjustable constants distinguishes the model from the other zero-dimensional or pseudo-multi-dimensional models. The success of the model is demonstrated by applying the technique to engines widely varying in bore size with single-shot fuel injection.

The almost infinite ability of the common rail diesel injection system spawned multiple injections, currently up to nine shots per cycle. It enables containing nitric oxide and particulate emissions as much as possible within the cylinder and very little treatment after the engine to meet some of the tightest emission standards. The model detailed in Chap. 9 has been morphed successfully to accept multiple injections in Chap. 10. Examples of predictions of heat release rate are provided for a commercial truck engine with pilot, main, and post-injections.

Hydrocarbon (HC) emissions from direct injection diesel engines are mainly due to fuel injected and mixed beyond lean combustion limit during ignition delay and fuel effusing from the nozzle sac at low pressure. The concept has been developed in Chap. 11 to provide an elegant model to predict HC emissions. To contrast the phenomenon of HC formation in a diesel and a spark-ignition engine, Chap. 12 is included. The absorption and desorption of fuel by cylinder lubricating oil films have been modelled using principles of mass transfer.

A new model for smoke explained in Chap. 13 characterizes the smoke emitted at higher loads from the wall–spray formed after impingement. The smoke has been treated by ignoring the fast chemistry, as the slow physical mixing seems to be controlling. A new phenomenological model for  $\text{NO}_x$  emission is developed based on mixing-controlled combustion incorporating localized wall heat transfer in Chap. 14. Based on the smoke formation and oil consumption, an estimate of the particulate matter is made in Chap. 15. In this chapter, some of the intricate relationships between smoke and soot are explored. Also, smoke, as measured by filter paper method and opacity, is compared and the usefulness of the different methods for the development engineer is explained.

Chapter 16 reviews the basic approach of multi-dimensional CFD modelling of diesel combustion, focusing on the advanced turbulence and combustion models. Recent efforts for reducing the computational expense of multi-dimensional CFD modelling are also discussed. CFD tools reveal details about invisible or technically difficult or costly to measure in-cylinder processes of diesel combustion so that guidance can be provided to improve engine designs in terms of emission reduction and fuel economy; innovative combustion concepts can be evaluated numerically before experimental tests to reduce the number of investigated parameters and thus costs; important design parameters can be discovered by modelling engines of different sizes to establish engine size-scaling relationships and thus non-dimensionalizing engine designs; by integration with optimization methodologies, CFD tools can also directly impact the design of optimum engine systems, such as piston geometry and injection parameters. Each of these aspects is described by relevant case studies in Chap. 17.

Even though the direct simulation of turbulence may be attractive, the cost and time of computation are prohibitive. Therefore, the closure of turbulence equations by RANS as explained in Chaps. 16 and 17 is used to obtain useful results. With the advent of faster computers, it is possible to graduate to the next step of simulating large eddies. Large eddy simulation (LES) gives insight into engine emissions that might be missed by RANS. Chapter 18 opens the door to the vista of LES with all the attendant equations and examples.

The appendix is numbered as a chapter in the second edition. Also, at the end of chapters, relevant nomenclatures are appended as suggested by the series editor of the Springer Mechanical Engineering Series.

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In the second edition, we enhanced the chapter on PM emissions bringing in recent publications on the subject. We hope it will enable developers to estimate the particulate mass during the development process.

The common rail fuel injection system made a direct injection diesel engine highly adaptable, offering a variety of combustion and emission solutions. Multiple injections of chosen durations with predetermined separation are the basis for the versatility. In this book, the heat release rate in a diesel engine is treated as the transformation of the rate of injection. This concept is developed successfully for engines of widely varying bores with single-shot injection. Then, a chapter is dedicated to extending the idea for multiple injections and authenticated. A good prediction of heat release leads to predicting many thermodynamic parameters of an engine.

