Chapter 2
Modelling Aspects for Adaptation of Alternative Fuels in IC Engines

Hardikk Valera, Dhananjay Kumar, Akhilendra Pratap Singh and Avinash Kumar Agarwal

Abstract Deteriorating environment and stricter emission norms are motivating researchers for finding sustainable transport solutions. Researchers are focusing on two approaches namely adaptation of alternative fuels, and exhaust gas after-treatment. Utilization of alternate fuels such as methanol, ethanol, and biodiesel etc. in internal combustion (IC) engines reduces inherent chemical components present in conventional fossil fuels. These chemical species are a major source of harmful pollutants such as particulate matter (PM), polycyclic aromatic hydrocarbons (PAHs), PM bound trace metals, etc. Advancement in after-treatment technologies such as optimization of hexagonal cells of substrate, use of noble metals, etc. are also effective in reducing pollutants from engine tail-pipe. However, developments for adaptation of these technologies in existing engines is a challenging task. For adaptation of any alternative fuel, engine components need to be modified according to fuel properties. However, optimization of design parameters of thousands of engine components is a tedious task, which cannot be done experimentally. This can be done easily using modelling techniques, in which a prototype engine can be developed to investigate the effect of engine design parameters and fuel properties on the engine performance and emission characteristics. In last few years, 1-D and 3-D simulation tools have been extensively explored for engine design and performance optimization. This chapter discusses basic modelling techniques, which can be used for engine research. This chapter also presents heat transfer models, which are important for in-cylinder combustion analysis. Few fluid-flow models have also been discussed in this chapter, which are mainly used for in-cylinder air-flow investigations, fuel flow in the fuel injection system, etc. Overall, this chapter discusses modelling aspects related to engine design so that alternative fuels can be adapted.

Keywords Transportation sector · Engines · Modelling · 1-D modelling · 3-D modelling

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2.1 Introduction

Internal combustion (IC) engines are primary choice for transport sector due to their proven durability, reliability, cost, and user friendliness. Now-a-days, new technologies such as electric vehicles (EVs), hybrid vehicles, etc. have been introduced in transport sector, however, these vehicles have certain limitations such as cost, complexity, limited range, etc. Therefore, IC engines still are the main choice in the transport sector. Since last few decades, IC engines are facing bad press because of energy security and environmental issues. To resolve these issues, IC engines have changed remarkably due to advancement in engine technologies, introduction of new fuels and development of emission compliance technologies. Development of oxidation catalysts for SI engines reduced carbon monoxide (CO) emission significantly. Introduction of three-way catalytic (TWC) converter reduced the toxic exhaust gases hydrocarbons (HC), oxides of nitrogen (NO_X), and CO emissions. However, these interventions are not enough for meeting upcoming emission norms.

Rapidly depleting fossil fuels and continuously increasing demand for these fossil fuels are the other challenges. International Energy Agency (IEA) reported that demand for petroleum may increase by 20% by 2035 compared to 2010 (Statistics by International Energy Agency 2018). In such a critical situation, automotive industry is desperately looking for alternative energy sources, which would improve ambient air quality, reduce greenhouse gas (GHG) emissions and contribute to national energy security (Knothe 2010; https://www.e-education.psu.edu/egee439/node/684; Agarwal 1998; Agarwal and Das 2001; Urja 2013). Therefore, researchers are exploring sustainable alternative fuels, which can be utilized in new engines as well as existing engines. Design of existing engines is the main constraint for adaption of alternative fuels because current engines are designed to operate on conventional fuels, which have fuel properties quite different from the alternate fuels. Therefore, 100% replacement of fossil fuels with alternate fuels is very challenging. In such a scenario, it is important to modify the design of engine component so that engines fuelled by alternative fuels can be operated efficiently and in an eco-friendly manner. These engine modifications are tedious tasks because an engine consists of hundreds of components. Modelling and simulation techniques make this task relatively easier compared to experimental techniques. Modelling is generally regarded as the process of describing the physical phenomena in a particular model with the help of mathematical equations and solution of these equations predicts the effects of new fuel, without actually performing any engine experiment. Using these techniques, initial effects of alternative fuels on engine performance and emissions can be predicted by making the computational models of the physical process involved in the engine using different simulation tools. Using sophisticated modelling techniques, more extensive analysis is also possible, which helps in understanding various phenomenons such as fuel-air chemical kinetics, fuel sprays, in-cylinder combustion, etc.

In last few decades, engine modelling efforts have primarily concentrated on engine performance improvements and reduction of emissions. There are numerous modelling studies available in open literature, which show the potential of modelling and simulations in the domain of IC engine research. Initially, researchers used these techniques for preliminary research studies however now-a-days, these techniques are used for solving complex engine problems, which are not solvable by experiments. Some features of modelling techniques are given below:

- Opens the door for exploring solutions, which never appeared in reality.
- Provides opportunity to generate new ideas and takes innovative decisions based on prepared models.
- Helps to understand the effects of proposed solution on each engine parts such as on the piston, cylinder, fuel injection equipment, muffler, etc.
- Provides comparison among different possible solutions using graphics/animations.
- Allows to perform tests on physical models without preparing expensive and complex engine test cells.
- Perform experiments without harming the person or the ambient environment.
- Modelling can show simultaneous effects of new design of different engine parts.

