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Fourth Edition

An Introduction to Combustion

Concepts and Applications

Stephen R. Turns
Daniel C. Haworth



Mc Graw Hill

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Concepts and Applications

Fourth edition

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AN INTRODUCTION TO COMBUSTION

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Stephen R. Turns received degrees in mechanical engineering from The Pennsylvania State University (B.S., 1970), Wayne State University (M.S., 1974), and the University of Wisconsin at Madison (Ph.D., 1979). He was a research engineer at General Motors Research Laboratories from 1970 to 1975. He joined the Penn State faculty in 1979 and is currently Professor Emeritus of Mechanical Engineering. Dr. Turns taught a wide variety of courses in the thermal sciences and received several awards for teaching excellence at Penn State. In 2009, he received the American Society of Engineering Education's Ralph Coats Roe award. Dr. Turns had conducted research in several combustion-related areas. He is a member of The Combustion Institute, the American Institute of Aeronautics, the American Society of Engineering Education, and the Society of Automotive Engineers. Dr. Turns is a Fellow of the American Society of Mechanical Engineers.

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This book is dedicated to Joan Turns and to the memory of Amy Haworth.

By contrast, the first fires flickering at a cave mouth are our own discovery, our own triumph, our grasp upon invisible chemical power. Fire contained, in that place of brutal darkness and leaping shadows, the crucible and the chemical retort, steam and industry. It contained the entire human future.

Loren Eiseley
The Unexpected Universe

Preface to the Fourth Edition

The fourth edition retains the same primary objectives as previous editions: first, to present basic combustion concepts using relatively simple and easy-to-understand analyses and second, to introduce a wide variety of practical applications that motivate or relate to the various theoretical concepts. To these, a third objective has been added in this edition: to introduce the use of modern combustion software and to use that as a vehicle to present material that supplements the text. The overarching goal remains to provide a textbook that is useful for both formal undergraduate and introductory graduate study in mechanical engineering and related fields and informal study by practicing engineers.

Three principal changes have been made in the fourth edition: Chapter 1 has been rewritten, a new chapter (Chapter 18) has been added, and new supplementary material has been included in the form of combustion software. The changes in Chapter 1 in addition to the new Chapter 18 are motivated by the increasing emphasis on sustainable energy systems and concerns over adverse environmental impacts of combustion-based energy conversion, including global climate change. In Chapter 18, the relevance of combustion in the anticipated low-carbon 21st-century energy portfolio is discussed, and entry points to the literature are provided for this rapidly evolving area of technology. Changes to Chapters 2–17 intentionally have been kept minimal, other than the introduction of the new combustion software. The computer software that had been provided with earlier editions also has been retained for those who would like to continue to use that. That software remains available for download from the Online Learning Center (OLC) at http://www.mhhe.com/turns4e. An instructor's solution manual is also available on the OLC.

The new combustion software and supplementary material are based on Cantera (https://cantera.org/). Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes. Several options are available for installing and running Cantera on different kinds of computers; the Python/Jupyter Notebook interface is used here. This requires two layers of software in addition to Cantera itself: Python (https://www.python.org) and Jupyter Notebook (http://jupyter.org/). Various other software packages are also used to facilitate mathematical operations, data analysis, and plotting. The Python/Jupyter Notebook approach has several advantages compared to other options for installing and running Cantera: all of the software is open source; Python is increasingly being adopted as a high-level programming language for scientific/engineering applications and provides access to other useful packages including math, data analysis, and plotting libraries; and Jupyter Notebook (formerly iPython Notebook) provides an interactive computational environment in which one can combine executable code with rich text and plots. We hope that the benefits will become clear as you progress through the tutorial Cantera/Jupyter Notebooks that have been developed to supplement this book.



To get started with the software, a file named "README.pdf" is posted on the OLC (http://www.mhhe.com/turns4e). In that file, the organization of the remaining files is explained. Those include installation instructions for computers that run Windows and macOS operating systems, and a "Getting Started" Notebook to help readers to come up to speed quickly with the software. The Notebooks are numbered sequentially by book chapter, and readers are encouraged to work through them sequentially, in parallel with the book. At the appropriate location in the book, the icon that is shown to the left appears in the margin, and a brief description is given in the text of the material that is covered in the Notebook.

A total of 35 Notebooks is provided with this edition. Each Notebook reviews one or more key concepts. In some cases, alternative and/or deeper explanations are given compared to those in the book. Examples are provided of how to use Cantera to solve various classes of combustion problems, and the examples can serve as templates that the reader can adapt to develop code to solve similar or related problems. The Notebooks have been designed such that no prior programming experience should be necessary. In addition to providing material on a specific combustion topic, each successive Notebook introduces progressively higher-level material on Python syntax and coding, plot generation, and other information that should help readers to develop their programming and analysis skills. Finally, in addition to the tutorial Notebooks, new Cantera-based end-of-chapter problems have been added in several chapters. Those also are available online.