The book is complete only with the two chapters on the reviews and applications of modern methods of simulating diesel engines by Dr. Yu Shi and Prof. Dr. Rolf Reitz of Engine Research Centre at the University of Wisconsin-Madison. They acceded to our request spontaneously and gracefully to provide the material. We express our gratitude to them for showing magnanimity. Large eddy simulation as an elegant closure for the turbulence flow equations helps in modelling combustion and emissions better with the help of new generation computers. Through Dr. Shi and Prof. Reitz, we were introduced to Dr. Haiwen Ge of Texas Tech University who could offer an excellent chapter on the subject.

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Yogesh V. Aghav

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## Contributors

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**Mr. Anirudh Jaipuria** completed his B.Tech. in mechanical engineering from the National Institute of Technology Surat, India, after which he joined Ashok Leyland Ltd. as Deputy Manager where he led the development of the BS-IV heavy-duty diesel engine family. Following that, he completed his master's in combustion engines from RWTH Aachen, Germany. In 2012, he joined MAN Diesel & Turbo as Simulation Engineer responsible for valvetrain development for 4-stroke large diesel engines. Since 2015, he has been with BMW M-GmbH, Munich, as SE-Team Leader and technical specialist responsible for all dynamic simulations and drivetrain development for high-performance sports cars. He has five publications and has been a speaker at two international conferences.

# Chapter 1

## Introduction



### Role of Internal Combustion Engines

Rapid increase in pollution levels, escalation of fuel prices, and depletion of hydrocarbon reserves of the world have forced the engineers to look for appropriate technology and alternative fuels to cater to the ever-increasing demands of energy. The internal combustion (IC) engines form an indispensable part of industrial growth. IC engines play a dominant role in the fields of propulsion, power, and energy. They also contribute to our modernized agricultural sector and the transportation of goods and passengers. It is impossible to do without the IC engines and hence means must be sought to improve the designs.

It has been estimated that the present fossil fuel demand is expected to double between now and 2050. At present, about two-thirds of world energy demand is met by fluid fossil fuels because of their availability and convenience of use in the existing design of several prime movers such as internal combustion engines. In the future, the energy scenario is likely to be several times worse than the two oil crises of the 1970s. The second predicament involving fossil fuels is the environmental damage caused by the combustion of fossil fuels. Technologies for fossil fuel extraction, transportation, processing, and particularly their combustion have harmful impacts on the environment. The fossil fuels which constitute carbon and hydrogen in addition to traces of sulphur and quality enhancer additives like oxygenates produce various gases, soot, ash, and other organic compounds during combustion and when released into the atmosphere cause degradation of air quality [1, 2]. These pollutants when mixed with water and other atmospheric compounds or triggered by sunlight change their form and become pollutants like ozone, aerosols, peroxyacetyl nitrates, various acids causing damage to the aquatic and terrestrial ecosystem, affecting humans, animals, vegetation, and structure.

In IC engines, the chemical energy of the fuel is released inside the cylinder to produce mechanical power. Spark-ignited (SI) gasoline and compression-ignited (CI) diesel engines are the main types of IC engines. In 1876, Otto invented the SI engine, and later in 1892 Diesel developed the CI engine. Traditionally, SI gasoline engines

are employed for light-duty applications, as they are compact with a simple construction for a lower power range. On the other hand, CI diesel engines are for heavy-duty usage as they can develop more power at lesser fuel consumption. Different methods of fuel supply are used for CI engines, namely indirect and direct types. Out of these different types of engines, the direct injection (DI) diesel engine exhibits the best fuel economy along with the lowest engine-out emissions. Therefore, it is emerging as the engine of the future. The packing of higher power also improves the power-to-weight ratio to make the engine more compact. Traditionally, considered heavy-duty, the DI diesel engines are also popular in the passenger car market. The best fuel economy car consuming only three litres of fuel for 100 km is developed with the modern DI diesel engine. This trend is facilitated by the development of contemporary injection systems that are more flexible and generate higher injection pressures for better spray atomisation and combustion characteristics than their predecessors. The modern DI diesel engines satisfy stringent emission norms of Euro III without after-treatment. The DI diesel engine is now recognized as environmentally friendly, powerful, and smooth running [3].