Basic procedure for engine modelling to study the effects of alternative fuels in an IC engine is given below:

Step 1: Conduct the engine experiments using baseline fuel and collect engine performance and emissions data at selected operating conditions.
Step 2: Prepare an engine model in 1-D/3-D simulation softwares and compute the engine performance and emissions data at tested conditions.
Step 3: Validate the computational model using the experimental data. Use calibration procedures, if required.
Step 4: Replace baseline fuel with alternative fuel in the validated engine model to compute the results.
Step 5: Analyse the effects of alternative fuels on engine performance and emissions.

Due to extensive research in IC engines, several commercial simulation softwares such as GT-Power, Converge, and KIVA, etc. are available, which are especially designed for solving problems related to IC engines, combustion and fluid flow. These softwares have a number of modules, which can solve complex problems of IC engines using governing mathematical equations (https://www.gtisoft.com/gt-suite-applications/propulsion-systems/gt-power-engine-simulation-software/, https://convergecfd.com/, https://www.mechanicalbooster.com/2017/10/spark-ignition-engine.html). Currently 1-D and 3-D modelling softwares are the most used simulation tools in the domain of IC engines. 1-D Modelling is used to simulate complex behaviour of entire engine systems as a whole, such as fuel injection system, gas exchange system, turbocharger, etc. On the other hand, 3-D Modelling focuses on a single component of the system (such as cylinder, injector, etc.) without considering their dynamic interaction with other components.

This chapter is based on these two modelling techniques with greater emphasis on 1-D modelling. This chapter includes general description of these modelling techniques and covers different modelling aspects of the IC engines. Thrust is given on modelling of essential components such as injectors, cylinders, valves, etc. using 1-D modelling. Required comprehensive details for each component has also been discussed. Attention is given to the heat transfer model since it calculates how the heat will transferred to the combustion chamber walls. In the last section, a 1-D model using GT-Power software is demonstrated.

2.2 General Architecture of IC Engines

There are two types of engines used in transportation sector. First type is spark ignition (SI) engines, operating on Otto cycle using a spark plug as an ignition source. SI engines use either carburetor or port fuel injectors for supplying the fuel in the engine intake manifold. Second type is compression ignition (CI) engines in which the engines, operating on diesel cycle and ignition is initiated by high-pressure and temperature generated during the compression stroke. In CI engines, fuel injectors are used to inject fuel directly into combustion chamber. During combustion, chemical energy of fuel is released and transferred as mechanical work to the piston, through which power comes as an output to move the wheels. Fuel supply system is the most important part of an engine, which supplies the required amount of fuel at a certain point of time in each engine cycle.

2.2.1 SI Engine

SI engines require an ignition source such as spark plug, which creates the spark inside the combustion chamber (https://www.mechanicalbooster.com/2017/10/spark-ignition-engine.html). Spark engines use gasoline like fuels (high octane fuels). Working of a typical SI engine is summarized below:

(i) Suction stroke: Air-fuel mixture enters the cylinder.
(ii) Compression stroke: Air-fuel mixture get compressed, resulting in high pressure and temperature.
(iii) Power stroke: Power generation due to combustion of fuel-air mixture.
(iv) Exhaust stroke: Burnt gases evacuate out of the engine.

Generally the fuel is injected via carburetor during the suction stroke, and is shown in Fig. 2.1.

Some essential features of the SI engines are mentioned below:

- The compression ratio of the engine is between 6 and 10.
- Lightweight makes these engines suitable for light-duty applications such as motorcycles and lawnmovers.

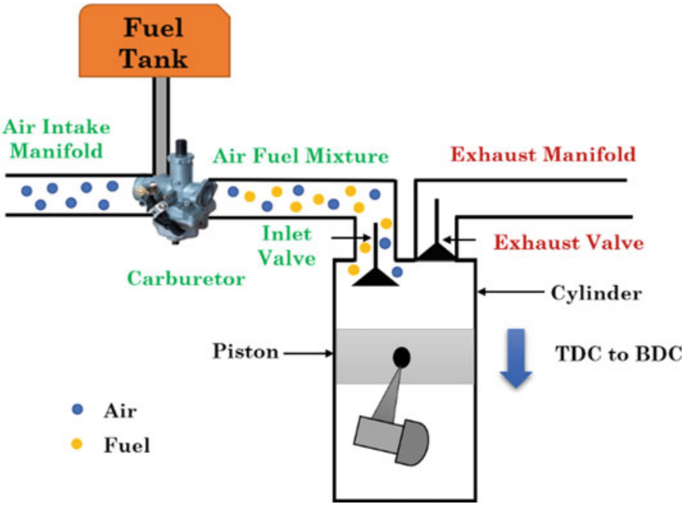


Fig. 2.1 Schematic of a SI engine system

- Higher maximum engine speed can be achieved due to their lightweight construction.
- Fuels having high self-ignition temperature (high octane fuels) are suitable for SI engines.