The authors hope that this new edition will continue to serve well those who have used previous editions and that the changes provided will enhance the usefulness of the book. By the end of your study of this book, including the associated tutorial Notebooks, it is hoped that you will be well prepared for further study of combustion and advanced use of Cantera.

Stephen R. Turns
Daniel C. Haworth
University Park, PA

ACKNOWLEDGMENTS

We would like to reaffirm our acknowledgments of all of the people cited in preceding editions. As previously detailed, many people contributed their support, time, and psychic energy to the creation and success of this book. Again, we are forever grateful to them for their contributions.

Several individuals and groups contributed to the development of the new Cantera/Jupyter Notebooks. That includes approximately 200 mostly undergraduate students at Penn State who took our senior-level undergraduate combustion course in 2018 and 2019. Those students endured the early iterations and provided constructive feedback that significantly improved both the installation instructions and the Notebooks themselves. We also are grateful to the members of the Cantera Users' Group (https://groups.google.com/forum/#!forum/canterausers). Draft versions of several of the Notebooks were posted to their online forum for comment, and their feedback resulted in much-improved products. We will not attempt to name everyone who provided input, but there are two individuals in particular who were especially generous with their time and expertise: Bryan Weber and Ray Speth, both of whom have been instrumental in promoting and supporting the development of this open-source combustion software.

Contact me in order to access the whole complete document. Email: solution9159@gmail.com
WhatsApp: https://wa.me/message/2H3BV2L5TTSUF1 Telegram: https://t.me/solutionmanual

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chapter

1

Introduction

MOTIVATION TO STUDY COMBUSTION

Combustion is the dominant technology by which we obtain the energy required to support the lives of approximately 7.7 billion people (in 2019) on our planet. In 2018, over 80 percent of the energy used, both in the United States and worldwide, came from combustion sources [1, 2]. Combustion touches our daily lives in multiple ways. More than likely, the heat for your room or home comes directly from combustion (either a gas- or oil-fired furnace or boiler), or indirectly, through electricity that was generated by combustion. Approximately two-thirds of U.S. and of global electricity generation is from combustion. Our global transportation systems rely almost entirely on combustion. And industrial processes rely heavily on combustion. Those include metal refining and processing, boilers, refinery and chemical fluid heaters, glass furnaces, solids dryers, surface-coating curing and drying ovens, organic fume incinerators, and rotary kilns in the cement manufacturing industry [3], to name a few examples. Combustion is also used at the other end of the product life cycle, as a means of waste disposal. Incineration is an old method, but it is being used with increasing frequency in some parts of the world because of the limited availability of landfill sites, and for its ability to dispose of some toxic wastes relatively safely.

Two organizations that compile energy statistics for the United States and the world, and that make projections about future energy use, are the U.S. Energy Information Administration (USEIA) [1] and the International Energy Agency (IEA) [2]. Their most recent reports and other information can be found on their respective websites. Examples from these two sources showing historical trends and projections are shown in Figs. 1.1 to 1.4. In making projections, each organization considers multiple scenarios: a baseline case, and several other cases that differ in their underlying assumptions. The baseline case is not necessarily the most likely nor the most desirable scenario. Rather, it is one that is consistent with the current world

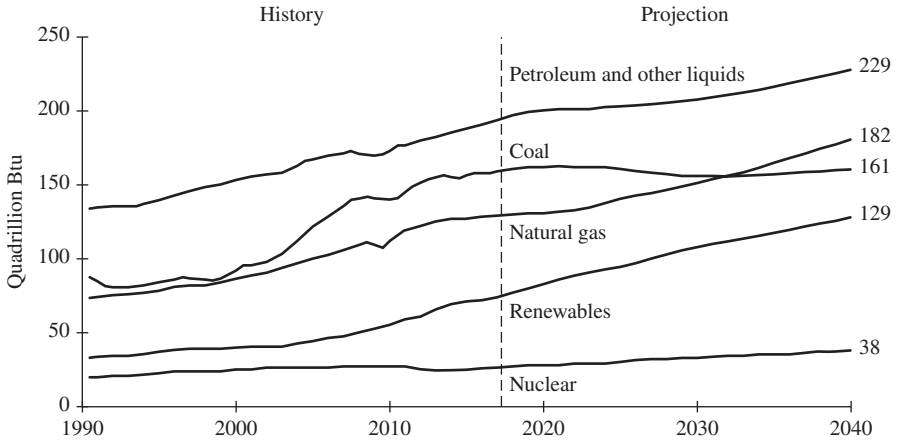


Figure 1.1 World energy consumption by energy source, with historical data to 2018 and projections to 2040. Projections are based on the USEIA Reference Case.
SOURCE: EIA, International Energy Outlook, 2018.

population, energy prices, economic situation, government policies, and technology available, with relatively conservative extrapolations into the future. The USEIA refers to their baseline case as the "Reference Case," and the IEA refers to theirs as the "New Policies Scenario." For alternative scenarios, the USEIA considers different assumptions regarding fossil energy prices and economic growth, while the IEA focuses mainly on different policies with respect to carbon dioxide emissions, which are discussed later in this section.