## Developments in DI Diesel Engines

In DI diesel engines, the fuel is sprayed at higher pressure directly into the main combustion chamber where it ignites by mixing with hot air produced by isentropic compression. The stoichiometric air-to-fuel ratio is 14.7 for diesel fuel. However, the diesel engines work satisfactorily above the air-to-fuel ratio of 19, i.e. always with some excess air. As the fuel is directly sprayed into the cylinder, sufficient time is not available for mixing, which results in smoke in zones of lower air-to-fuel ratios. The higher compression ratio helps improve the efficiency of diesel engines at higher loads. They are also more economical than gasoline engines at lower loads because they can work at very lean mixtures avoiding throttling losses of charge air. Due to their lower heat losses, diesel engines have a lower risk of gradually over-heating if left idling for long periods. In many applications, such as marine, agriculture, and railways, diesel is left idling unattended for many hours. These advantages are especially attractive in locomotives.

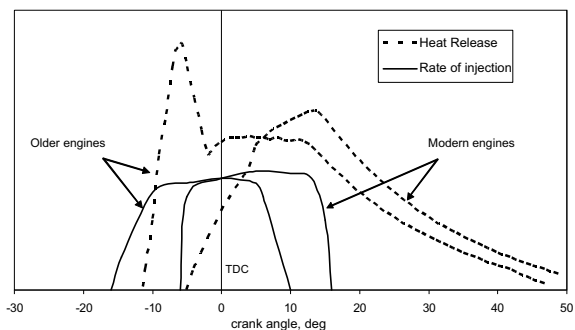
A naturally aspirated diesel engine produces less power density, i.e., power in a given volume, compared to gasoline engines. The power of the diesel engine is always limited by the air available. Therefore, they are often turbocharged to improve power density. The turbocharged versions can produce more power than petrol engines, limited by mechanical capability. The diesel engines do not face knocking problems. A turbocharger consists of a turbine and a compressor linked by a shared axle. The turbine inlet receives exhaust gases from the engine exhaust manifold causing the turbine wheel to rotate. This rotation drives the compressor, compressing ambient air, and delivering it to the intake of the engine; this allows more fuel to burn in the cylinder. At a higher boost, the benefit of more air mass diminishes as the density drops substantially. Inter-cooling by using atmospheric air

or engine jacket water helps to recover the density by bringing down the temperature of the charge. The charge air is not throttled in diesel engines; therefore, a governor is used to control fuel supply quantity. A sophisticated fuel supply system consisting of a pumping unit, multi-hole injector, and governor are employed in DI diesel engines to inject the correct amount of fuel at the required time under favourable conditions for combustion.

Early DI diesel engines operated at relatively low compression ratios and low injection pressures. Hence, they demanded very advanced injection timings commensurate with the large ignition delay. During the ignition delay period at the beginning of combustion, up to about 20% of the injected fuel is prepared to stoichiometric proportion. Due to high flame speed, the prepared mixture burns at high temperatures to produce nitrogen oxides and explosive noise characteristic of a diesel engine, Fig. 1.1. This period of combustion is said to be the premixed phase governed by chemical kinetics. On the other hand, the rest of the fuel burns as and when the mixture is prepared because the delay is absent with hot gases and radicals available in the vicinity, a remnant of the fuel burnt earlier. This second part is called the diffusive phase, and the rate of combustion of the majority of fuel is controlled by the physical mixing processes in the spray. The third or the last stage corresponds to the tail of the heat release diagram in which a small but distinguishable rate of heat release persists late into the expansion stroke [4]. Such a design was the result of the available technology and lack of norms for noise and emissions.