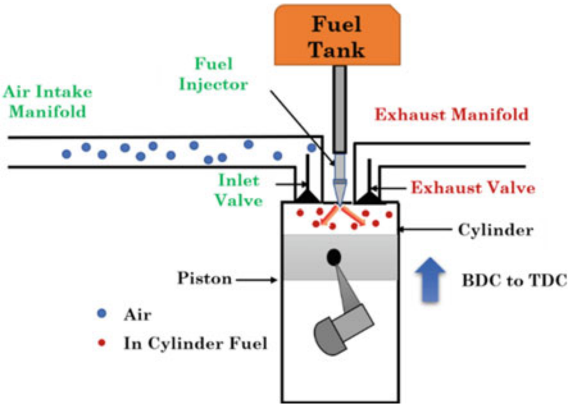
2.2.2 CI Engine

In CI engines, fuel is ignited due to its injection in the heated and pressurised air at the end of the compression stroke (https://www.howacarworks.com/basics/how-a-diesel-engine-works). In CI engines, diesel like fuels with high cetane numbers are preferred due to their low knock tendency. General working of diesel engines is given below:

(i) Suction stroke: Air enters into the cylinder.
(ii) Compression stroke: Air is compressed, and fuel is directly injected into the cylinder in high temperature and pressure air at the end of the compression stroke.
(iii) Power stroke: Power generation due to combustion of fuel-air mixture.
(iv) Exhaust stroke: Piston pushes the burnt gases out of the engine cylinder.

Generally fuel is injected directly into the combustion chamber through an injector at the end of the compression stroke (Fig. 2.2). Other features of the CI engines are given below:

Fig. 2.2 Schematic of a CI engine system



- Compression ratio of the engine is between 14 and 22.
- Heavyweight due to high injection pressure makes it suitable for heavy-duty applications such as buses, trucks and tractors.
- Relatively low engine speeds are preferred due to its heavy-weight construction.
- Fuel having low self-ignition temperature are desirable.

In the next section, modelling of different engine sub-systems are discussed.

2.3 Modelling of IC Engines

The engine consists a large number of components such as fuel injector, cylinder, cranktrain, valves, etc. Each part affects the performance and emission characteristics of the engine. Therefore it is very important to model each part carefully for simulating the engine experiments. Simulation softwares require a set of minimum information about each part before starting the modelling. Next sub-section discusses required critical information about the engine components and explains the modelling aspects of these components.

2.3.1 Fuel Injector

Fuel injector is used to deliver the fuel into the port or into the engine cylinder for powering the engine. Injector contains one needle, which acts as a valve to open or close the injector passage hole through which fuels comes out at certain fuel injection pressure (FIP). Injector nozzle performs two important functions namely fuel atomization and fuel distribution inside the combustion chamber. Fuel distribution is also affected by several other parameters such as FIP, ambient air density at the time of fuel injection, and physical properties of the fuel. High FIP leads to improved fuel atomization and fuel spray penetration however, high air density inside the combustion chamber results in superior dispersion of fuel. Fuel properties such as vapour pressure, viscosity, and self-ignition temperature also play a vital role in fuel spray characteristics. In a pressure-activated injector, one end is exposed to the fuel pressure, and the another end is exposed to preloaded spring. Needle is in closed condition, when spring force is greater than the fuel pressure. Fuel pump is connected to injectors via a high pressure pipe. Fuel injection starts with upward movement of needle from the needle seat, until the fuel pressure is sufficient to overcome the spring force. In a pneumatically-activated injector, one end is exposed to the fuel pressure, and the other end is connected to the needle. Opening and closing of the needle can be done by changing the hydraulic pressure. Injector modelling requires some essential inputs, as shown in Table 2.1.

2.3.2 Cylinder

Cylinder is the most critical part of engine, which can be sleeved and sleeveless. Sleeved cylinders are lined with a harder metal compared to block metal, and sleeveless cylinders are coated with wear resistant materials. A cylinder's displacement is calculated by multiplying its cross-sectional area and stroke length. Multi-cylinders

Table 2.1 Required inputs for injector modelling

Parameter	Description
Start of injection (SoI)	Time at which fuel injection starts. Usually expressed as crank angle degree (CAD) relative to TDC
End of injection (EoI)	Time at which fuel injection stops. Usually expressed as CAD relative to TDC
Injected fuel mass	Mass of fuel injected into the cylinder. Usually expressed in terms of mg/stroke or mg/cycle
Injection duration	Time period during which fuel is injected into the combustion chamber. Injection duration can be expressed as time difference between EoI and SoI
Injection profile	Fuel injection rate, which can be expressed as injection shape such as boot, ramp, square etc.
Nozzle discharge coefficient	It is a correction factor used to define the actual mass injected into the cylinder
Number of holes	Number of holes available at the nozzle tip
Type of fluid	Diesel, gasoline, methanol, ethanol, etc.
Injected fuel temperature	Temperature of fuel at the time of injection
Nozzle/atomizer hole diameter	Individual nozzle hole diameter
Injector location	In case of port injection, it is the distance between injector and the intake valve/port

displacement is calculated by following the above mentioned procedure and further multiplying with the number of cylinders. Modelling of cylinders is quite complex because it involves the simultaneous motion of several components. Generally, three combustion models are used for cylinder modelling (Hariram and Bharathwaaj 2016).