Figures 1.1 and 1.2a show global and U.S. energy consumption historical trends and projections (for the USEIA Reference Case) by fuel type. Figure 1.2b breaks down

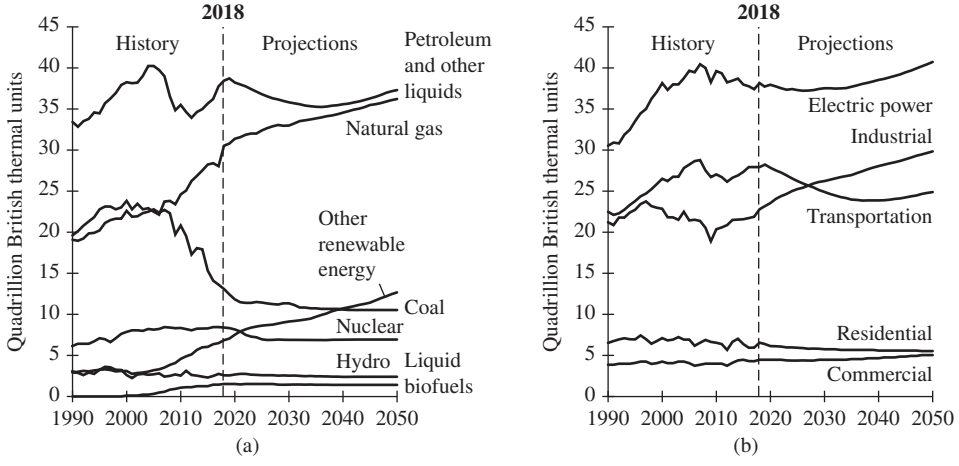


Figure 1.2 U.S. energy consumption, with historical data to 2018 and projections to 2050. Projections are based on the USEIA Reference Case. (a) By fuel and (b) by end-use sector.
SOURCE: https://www.eia.gov/pressroom/presentations/capuano_01242019.pdf.

the U.S. data by end-use sector. The units of energy here are quads: 1 quad = 1 quadrillion Btu = 10^{15} Btu = 1.055×10^{18} J = 1.055 EJ (exajoules). Several observations can be made. First, the 2018 data are consistent with the statements made in the first paragraph of this section. Second, there has been a significant shift from coal to natural gas in the United States since approximately 2010, and that trend is expected to continue (albeit at a slower pace) through mid-century. A similar trend is anticipated globally over the next 10–20 years. Third, modest growth is anticipated for nuclear energy. And fourth, the rate of increase in renewable energy (mainly wind and solar photovoltaic) that has been seen over the past approximately 10 years is expected to continue through mid-century. In this scenario, combustion would continue to account for over three-quarters of global energy consumption (somewhat higher in the United States compared to the rest of the world) in 2040–2050. Most of the growth in total energy consumption is anticipated to be for electric power generation and industrial processes.

There has been a general trend toward electrification in light-duty transportation vehicles, in particular, as well as in other applications heretofore dominated by combustion, and that is expected to continue. This, by itself, does not decrease the ultimate reliance on combustion. Trends and projections with respect to electrical power generation are shown in Figs. 1.3 and 1.4. Figure 1.3 shows historical trends and projections for two of the IEA scenarios: their baseline case ("New Policies Scenario"), and a scenario in which policies are enacted to reduce carbon dioxide emissions to levels consistent with limiting the increase in global average temperature to less than 2°C ("Sustainable Development Scenario"). Carbon dioxide emissions are discussed later in this section. Figure 1.4 shows similar data and projections for the United States from two of the USEIA scenarios: their baseline case ("Reference Case"), and a scenario that would reduce reliance on fossil fuels ("Low Oil and Gas Resource and Technology Case"). Note that power (GW) is plotted in Fig. 1.3, while energy (billion kilowatt-hours) is plotted in Fig. 1.4. The recent shift in the United States from coal to natural gas for electricity generation is evident in Fig. 1.4. In their respective baseline cases, the IEA and the USEIA project that combustion will continue to be relied on for approximately 42 percent globally, and 56 percent in the United States, of electrical power generation in 2040–2050. Even in the scenarios with significant reductions in fossil-energy-based electrical generation, the percentages from combustion remain approximately 26 percent (globally) and 44 percent (United States).

A key issue in combustion is the environmental impact of pollutant emissions from combustion systems. For historical and technical purposes, we consider two different classes of emissions: criteria air pollutants (CAPS) [4], and greenhouse gases (GHGs) [5].