During the last 50 years, the design of DI engines has undergone a sea change because of social and economic aspects [5]. With the advent of new emission norms, reduction in ignition delay held the key to solve twin problems of NO<sub>x</sub> emission and noise. The higher temperature at the beginning of injection by increased compression ratio reduced the delay period and subsequent premixed combustion phase substantially. Higher injection pressures and turbulence were introduced to improve the mixing rate and hence to maintain the combustion duration within a reasonable limit, in spite of the loss of the fast-burning premixed combustion process. User demands of improving fuel economy and legal requirement of reduction in emissions are driving the engine development persistently. The advancements in the design are summarized in Table 1.1.

**Fig. 1.1** Combustion in DI diesel engine



**Table 1.1** Advancements in DI diesel engines

Period	Advancements	Events
The early 1970s	The main problems were the life of an engine and visible smoke	Improve design engine components, avoid secondary injection
The late 1970s to early 1980s	Improve fuel economy	Improved design of the combustion chamber, valve train
The mid-1980s to early 1990s	Reduction in noise Reduction in NO <sub>x</sub> , HC, CO	Improved compression ratios Very low nozzle sac volumes or valve-closed orifice (VCO) nozzles Increase injection pressure capability even more, especially at a lower speed Increase injection timing flexibility
1990–2000	Reduction in particulate Improving power packing	Turbo-charging, electronic control of injection rate, injection timing
2000–2006	Stricter emission laws, rapid escalation, and shortages of fuel	Heavy boosting and inter-cooling, higher injection pressure, oxygenated fuels

The DI diesel engines are regulated by government laws for gaseous emissions like HC, CO, and NO<sub>x</sub> as well as for solid emissions known as particulate matter and smoke. In diesel engines, both HC and CO emissions are a small fraction of those found in a gasoline engine. Even engine-out NO<sub>x</sub> emissions in a diesel engine are less than their corresponding gasoline emissions. However, modern gasoline engines operate at a stoichiometric ratio where the three-way catalyst performs at its highest conversion efficiency resulting in extremely low HC, CO, and NO<sub>x</sub> emissions. Unfortunately, diesel exhaust is very lean, and reducing NO<sub>x</sub> in an oxygen-rich environment is a very challenging task. The catalyst industry is developing solutions like DeNO<sub>x</sub> catalyst or selective catalytic reduction (SCR) for the diesel NO<sub>x</sub> problem. Another problematic pollutant associated with diesel engines is particulate matter. The casual observer is made aware of this pollutant in the form of black smoke or soot emitted from either the tailpipes of many diesel-equipped passenger cars or the stacks of diesel-powered heavy-duty vehicles. Emission of soot is also accompanied by other matter suspended in the exhaust, such as unburned lube oil, unburned fuel, trace metals, and sulphur by-products. Emission of soot in particulate matter results from the nature of the heterogeneous combustion process or diffusion-type combustion that is prevalent in diesel engines. The preparation of fuel and air mixture in modern diesel engines has greatly reduced this problem. The development of diesel particulate filters promises to eliminate it.

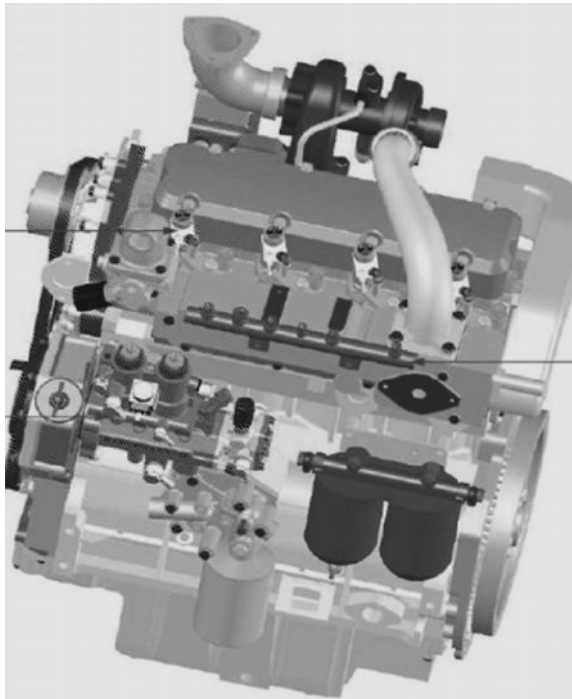
There are several serious reasons for considering biofuels like vegetable oil-based biodiesel, alcohols, as alternatives for petroleum-based diesel fuel, e.g. expected