(i) Zero-dimensional model
(ii) Quasi-dimensional model
(iii) Multi-dimensional model

Zero-dimensional models are the most suitable and simple models for understanding the effects of engine operating parameters on overall heat release rates and in-cylinder pressure. These models use various assumptions and simplifications and do not consider complex flow-field dimensions. Zero-dimensional model is an open system, which generally evaluates the instantaneous in-cylinder combustion characteristics such as pressure, temperature, heat release rate, etc. by utilizing mass and energy conservation equations (Payri et al. 2011). Single composition of the cylinder contents and uniform state is assumed throughout the control volume, which leads to limitation in terms of emission predictions. Overall, this is a good tool for predicting combustion parameters for different engines and operating conditions (Payri et al. 2011). Due to complications of the engine, various input constraints such as injection timing/spark timing, EGR, etc., can not be incorporated in this model, leading to inaccurate predictions. Zero-dimensional models are further classified into single-zone models, two-zone models and multi-zone models (Neshat et al. 2017). Single zone models are the ones, in which working fluid is considered as one thermodynamic system, and energy released from the fuel combustion is calculated by using first law of thermodynamics applied to the system. In two-zone models, the working fluid is considered in two zones, namely burned zone and unburned zone (Fig. 2.3). These zones act like two different thermodynamic systems with energy and mass interactions having common surrounding of cylinder walls. However, two-zone models have several assumptions as mentioned below.

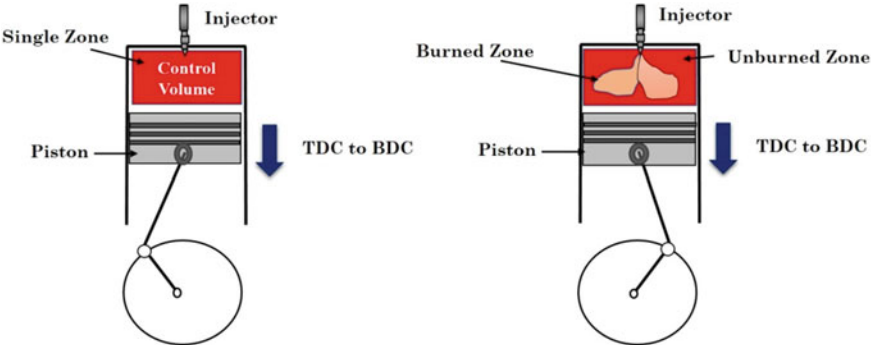


Fig. 2.3 Burned and unburned zones in the engine cylinder

- The burned and unburned zones are modelled as ideal gases with different physical properties.
- Unburned zone is modelled as a premixed fuel-air mixture. Therefore it is more accurate/realistic to model SI engine combustion rather than CI combustion.
- Characteristic gas constants for both zones do not vary with temperature and pressure in the modelling. If it varies up to certain extent, then it is modelled using explicit relationship between gas constant and involved gas properties (T, P, etc.)
- Heat does not transfer from burned to unburned zone and vice versa in modelling.
- Enthalpy of fuel is ignored during modelling, since it is not significant.
- Crevice losses are not considered.
- Instantaneous pressure in both zones is considered to be the same.

Based on the assumptions as mentioned earlier, combustion is modelled in the following manner using two different equations.

1. Cylinder acts like two divided chambers namely burned zone and unburned zone. It also contains residual gases from the previous cycle (https://www.gtisoft.com).
2. As combustion progresses, air-fuel mixture is transferred from the unburned zone to the burned zone. Rate of transfer of air-fuel mixture from unburned zone to burned zone is considered as 'burn rate', which is an important parameter for modelling.
3. Chemical equilibrium calculations start once air-fuel mixture transfers from the unburned zone to the burned zone and calculate thirteen combustion product species, i.e., H_2O, CO_2, N, O, H, CO, H_2, OH, NO, SO_2, Air, N_2, O_2.