The combustion of carbon-containing fuels with air is a major (the dominant, in some cases) contributor to several of the regulated criteria air pollutants. Pollutants produced by combustion include unburned and partially burned hydrocarbons, carbon monoxide (CO), nitrogen oxides (nitric oxide – NO, and nitrogen dioxide – NO_2; together denoted as NO_x), sulfur oxides (sulfur dioxide – SO_2, and sulfur trioxide – SO_3), and solid particulate matter (PM). For the latter, ultrafine particles having diameters of 2.5 μm and smaller ($PM_{2.5}$) are of particular concern, as those penetrate deeply into the lung when inhaled. The reasons why each of these is regulated as a pollutant, the mechanisms by which each is formed in combustion processes, and

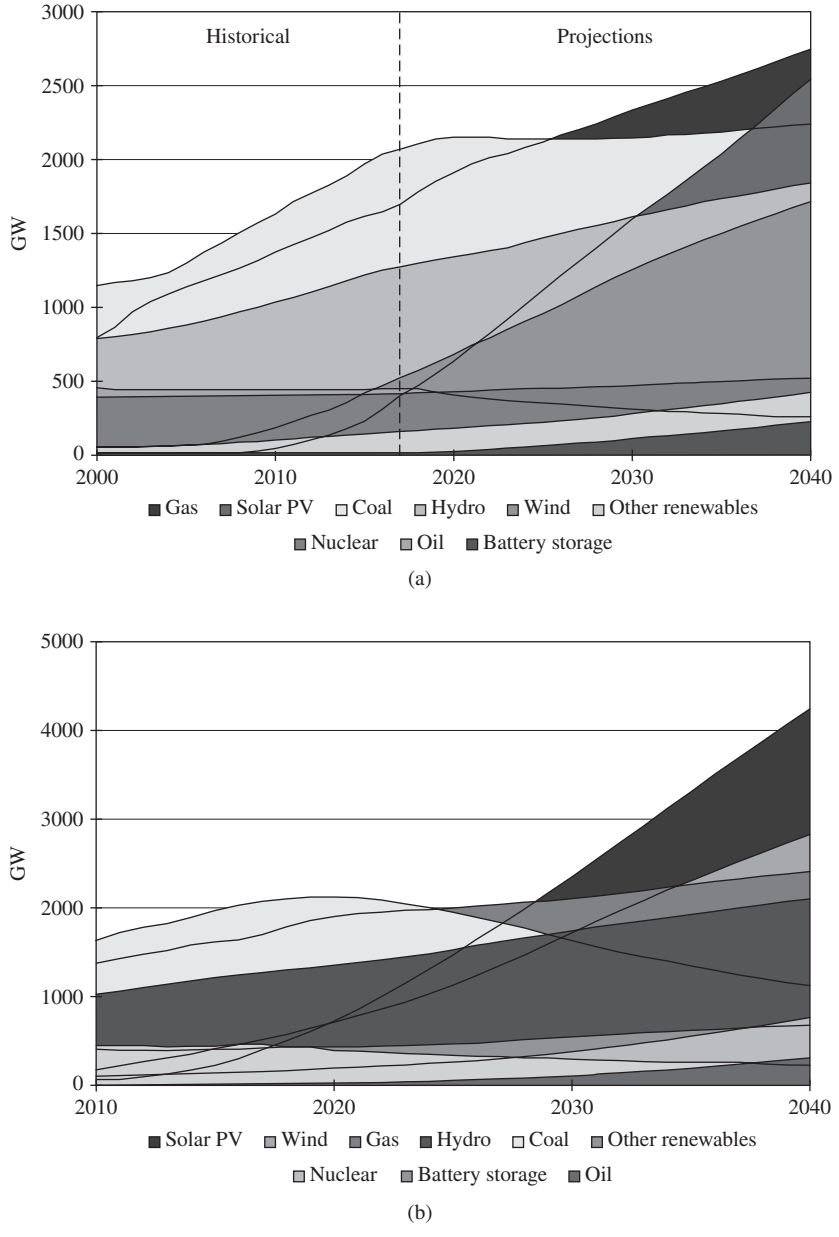


Figure 1.3 World electrical power generation capacity by source, with historical data to 2017 and projections to 2040. Projections are based on (a) the IEA New Policies Scenario and (b) the IEA Sustainable Development Scenario.
SOURCE: International Energy Agency.

