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Introduction

The internal combustion (IC) engine is a spectacular, complex device that has been an unqualified success. The IC engine is probably best known as the power plant for vehicles, but, of course, is also successfully used in a variety of other applications. These other applications include, for example, simple garden equipment, stationary electrical power generation, locomotives, and ships. A powerful approach to aid in the design and understanding of these engines is through the use of mathematical simulations.

Engine cycle simulations have been developed and used to study a variety of features and issues relative to IC engines since the 1960s. In the beginning, engine cycle simulations were fairly elementary, and were limited by both computing capabilities and a lack of knowledge concerning key sub-models. In time, these simulations have become more complete and more useful.

Today, engine cycle simulations are sophisticated, complex computer programs that provide both global engine performance parameters as well as detailed, time-resolved information. Many of these simulations contain advanced and detailed sub-models for the fluid mechanics, heat transfer, friction, combustion, and chemical kinetics. The most advanced simulations include calculations in three dimensions. Some of these simulations are grouped in the general category of computational fluid dynamics (CFD). Some comments on the early history (pre-1990) of the development of engine simulations may be found in References 1–3.

1.1 Reasons for Studying Engines

As mentioned above, IC engines have been an unqualified success in several major economic markets. Certainly, as the propulsion unit for light duty vehicles, the IC engine has been a significant accomplishment. The number of such vehicles and their engines is estimated at one billion throughout the world, and is expected to be about two billion by 2020. For a rather complex, major device, these are exceptional numbers. Other applications of IC engines include stationary power generation, marine propulsion, small utility, off-road, and agriculture.

The reasons for the success of the IC engine have been well documented (e.g., References 2, 4, and 5). These reasons include relatively low initial cost, high power density, reasonable

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driving range (say, more than 200 miles for a standard fuel tank size), able to refuel on the order of minutes at many locations, robust and versatile, reasonably efficient, able to meet regulated emission limits, and well matched to available fuels. This last item is particularly important and results in some of the other favorable features.

Liquid hydrocarbon fuels (such as gasoline and diesel) possess relatively high energy densities, are relatively safe and stable, and (currently) are widely available. In addition, these fuels possess excellent characteristics for combustion processes utilized by spark-ignited and compression-ignited engines.

Current (2015) engine technology spans a wide range from fairly basic to relatively advanced. Some engines are still based on the use of carburetors, mechanical valve trains, and large displacements. More advanced engine designs include direct fuel injection, variable valve timings, turbocharging, and the capability to deactivate some cylinders for part load operation. Most spark-ignition engines are designed for operation at or near stoichiometric with compression ratios less than about 11 (to avoid spark knock).

The demise of the IC engine is often a popular topic in the lay press due to the perception that it is based on "old" technology. Despite this perception, the IC engine remains a successful device. Alternative power plants for light-duty vehicles include electric motors operated with batteries or fuel cells. Some advances have been accomplished regarding these technologies, but these alternatives are still many years away from displacing the IC engine. Especially considering the long time frame for replacement of existing vehicles in the current fleet, IC engines are expected to be the dominant power plant for many decades into the future.

1.2 Engine Types and Operation

Several versions of the IC engine exist. The two major categories are spark-ignition engines and compression-ignition (diesel) engines. The spark-ignition engine is based largely on a (nearly) homogeneous mixture of fuel and air, and on a more-or-less organized flame propagation. To satisfy this type of ignition and combustion process, the fuel must vaporize relatively easily and resist autoignition. Fuels with these characteristics include gasoline, natural gas, propane, and alcohols. The spark-ignition engine is often restricted to moderate compression ratios to avoid spark knock. Almost all spark-ignition engines for today's light-duty vehicles operate with stoichiometric mixtures and utilize three-way catalyst systems to meet emission regulations.

The compression-ignition engine, on the other hand, is based on the injection of the fuel into a cylinder with air, and on the self-ignition of the fuel due to the temperature of the compressed air. For the compression-ignition engine, combustion occurs in various locations throughout the cylinder with no organized flame propagation. To satisfy this type of ignition and combustion process, the compression ignition engine must utilize a fuel that can readily self-ignite. This fuel is typically a diesel fuel, but jet fuel and other oils can be used. The compression-ignition engine generally requires a relatively high compression ratio to generate sufficiently high temperature air for the auto-ignition process. These engines typically must operate with excess air (fuel lean) to ensure all the fuel is burned. In many applications, the compression-ignition engine uses intake air compression (turbochargers and superchargers) to increase its power density.

Another important classification of engines is the number of strokes the engine uses per power event. The four-stroke cycle engine uses four (4) strokes (two revolutions) for each cycle, while the two-stroke cycle engine uses two (2) strokes (one revolution) for each cycle. Almost all engines for light-duty vehicles use four-stroke cycle engines. Utility engines and some engines for small scooters and motorcycles use two-stroke cycle engines. This book will consider only the four-stroke cycle engines.