growth of prices of fossil liquid fuels soon and gradual exhaustion of crude oil sources in the next 80–100 years. Governments of many countries have started thinking that biofuels will provide a boost to the agricultural industry. Also, oxygenated fuels have attracted increasing attention in engine development owing to their excellent combustion characteristics in reducing emissions [6, 7]. Therefore, oxygenated fuels would find a way as a supplement and substitute for diesel fuels for regular usage.

Heavy turbocharging along with inter-cooling, higher injection pressures with finer sprays, flexible injection timing, exhaust gas recirculation, and electronic control unit are the main features of modern DI diesel engines. The modern DI diesel engines are compact, smooth, reliable, and sturdy as shown in Fig. 1.2. To accomplish improved air–fuel mixing, reduced premixed phase of combustion, and minimize the tail in the heat release diagram modern DI diesel engine employ:

- Higher compression ratios
- Turbocharging and inter-cooling
- Down-sizing and up-rating
- Smaller fuel orifice sizes and sac volume
- Oxygenated fuels.

**Fig. 1.2** Modern DI diesel engine



## Modelling of Combustion in DI Diesel Engines

The complex task of improving IC engines, which have reached a higher degree of sophistication, can be achieved by a combination of advanced experiments and computational studies. Despite the quantitative uncertainties of numerical simulations, which are often greater than those of experiments, the modelling of combustion engine processes has some significant advantages that make its utilization in engine development a necessity. In this regard, it is obvious that numerical simulations are especially suited to carry out extensive parametric studies since they are more effective than the alternative construction and investigation of numerous prototypes [8].

The advantages of engine modelling are: (a) parametric studies of each variable can be done, (b) a wide range of boundary conditions can be analysed, (c) separation of each sub-process from other, (d) detailed information is available as output, and (e) effective in terms of time and cost.

Depending on the various possible applications, different types of models for engine combustion processes have been developed. Three different model categories are typically distinguished. In an order of increasing complexity and increasing requirements of computing power, these are zero-dimensional thermodynamic models, quasi-dimensional phenomenological models, and multi-dimensional computational fluid dynamics (CFD) models.

In thermodynamic models, the heat released by combustion cannot be easily derived by detailed modelling of physical and chemical sub-processes, because these processes are strongly affected by the distribution of unresolved spatial temperature and composition. Because the combustion chamber is taken as zero-dimensional, it is mandatory to model the heat release rate by empirical sub-models using simple mathematical equations. On the other hand, the multi-dimensional CFD models are based on the locally resolved solution of conservation of mass, energy, momentum, and include detailed sub-models for spray and combustion phenomena. With these models, the gas flow patterns can be predicted best and the prediction of fuel spray is less complete, and combustion calculations present considerable difficulties. The CFD models are of immense use to appreciate the inner mechanism of diesel sprays but are very difficult to comprehend during the complete simulation of a diesel engine. Therefore, there is a need for a third category of the model that allows executing efficient, fast, and economic preliminary calculations of heat release models and exhaust emissions as a function of important engine parameters like injection pressure, injection timing, swirl ratio, and boost pressure. These models based on physical and chemical sub-models, for local processes like spray formation, air–fuel mixing, ignition, and combustion including emission formation are termed phenomenological models. These models are more comprehensive compared to thermodynamic models and consume less computational resources compared to CFD models. It should be noted that phenomenological models are the most practical to describe diesel engine combustion [8]. 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. Therefore, these models are widely used as predictive tools for carrying out parametric studies during engine development.

Many experimental investigations are also being carried out to provide a better insight into the combustion process happening under the engine environment. More recently, the development of laser-based diagnostics has provided a means for making detailed in situ measurements of the processes occurring inside a reacting diesel fuel jet. These diagnostics allow specific species within the reacting jet to be measured at multiple points simultaneously with high spatial and temporal resolution.