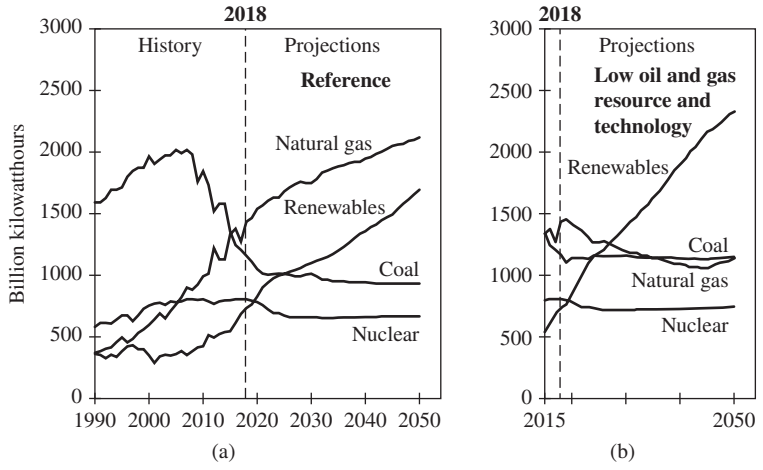


Figure 1.4 U.S. electricity generation from selected fuels, with historical data to 2018 and projections to 2050. Projections are based on (a) the USEIA Reference Case and (b) the USEIA Low Oil and Gas Resource and Technology Case.
SOURCE: Energy Information Administration.

strategies to reduce their formation, are discussed in Chapter 15. In a properly functioning modern combustion system, the mass of each criteria pollutant formed is a small fraction of the mass of the fuel consumed: usually well under 1 percent. The United States historically has had among the strictest CAPS regulations in the world; the examples of U.S. emissions trends in Figs. 1.5 to 1.8 are taken from [6].

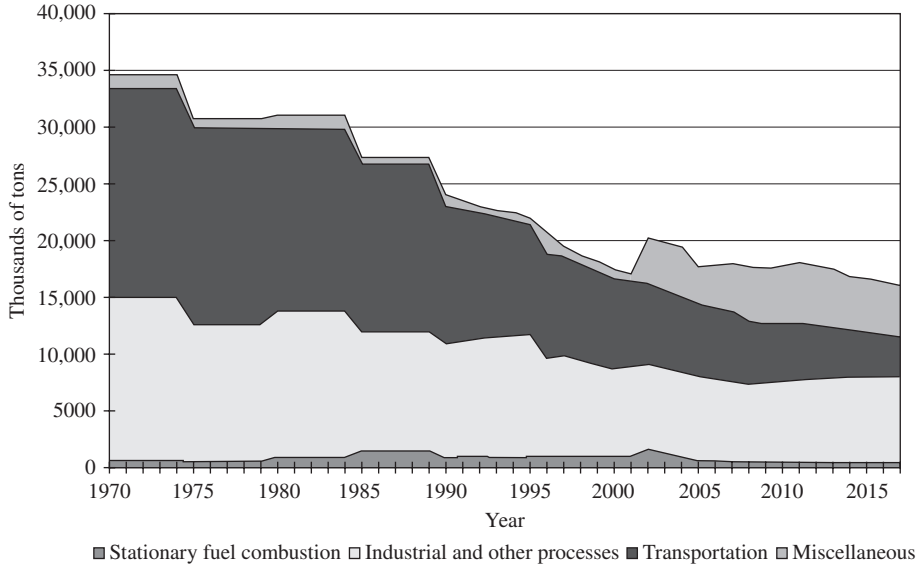


Figure 1.5 Trends in emissions of volatile organic compounds for the United States, 1970–2017. Reading legend left to right corresponds to plotted series bottom to top.

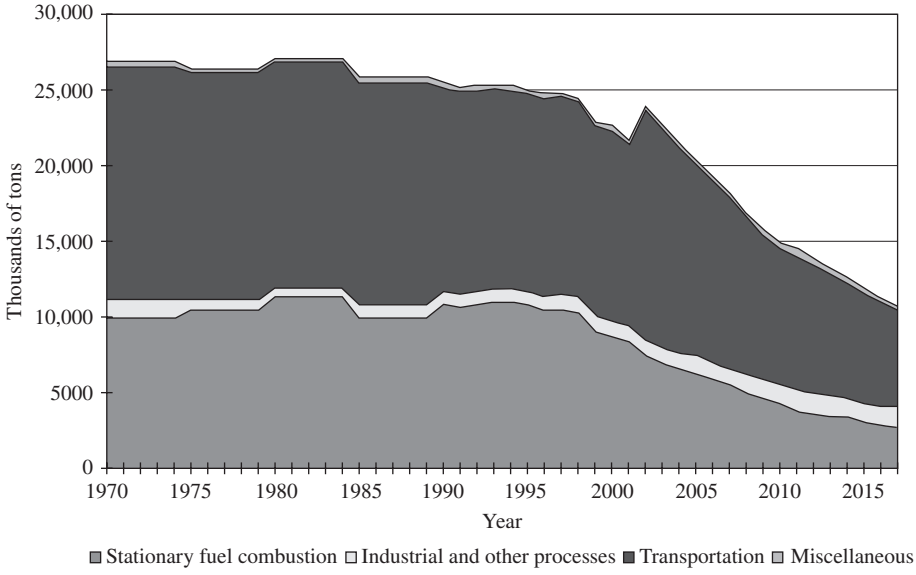


Figure 1.6 Trends in emissions of nitrogen oxides for the United States, 1970–2017. Reading legend left to right corresponds to plotted series bottom to top.