The IC engine is not a heat engine,[1] and is more accurately described as a chemical conversion device. This means that the "Carnot limitation" is not applicable. In fact, the IC engine may potentially approach 100% efficiency and still be consistent with the first and second laws of thermodynamics [2, 6]. This book will provide quantitative information on this feature of IC engines.

The IC engine consists of a series of processes which include induction, compression, combustion, expansion and exhaust. Each of these processes (and their sub-processes) are subject to real effects (irreversibilities and energy losses) which prohibit the engine from achieving 100% efficiency. For example, heat transfer from the cylinder gases is an energy loss that reduces the maximum possible efficiency. The implications of minimizing heat losses for higher efficiency are described in subsequent parts of this book.

Another, more severe, limitation is the irreversibility associated with the combustion process. For an adiabatic conversion of chemical energy to thermal energy, energy losses can approach zero. But the second law of thermodynamics describes that this process is highly irreversible and results in lower grade energy, and a loss of the potential to produce work. This, then, is the key thermodynamic fact that limits IC engine efficiency (and not the "Carnot limitation").

1.3 Reasons for Cycle Simulations

The focus of this book is the development and use of zero-dimensional, thermodynamic engine simulations. The overall goal of such thermodynamic engine simulations is to mathematically simulate the significant processes, and to predict engine performance and engine operation details including certain emission parameters. Benefits of developing and using these engine simulations are multiple. Examples of these benefits are described next.

1.3.1 Educational Value

The development of engine cycle simulations forces engineers to understand the fundamentals of engine operation, and to recognize the complex interaction of the various processes. The engineers obtain a much deeper appreciation for the role of thermodynamics, fluid flow, heat transfer, and combustion on engine performance and emissions.

1.3.2 Guide Experimentation

Since experimentation is a highly intensive activity involving many people, facilities, and funds, methods to minimize unnecessary experiments and to more efficiently conduct the

[1] Further discussion of the "heat engine" concept relative to IC engines is provided in Section 19.2.

experiments are important. Although thermodynamic engine cycle simulations may never completely eliminate experimentation, such simulations do help guide experimentation. This is accomplished in a number of ways, but the main result is that less experimentation will be needed. By calibrating an engine cycle simulation, fairly detailed and reliable results may be obtained. The use of these types of simulations and careful, efficient experimentation are a highly effective and systematic way to develop engines, and engine concepts and technology.

1.3.3 Only Technique to Study Certain Variables

Certain variables are difficult to study experimentally either because access is difficult or the very act of measurement will change the variable's value. For example, the overall spatial-average gas temperature (particularly during combustion) is difficult if not impossible to obtain. The cylinder pressure, however, may be measured and with the proper algorithm, the average gas temperature may be obtained using this pressure. Another example is the completion of second law analyses which are dependent on detail thermodynamic parameters.[2]

1.3.4 Complete Extensive Parametric Studies

To complete cost-effective, extensive parametric studies, the use of thermodynamic simulations is a proper choice. Since multiple sets of engine operating conditions are of increasing interest, experimentation could be prohibitively expensive. As an alternative, thermodynamic simulations can be used in a cost-effective manner to examine extensive sets of parameters.

1.3.5 Opportunities for Optimization

The use of the cycle simulations is ideal for determining optimal combinations of engine parameters for a given set of operating variables such as load, speed, spark timing, equivalence ratio, and so forth. Either a simple manual search or a more complex algorithm can be used to find the optimum set of parameters for a given set of constraints.

1.3.6 Simulations for Real-time Control

Versions of engine cycle simulations may be used as algorithms for engine control. An advantage of this approach is that the engine control will be able to accommodate a much wider range of variables. The control algorithm can employ a degree of intelligence in selecting the combination of operating parameters to meet specific goals. In addition, the controls and diagnostics can be integrated into a single, common system.

[2] Some authors have reported experimentally based second law analyses, but in these cases the authors have used their experimental data as input to analyses which contain at least some of the portions of thermodynamic cycle simulations.

1.3.7 Summary

The above are examples of the motivations which drive the interest in cycle simulations. From a practical perspective, the use of engine cycle simulations offers shorter engine development times, reduces development costs, minimizes emissions, maximizes fuel efficiency and performance, and provides a data base for current and future development efforts.

The development of engine cycle simulations is a challenging task largely because the IC engine is a complex device. The characteristics of IC engines which contribute to this complexity include turbulent, unsteady flow, non-uniform mixture composition, highly exothermic chemical reactions, two or three phase compositions, and pollutant species (typically with low relative concentrations). In addition, the important time scales have a large dynamic range of between 1 μs and 1 s, and the important length scales range roughly between 1 μm and 1 m.

1.4 Brief Comments on the History of Simulations

Chapter 3 provides a detailed description of the evolution of engine cycle simulations, but for completeness, this introductory chapter will summarize this evolution (e.g., References 1–3.) From the beginning of reciprocating engine development, engineers and scientists have attempted to model the overall engine operation to help understand and improve the technology. The earliest such models were the ideal air standard cycles which were first presented in the late 1800s. Although these were very crude, they helped the early engineers understand engine operation and actually provided some trend-wise insight. The history of engine model development shows a continual improvement of these models.