Governing Equation for Unburned Zone (https://www.gtisoft.com):

$$\frac{d(m_{ub}e_{ub})}{dt} = -p\frac{dV_{ub}}{dt} - Q_{ub} + \left(\frac{dm_f}{dt}h_f + \frac{dm_a}{dt}h_a\right) + \frac{dm_{fi}}{dt}h_{fi} \tag{2.1}$$

where,
m_{ub} = Mass of the unburned zone, v_{ub} = Volume of zone
m_f = Mass of fuel, Q_{ub} = Heat transfer rate in unburned zone
m_{fi} = Mass of injected fuel, h_a = Enthalpy of air mass
m_a = Mass of air, h_f = Enthalpy of fuel mass
e_{ub} = Unburned zone energy, h_{fi} = Enthalpy of injected fuel mass
m_a = Mass of air, h_f = Enthalpy of fuel mass
e_{ub} = Unburned zone energy, h_{fi} = Enthalpy of injected fuel mass
p = Cylinder Pressure

ub denotes the unburned zone.

Governing Equation for Burned Zone (https://www.gtisoft.com):

$$\frac{d(m_b e_b)}{dt} = -p\frac{dV_b}{dt} - Q_b + \left(\frac{dm_f}{dt}h_f + \frac{dm_a}{dt}h_a\right) \tag{2.2}$$

where b denotes the burned zone, and remaining symbols are similar to that of unburned zone.

Multi-zone models give results closer to reality since it considers the energy and mass balance between the two zones. However for modeling, some additional parameters are required as shown in Table 2.2.

2.3.3 Heat Transfer Models

There are various heat transfer models used for 1-D modelling. In GT Power, WoschniGT model is used for calculating the heat transfer coefficients if measured swirl data is not available. This model uses following equation for calculating the heat transfer coefficient (Heywood 1988).

$$h_c = \frac{3.01426 p^{0.8} w^{0.8}}{D^{0.2} T^{0.50}} \tag{2.3}$$

Table 2.2 Required input parameters for cylinder modeling

Parameter	Description
Fluid initial state	Initial condition of the cylinder
Wall temperature	Initial temperature of cylinder before starting of combustion
Heat transfer model	There are some models, which are used to calculate the heat transfer coefficients such as WoschniGT, WoschniClassic, WoschniSwirl, WoschniHuber and Hohenberg. These models use different coefficients to calculate heat transfer in the cylinder
Flow object	Comprehensive data of piston geometry is used for calculating the inside flow behavior
Combustion object	Object which gives fuel burn rate profile as input
Head initial temperature	Initial temperature of head mass, which are in contact with the combustion gases
Piston initial temperature	Initial temperature of entire piston including piston rings
Cylinder initial temperature	Initial temperature of the cylinder liner
Inlet valve initial temperature	Initial temperature of an inlet valve including associated valve guides
Exhaust valve initial temperature	Initial temperature of an exhaust valve including associated valve guides
Cylinder coolant temperature	Temperature of the coolant, which flows on the back-side of the cylinder walls
Head oil temperature	Temperature of the lubricating oil, which flows over the head surface
Head oil heat transfer coefficient	Heat transfer coefficient of the oil, which flows over the head surface

The WoschniClassic model calculates the heat transfer coefficient without considering the effect of swirl and uses the following equation for calculating the heat transfer coefficient (Heywood 1988).

$$h_c = \frac{3.26p^{0.8}w^{0.8}}{D^{0.2}T^{0.53}} \tag{2.4}$$

where,
h_c = Convective heat transfer coefficient (WK/m^2)
D = Cylinder bore (m)
p = Cylinder pressure (kPa)
T = Cylinder temperature (K)
W = Average cylinder gas velocity (m/s)

WoschniSwirl and WoschniHuber model uses the same equation as used by WoschniClassic model, but these models utilize swirl number from the center region.

2.3.4 Engine Crank-Train

Crank-train translates the reciprocating motion of the pistons into the rotary motion. This is comprised of three parts namely connecting rod, crankshaft and flywheel. Connecting rod is modeled as a simple beam, which connects the piston and the crankshaft via rotating bearing. Crankshaft drives the cooling system and valve train of the system.

It is a most stressed component of the system as it is subjected to the high tensile, bending and compressive stresses. Flywheel performs multiple functions in the engine. It adds additional inertia on the crankshaft to minimizes the cyclic variations produced by the reciprocating motion of the piston. Some additional parameters have to be defined for modelling the crank-train (Table 2.3).

2.3.5 Valves

Accuracy in valve modelling is very important because it affects the volumetric efficiency, engine noise, mechanical friction and pumping loss. Valve controls the inlet and outlet movements of charge and exhaust gases in the cylinders concerning different piston positions. Valves are located in the cylinder head on all the engines. The most popular shape of poppet-valve for automobile application is a small cup at one end of the stem. A valve stem is placed in a circular passage in the cylinder head. Valve disc head basically opens and closes the ported passage during the in and out movement of the stem. However, some additional parameters have to be defined for modelling the valvestrain as shown in Table 2.4.

2.3.6 Orifice Connection

Orifice connections is used to measure the flow rate of fuel or exhaust gas, which mainly work on the differential pressure measurement principle. This connection is used at the location, where flow-rate measurements are required. The orifice connection offers the following advantages.