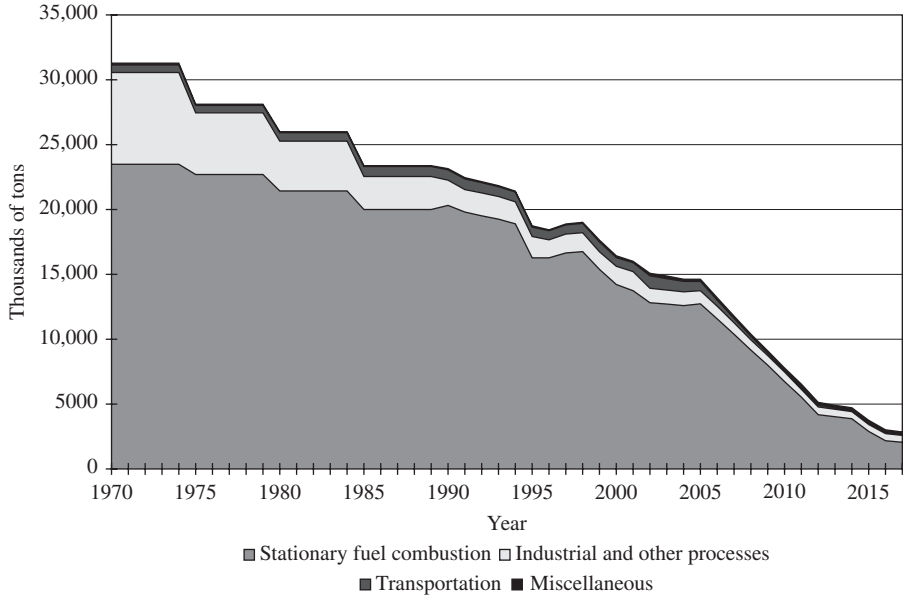


Figure 1.7 Trends in emissions of sulfur dioxide (SO_2) for the United States, 1970–2017. Reading legend left to right corresponds to plotted series bottom to top.

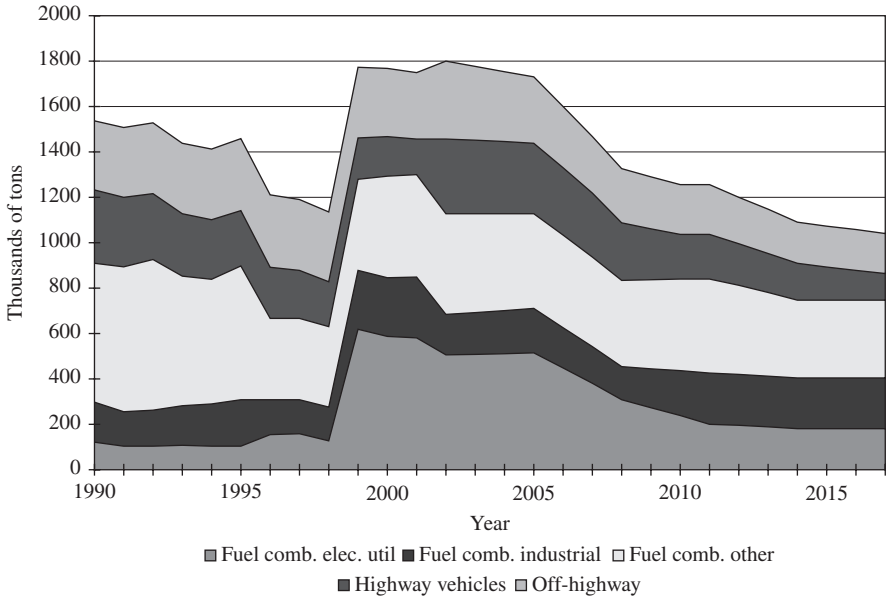


Figure 1.8 Trends in emissions of ultrafine particulate matter ($PM_{2.5}$) from combustion for the United States, 1990–2017. The increase for electrical utilities from 1998 to 1999 is a consequence of changes in reporting methods. Reading legend left to right corresponds to plotted series bottom to top.

Significant progress has been made in reducing the emissions of these pollutants since the enactment of the Clean Air Act and its subsequent amendments [7]. In most cases, this has been accomplished while maintaining and even improving fuel efficiency and performance. For example, U.S. light-duty vehicle unburned hydrocarbon, CO, and NO_x emissions have been reduced by 98–99 percent since pre-emissions-regulations levels, while fuel economy and performance both have increased substantially.