Even though the IC engine was invented a century ago, its development is continuing, as new technology is available and new demands are arising. Although the DI diesel engine is a better choice among different types of IC engines as a prime mover considering fuel economy and exhaust emissions, efforts are being put to improve them further to meet future stringent demands of fuel economy and pollution. Alternative technologies and fuels are being implemented in these engines. Therefore, theoretical and applied understanding of the engine processes is also developing at a faster rate.

## References

1. Walsh MP (2000) Global trends in motor vehicle pollution control, accomplishments to date and challenges for new millennium. Paper No. F2000PH02, Proceedings of FISITA-2000, Seoul, Korea
2. Fiaz A, Sturm PJ (2000) New directions, road traffic in developing countries. *J Atmos Environ* 34:4745–4746
3. Krieger K, Hummel HG, Naik LM (2000) Diesel fuel injection technology: an essential contribution towards an environment-friendly powerful diesel engine. SAE 2000-01-1429
4. Heywood JB (1988) A textbook on internal combustion engine fundamentals. McGraw-Hill International edition
5. Bosch Automotive Handbook (2000) Bosch, 5th edn
6. Miyamoto N, Ogawa H, Nurun NM, Obata K, Arimes T (1998) Smokeless, low NO<sub>x</sub>, high thermal efficiency, and low noise diesel combustion with oxygenated agents as the main fuel. SAE 980506
7. Xiao Z, Ladommatos N, Zhao H (2000) The effect of aromatic hydrocarbon and oxygenates on diesel engine emissions. *IMechE* 214, Part D
8. Stiesch G (2003) Modelling engine spray and combustion processes. Springer

# Chapter 2

## Phenomenology of Diesel Combustion and Modelling



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

The combustion in modern DI diesel engines is mainly divided into two phases (a) a small ignition delay event in which preflame activities take place followed by (b) the main heat release event in which actual combustion happens. These events are modelled differently considering the prominent role of chemical kinetics during ignition and physical mixing rate during heat release. This approach is described in detail in the following sections. This chapter summarizes different types of models along with a 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 a high compression ratio and highly retarded injection timing enabling a substantial reduction in noise,  $\text{NO}_x$ , 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. In 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  $\text{NO}_x$ . 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 atomization, vaporization, and mixing of air–fuel occur and (b) chemical delay attributed to precombustion 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 commensurate with the large ignition delay [35]. Reduction in ignition delay held the key to solving emission and noise problems. The 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 [54] developed the earliest correlation for predicting ignition delay. The equation was in the form of an Arrhenius expression representing a single-stage reaction. Kadota et al. [29] related results of combustion bomb experiments to an Arrhenius-type expression by introducing dependence of equivalence ratio. Lahiri et al. [34] 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 [21, 53]. 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. [4] 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 the overall equivalence ratio makes the correlation more dynamic.

The time taken for the visible fire to appear in the premixed zone of spray is a strong function of pressure and temperature of the ambient. Also, the physical properties such as Cetane number, the viscosity of fuel, nozzle hole size, injected quantity, and injection pressure contribute to the delay phenomenon in diesel engines [11].

## ***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 temperatures after compression. The variety of combustion chambers and types of fuel injection equipment influence the heat release rate characteristically.

### Models Based on Fluid Dynamics

These types of models are often called multi-dimensional 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 a simplified model for predicting combustion, which is mixing controlled and kinetically controlled [33]. 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 [6, 19, 40] described 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. Also, their sub-models require a thorough validation with detailed experiments before employing them confidently in engine design work [13, 14, 49].

### Phenomenological Models

In these types of models, details of different phenomenon happening during combustion are added to the basic equation of energy conservation. In the simplest approach, Rife and Heywood [45] 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. [46], Dent and Mehta [16] and Hiroyasu et al. [24] 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 the high shear velocity of the jet as shown in 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