- It measures a wide range of flow rates in a pipe.
- Most suitable for measuring the fuel and exhaust flow rates.
- Offers very small amount of pressure drops across the sides of orifice plates.

For modeling, some additional parameters are required as given in Table 2.5.

2.4 Model Demonstration

This section describes the simple model preparation using commercialized 1-D software GT-Power. GT-SUITE have a comprehensive set of automotive components in their libraries, which are used to simulate the physics of fluid flow, thermal,

Table 2.3 Required input for crank-train modelling

Parameter	Description
Engine type	2-stroke; 4-stroke
Speed or load specifications	It depends on the study objective of the model. Either it is for different speeds or percentage of total load
Start of cycle (CA at IVC)	It is a value after the closing of the inlet valve and before the start of combustion
Cylinder geometry	It is a detailed geometry of the cylinder such as bore, stroke and compression ratio
Firing order	This value is necessary during the modelling of multi-cylinder engine
Cylinder number	It shows the sequence of cylinder firing
Firing intervals	It is an angle of the firing relative to the preceding cylinder
Geometry of connecting rod	All dimensions are required such as big end bore, main rod length and connecting rod length

Table 2.4 Required inputs for valves

Parameter	Description
Cam timing angle	Angle between the cam timing anchor reference and cam timing lift array
Valve lift	Distance through which valve is opened maximum from its seated position
Valve lash	Clearance between valve and camshaft

Table 2.5 Modelling of orifice connections

Parameter	Description
Hole diameter	Diameter of the orifice
Geometric area	Total area of the orifice
Forward discharge coefficient	Discharge coefficient of the orifice in the forward direction
Reverse discharge coefficient	Discharge coefficient of the orifice in the reverse direction

mechanical, electrical, magnetic properties of materials and controls (https://www.gtisoft.com/). These libraries are used to build accurate models of entire vehicle, engine, driveline, transmission, general powertrain, mechanical systems, hydraulics, lubrication, friction, thermal management, cooling, chemistry, after treatment and much more (https://www.gtisoft.com/). GT-SUITE provides 1-D modeling solutions for real-time, HiL/SiL, and control system simulations. Also, a broad array of built-in advanced features such as design of experiments (DoE), optimization. In addition, distributed and parallel processing enhance user productivity and effectiveness. The software is designed around a series of icons and connectors that define each engine components and a logical interface for their use (Kmec et al. 2009). There are two main operating domains of this software called GT-ISE and GT-POST. GT-ISE provides an environment, where various components are taken out in project map to make the model, simulations setting are declared, simulations are launched in single or batch mode. 1-D model is then prepared using the following steps where dummy values are selected to present the demonstration model. Typical view of the model is shown in Fig. 2.4.

Step 1: Inlet end environment is selected from the template library and different boundary conditions such as pressure, temperature, humidity are defined in the inputs.

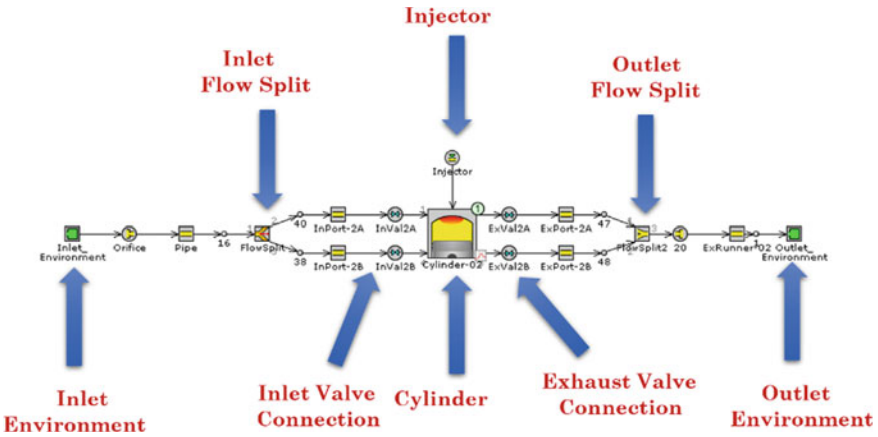
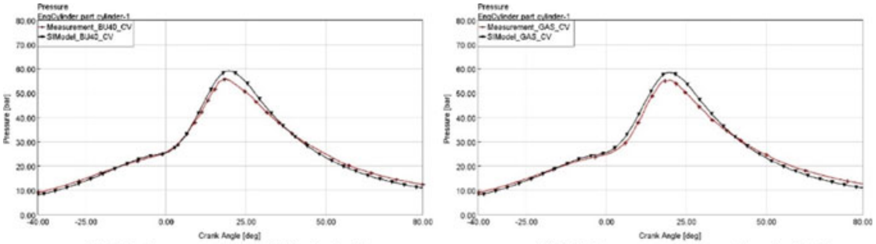