A more recently recognized problem, and one that is (arguably) more technically challenging compared to CAPS, is GHG emissions. Greenhouse gases are gases that trap heat in the earth's atmosphere [5], resulting in a rise in temperature. A general consensus of world scientific and political opinion, codified in the "Paris Agreement" of 2015/2016 [8], is that the increase in global average temperature should be kept to well below 2°C above pre-industrial levels, to reduce the risks and effects of climate change to a manageable level. Carbon dioxide (CO_2) is the primary GHG emitted through human activities, and the combustion of any carbon-containing fuel with air results in CO_2 emissions. In contrast to CAPS emissions, the amount of CO_2 produced in the combustion of a carbon-containing fuel with air is large, and is directly proportional to the efficiency of the combustion process. For example, for each liter of gasoline (approximately 0.7 kg) burned in an automotive engine, approximately 2.3 kg of CO_2 are released into the atmosphere; the mass of

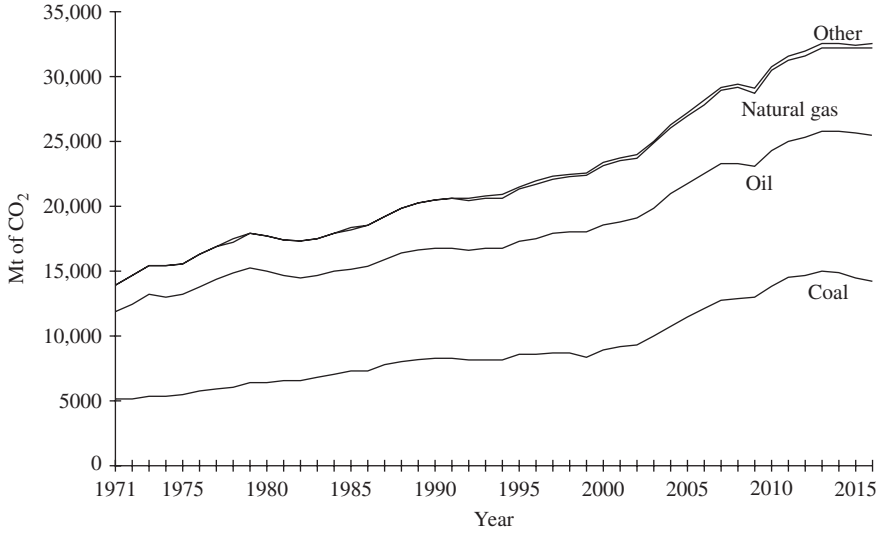


Figure 1.9 World CO_2 emissions by fuel, 1971–2016. Reading legend left to right corresponds to plotted series bottom to top.
SOURCE: International Energy Agency, "World Energy Outlook 2018." Accessed 5/29/2019. https://www.iea.org/weo/.

CO_2 released is over three times the mass of the fuel that is burned. This is possible because most of the mass of the CO_2 comes from oxygen in the ambient air. This is discussed further in Chapter 2. In the United States, new light-duty-vehicle efficiency and emissions standards were introduced in 2012 to improve fuel economy and reduce GHG emissions [9]. These were the first national GHG emissions

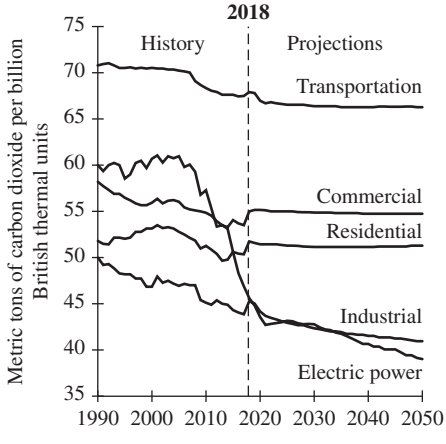


Figure 1.10 U.S. CO_2 emissions intensity (metric tons of CO_2 per billion Btu) by end-use sector, with historical data to 2018 and projections to 2050. Projections are based on the USEIA Reference Case.
SOURCE: Energy Information Administration.

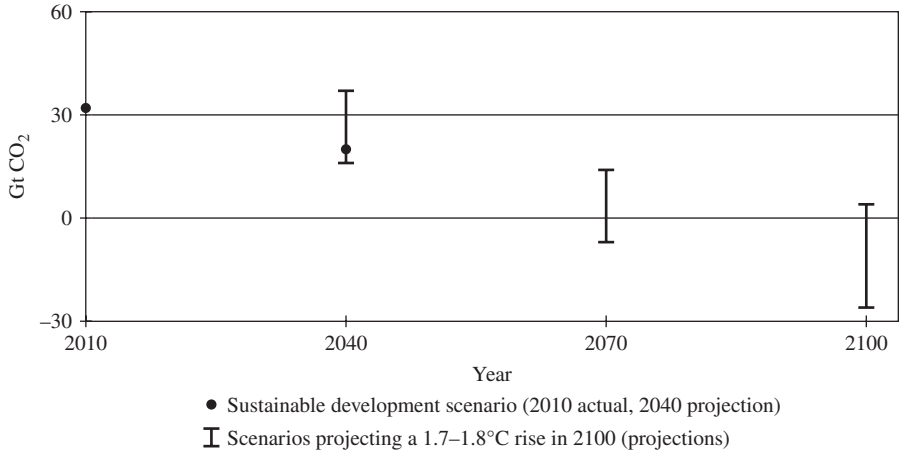


Figure 1.11 World CO_2 emissions projections for the IEA Sustainable Development Scenario (through 2040), and for several other scenarios that are intended to result in a global average temperature rise of 1.7–1.8°C relative to pre-industrial levels by 2100.
SOURCE: International Energy Agency.