These ideal (air-standard cycle) models are based on the simple application of the first law of thermodynamics, and a set of simplifying assumptions and approximations. Improvements to the air standard cycle analysis were adopted in the 1930s. These improvements included using more realistic thermodynamic properties based on more realistic mixtures. Although this was a much more realistic model for the working gases, the predictions were improved only in a modest manner since the other assumptions and approximations were still present.

A great improvement relative to the air-standard cycle models was the development of thermodynamic engine cycle simulations. These developments have been reported since the early 1960s. These types of cycle simulations could not be developed prior to this time due to the lack of sufficient computer capability and, to a lesser degree, the lack of understanding of the important engine processes. The original simulations were based on one-zone and two-zone formulations, and then these types of simulations were extended to include three or more zones.

Beginning in the late 1970s, thermodynamic engine cycle simulations were more complete and many included predictions of emissions, particularly nitric oxides. An important improvement in these simulations was a more complete description of the combustion process using three or more zones. Several researchers have mentioned the importance of multiple zones for predicting nitric oxide emissions.

Thermodynamic engine simulations can provide important and detailed information on engine operation. Although the simplest thermodynamic simulations generally provide no detail spatial information, they do provide time (or crank-angle) varying quantities such as cylinder gas pressure and temperature, heat release, heat loss, intake and exhaust flow rates, and cylinder mass. In addition, these simulations are typically more practical than the multi-dimensional simulations for extensive parametric studies and other related investigations.

In summary, the development of engine cycle simulations may be described as continual improvements in two related aspects: (i) the detail descriptions of the thermodynamic properties, and (ii) the descriptions of the processes. These improvements continue as more understanding is obtained on the various engine processes. In addition, these simulations continue to be extended to include other features (such as second law analyses), and continue to find new applications (such as onboard engine control). Chapter 3 will expand on the above history for thermodynamic simulations, and also include some comments about multidimensional simulations.

1.5 Overview of Book Content

This book has been divided into a number of chapters to cover the formulation of engine simulations, required items and procedures for solutions, detailed and performance results, and case studies. The following are descriptions of each chapter:

Chapter 1: Introduction. This chapter is a brief summary of the role of engine simulations relative to designing and understanding IC engines.

Chapter 2: Overview of Engines and Their Operation. This chapter provides a brief overview of engine fundamentals, terminology, components, operation, and performance parameters.

Chapter 3: Overview of Engine Cycle Simulations. This chapter provides a description of the evolution of thermodynamic engine cycle simulations. The description begins with the simple ideal (air-standard) cycle analyses, and continues with the historical development of the thermodynamic simulations. Brief comments are included on quasi-dimensional thermodynamic simulations, and multi-dimensional (CFD) simulations.

Chapter 4: Properties of the Working Fluids. This chapter is a fairly comprehensive presentation on the development of the algorithms needed to determine the composition of the unburned and burned mixtures. Chemical equilibrium compositions for combustion products are described. The chapter ends with results for various properties for typical engine conditions.

Chapter 5: Thermodynamic Formulations. This chapter includes the details for developing the governing thermodynamic relations for the cylinder contents. The chapter ends with a concise summary of a set of differential equations for the cylinder pressure, zone temperatures, zone volumes and zone masses.

Chapter 6: Items and Procedures Required for Solutions. This chapter outlines all the required items to solve the governing differential equations developed in Chapter 5. These items include cylinder volumes, fuel burning rates, heat transfer, flow rates, friction, and other sub-models as needed. The chapter ends with comments on solution procedures and convergence to final answers.

Chapter 7: Basic Results. This chapter starts the second part of the book which is focused on presenting results using the engine cycle simulation. This chapter presents detailed, time resolved results for the base case condition. Included are results for pressures, temperatures, species, and residual fractions.

Chapter 8: Performance Results. This chapter provides a fairly complete presentation of overall global performance metrics as functions of engine operating and design parameters. Overall performance metrics include power, torque, thermal efficiency, and mean effective pressure. Engine operating and design parameters include inlet pressure, speed, load, combustion variables, compression ratio, equivalence ratio, EGR, and combustion timing.

Chapter 9: Second Law Results. This chapter includes the development of the aspects needed to complete second law assessments of IC engines. This includes the property exergy which allows the irreversibilities of the engine processes to be quantified. Results for these irreversibilities are presented as functions of engine operating and design parameters.

Chapter 10–18: Case Studies. These chapters consist of a number of case studies using the engine cycle simulations. These cases include studies of combustion, cylinder heat transfer, fuels, oxygen enriched reactants, over-expanded engines, nitric oxide emissions, and high efficiency engines.

Chapter 19: Summary: Thermodynamics of Engines. This final chapter highlights the thermodynamic features of IC engines. Many of these features are quantified by the cycle simulation results reported in this book.

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