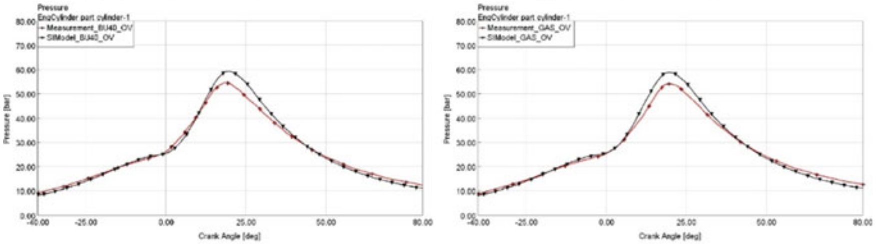
Fig. 2.4 Typical map view of the 1-D model of a single cylinder engine

Step 2: Pipe round object is selected to define a pipe connections, which are generally used in the air intake. Cross-section area is given as input.
Step 3: Bend pipe round is selected to define a bend pipe connections, where bend angle is given as input.
Step 4: Orifice is selected from the library to calculate the mass flow rate between the adjacent flow volumes, where orifice diameter and discharge coefficients are given as inputs.
Step 5: Cylinder is selected from the library to specify the attributes of the engine cylinder. Required inputs are given as mentioned in Table 2.2.
Step 6: Valve cam connections are selected to define characteristics of a cam-driven valve where essential inputs such as geometry, lift profile, and flow characteristics are defined.
Step 7: Engine crank-train is selected from the library to model the kinematics and rigid dynamics of a common reciprocating IC engine crank-train. Required inputs are given as mentioned in Table 2.3.
Step 8: Injector is selected to define the required parameters such as injection of a periodic mass flow rate or pressure profile of fuel.

Da Silva Trindade and dos Santos prepared 1-D model using GT-Power to validate the simulation results. Figure 2.5 (da Silva Trindade and dos Santos 2018) shows the in-cylinder pressure variations w.r.t. crank angle degree (CAD) position of an engine fuelled with BU40 (60% gasoline and 40% butanol on volume basis) and gasoline. Good correlation between experimental and computational results was reported (8% deviation between experimental and simulation results). The maximum value of



(a) Cylinder pressure in bar, BU40, closed valve. (b) Cylinder pressure in bar, gasoline, closed valve.



(c) Cylinder pressure in bar, BU40, open valve. (d) Cylinder pressure in bar, gasoline, open valve.

Fig. 2.5 In-cylinder pressure versus CAD for BU40 and gasoline (da Silva Trindade and dos Santos 2018) (experimental results: red lines and computational results: black lines) experimental results was slightly lower than simulation results because of pressure losses in the real engine.

Several other researchers performed comparative investigations of alternate fuels vis-à-vis baseline petroleum based fuels to investigate the effects on engine performance parameters. Table 2.6 shows the modelling results for performance and emissions of the engines fuelled with different alternative fuels. Preliminary results of modelling can be validated using experimental results and after the validation of model, more extensive investigations can be done using modelling and simulation tools, making the development process quicker and cheaper.

2.5 Conclusions

Modelling techniques help extensively in feasibility studies and preliminary investigations of new fuels in IC engines and these studies can be done without extensive engine experiments. This chapter presents a review of the requirements IC engine modelling. Suitability of methanol in CI engines is also discussed in this chapter briefly. Two main tools namely 1-D modelling and 3-D modelling are touched upon. 1-D modelling shows the effects of possible alternate fuels on engine performance and emissions however, 3-D modelling provides a platform for exploring the effect of alternate fuels on specific engine components. Using 3-D modelling, different components of the engine such as injector, cylinder head, etc. can be optimally designed to improve the engine performance and lower emissions. Finally, modelling in engine research can reduce the efforts required for adaptation of alternate fuels. These techniques help in preliminary investigations of performance and emissions studies of alternative fuels and play an important role in feasibility studies for new technology adaption.

Table 2.6 Typical results of 1-D simulation studies

Team	Aim	Procedure followed for modelling	Results
Chougule et al. (2013)	Determine the potential of dual fuel (CNG and Diesel) to improve the engine fuel economy	**Step 1**: Experiments were performed using diesel in a 4-cylinder, 2500 cc engine	Deviations between the experimental and simulation results were less than 10% and 5% for torque and BSFC respectively
		Step 2: Engine model was prepared using GT-Power	

(continued)

Table 2.6 (continued)

Team	Aim	Procedure followed for modelling	Results
		Step 3: Validation of simulation results using experimental results	
		Step 4: CNG was injected along with diesel in the validated engine model	BSFC increased by 13 and 9 for 50 and 70% load respectively using CNG as fuel
		Step 5: Results of engine performance were discussed	Fuel economy improved by 10% in a dual fuel engine, where diesel was injected as a pilot
Mtui (2013)	Determine the performance of dual fuel (Natural Gas/diesel) using 1-D/3-D simulations	**Step 1**: 1-D model of 18-cylinder engine was prepared using GT-Power	Natural gas can be used as a fuel for replacement of up to 60% baseline fuel
		Step 2: Prepared model was coupled with 3-D based KIVA software to provide accurate boundary conditions to the intake and exhaust valves during transients	Beyond 40% diesel replacement, engine power output decreased
Jadhav et al. (2017)	Determine the engine performance of dual fuel (Diesel-CNG) using GT Power	**Step 1**: Experiments on diesel fuel using 4-cylinder, 3000 cc engine	**Performance**: BSFC, and volumetric efficiency decreased by 8% and 5% respectively for dual fuel model compared to baseline fuel model **Emissions**: CO and HC emissions increased for dual fuel model, whereas PM emissions increased compared to baseline fuel model
		Step 2: Baseline 1-D model was prepared	
		Step 3: Simulation results were validated with the experimental results	
		Step 4: CNG was injected along with diesel in a validated baseline model (Port Injection)	

(continued)

Table 2.6 (continued)

Team	Aim	Procedure followed for modelling	Results
Soid et al. (2015)	Determine the performance of methane-fuelled engine	**Step 1**: Experiments on 4-stroke, single cylinder, 100 cc SI engine	Engine torque, BMEP, brake power, and peak cylinder pressure decreased for methane-fuelled model compared to gasoline-fuelled model Optimization was done using different inlet valve openings and outlet valve openings They retarded exhaust valve timing by 10° and found comparable results to gasoline-fuelled model
		Step 2: Baseline 1-D model was prepared using the engine data	
		Step 3: Simulation results were validated using calibration methods	
		Step 4: Methane was injected in a validated baseline model using port fuel injection method	

References

Statistics by International Energy Agency. https://www.iea.org/weo2018/

Knothe G (2010) Biodiesel and renewable diesel: a comparison. Prog Energy Combust Sci 36(3):364–373. https://doi.org/10.1016/j.pecs.2009.11.004

Web Source: https://www.e-education.psu.edu/egee439/node/684

Agarwal AK (1998) Vegetable oils versus diesel fuel: development and use of biodiesel in a compression ignition engine. Tide 8(3):191–204

Agarwal AK, Das LM (2001) Biodiesel development and characterization for use as a fuel in compression ignition engines. J Eng Gas Turbines Power 123(2):440–447. https://doi.org/10.1115/1.1364522

Urja A (2013) Ministry of New and Renewable Energy, Government of India, New Delhi, vol 7(1)

GT Power Software. https://www.gtisoft.com/gt-suite-applications/propulsion-systems/gt-power-engine-simulation-software/

Converge Software. https://convergecfd.com/

KIVA Software. https://en.wikipedia.org/wiki/KIVA_(software)

SI Engine. https://www.mechanicalbooster.com/2017/10/spark-ignition-engine.html

CI Engine. https://www.howacarworks.com/basics/how-a-diesel-engine-works

Hariram V, Bharathwaaj R (2016) Application of zero-dimensional thermodynamic model for predicting combustion parameters of CI engine fuelled with biodiesel-diesel blends. Alexandria Eng J 55(4):3345–3354. https://doi.org/10.1016/j.aej.2016.08.021

Payri F, Olmeda P, Martín J, García A (2011) A complete 0D thermodynamic predictive model for direct injection diesel engines. Appl Energy 88(12):4632–4641. https://doi.org/10.1016/j.apenergy.2011.06.005

Neshat E, Honnery D, Saray RK (2017) Multi-zone model for diesel engine simulation based on chemical kinetics mechanism. Appl Therm Eng 121:351–360. https://doi.org/10.1016/j.applthermaleng.2017.04.090

Engine Performance Manual. https://www.gtisoft.com

Heywood JB (1988) Internal combustion engine fundamentals

Gamma Technologies. The standard in multi-physics system. https://www.gtisoft.com/

Kmec JF, Kassebaum DA, Noerenberg RL (2009) First-time experience with engine simulation software in an internal combustion engines course. College of Technology, Purdue University, West Lafayette, IN, 47907

da Silva Trindade WR, dos Santos RG (2018) 1D modeling of SI engine using n-butanol as fuel: adjust of fuel properties and comparison between measurements and simulation. Energy Convers Manag 157:224–238. https://doi.org/10.1016/j.enconman.2017.12.003

Chougule VP, Vora KC, Suryavanshi Y (2013) Design and Simulation of 2.5 L Dual Fuel (Diesel-CNG) Engine for Performance Parameters (No. 2013-01-2885). SAE Technical Paper. https://doi.org/10.4271/2013-01-2885

Mtui PL (2013) Performance and emissions modeling of natural gas dual fuelling of large diesel engines. Int J Sci Technol Res 2(11):317–323

Jadhav AA, Hulwan DB (2017) Simulation of dual fuel (Diesel-CNG) engine of off road vehicle. Simulation 1(3)

Soid S, Amir S, Ismail M, Hamid M, Amzari M, Said M (2015). Simulation studies on the performance of small engine fuelled by methane and the effect of various valve timings. Indian J Sci Technol 8. https://doi.org/10.17485/ijst/2015/v8i30/87250