standards to be established in the United States since the 2007 Supreme Court decision [10] that ruled that CO_2 and three other greenhouse gases are air pollutants as defined in the Clean Air Act.

Examples of historical data and projections related to CO_2 emissions are shown in Figs. 1.9 to 1.11. The switch from coal to natural gas in electrical power generation has resulted in a reduction of CO_2 emissions, because natural gas (which consists mostly of methane) emits less CO_2 compared to coal, per unit of energy released. This is a major reason why CO_2 emissions (Figs. 1.9 and 1.10) have not increased as rapidly as electrical power generation capacity (Figs. 1.3 and 1.4) and total energy consumption (Figs. 1.1 and 1.2) since 2010, especially in the United States. Looking ahead, the reductions in CO_2 intensity (CO_2 released per unit of energy available) anticipated in the United States through 2040 in the USEIA Reference Case are mainly from the increase in renewables and the shift from coal to natural gas (Figs. 1.2, 1.4, and 1.10). However, to limit the global average temperature rise to less than 2°C in 2100, most projected scenarios require "negative emissions" technologies at some point starting in the second half of the century (Fig. 1.11), where CO_2 is withdrawn from the atmosphere on a scale that is significant enough to affect global temperatures. The role of combustion in a likely "low-carbon" energy future in the 21st century (i.e., one that will require low, zero, or even negative net CO_2 emissions) is discussed in Chapter 18.

Finally, we note that, in addition to the important motivations for studying combustion that have been discussed up to this point, the subject is in itself intellectually stimulating in that it nicely integrates the thermal-fluid sciences (thermodynamics, heat and mass transfer, and fluid mechanics), as well as bringing chemistry into the practical realm of engineering.

A DEFINITION OF COMBUSTION

Webster's Dictionary provides a useful starting point for a definition of **combustion** as "rapid oxidation generating heat, or both light and heat; also, slow oxidation accompanied by relatively little heat and no light." For our purposes, we will be interested mainly (although not exclusively) in the rapid oxidation regime, since most practical combustion devices belong in this realm.

This definition emphasizes the intrinsic importance of chemical reactions to combustion. It also emphasizes why combustion is so very important: combustion transforms energy stored in chemical bonds between adjacent atoms in molecules to heat that can be utilized in a variety of ways. Throughout this book, we illustrate the many practical applications of combustion.

COMBUSTION MODES AND FLAME TYPES

Combustion can occur in either a **flame** or **nonflame** mode, and flames, in turn, can be categorized as being either **premixed flames** or **nonpremixed (diffusion) flames.** The difference between flame and nonflame modes of combustion can be illustrated by the processes occurring in a knocking spark-ignition engine (Fig. 1.12). In Fig. 1.12a, we see a thin zone of intense chemical reaction propagating through the unburned fuel–air mixture. The thin reaction zone is what we commonly refer to as a flame. Behind the flame are the hot products of combustion. As the flame moves across the combustion space, the temperature and pressure rise in the unburned gas. Under certain conditions (Fig. 1.12b), rapid oxidation reactions occur at many locations within the unburned gas, leading to very rapid combustion throughout the volume. This essentially volumetric heat release in an engine is called **autoignition,** and the very rapid pressure rise leads to the characteristic sound of engine knock. Knock is undesirable, and a challenge to engine designers has been how to minimize the occurrence of knock while operating with lead-free gasoline and maintaining high efficiency.[1] In compression-ignition or diesel engines, however, autoignition initiates the combustion process by design.

The two classes of flames, premixed and nonpremixed (or diffusion), are related to the state of mixedness of the reactants, as suggested by their names. In a premixed flame, the fuel and the oxidizer are mixed at the molecular level prior to the occurrence of any significant chemical reaction. The spark-ignition engine is an example of where premixed flames occur. Contrarily, in a diffusion flame, the reactants are initially separated, and reaction occurs only at the interface between the fuel and oxidizer where mixing and reaction both take place. An example of a diffusion flame is a simple candle. In practical devices, both types of flames may be present in different degrees. Diesel-engine combustion is generally considered to have significant amounts of both premixed and nonpremixed or diffusion burning. The term

[1]The discovery that tetraethyl lead reduces knock, made by Thomas Midgley in 1921, allowed engine compression ratios to be increased, and thereby improved efficiency and power.

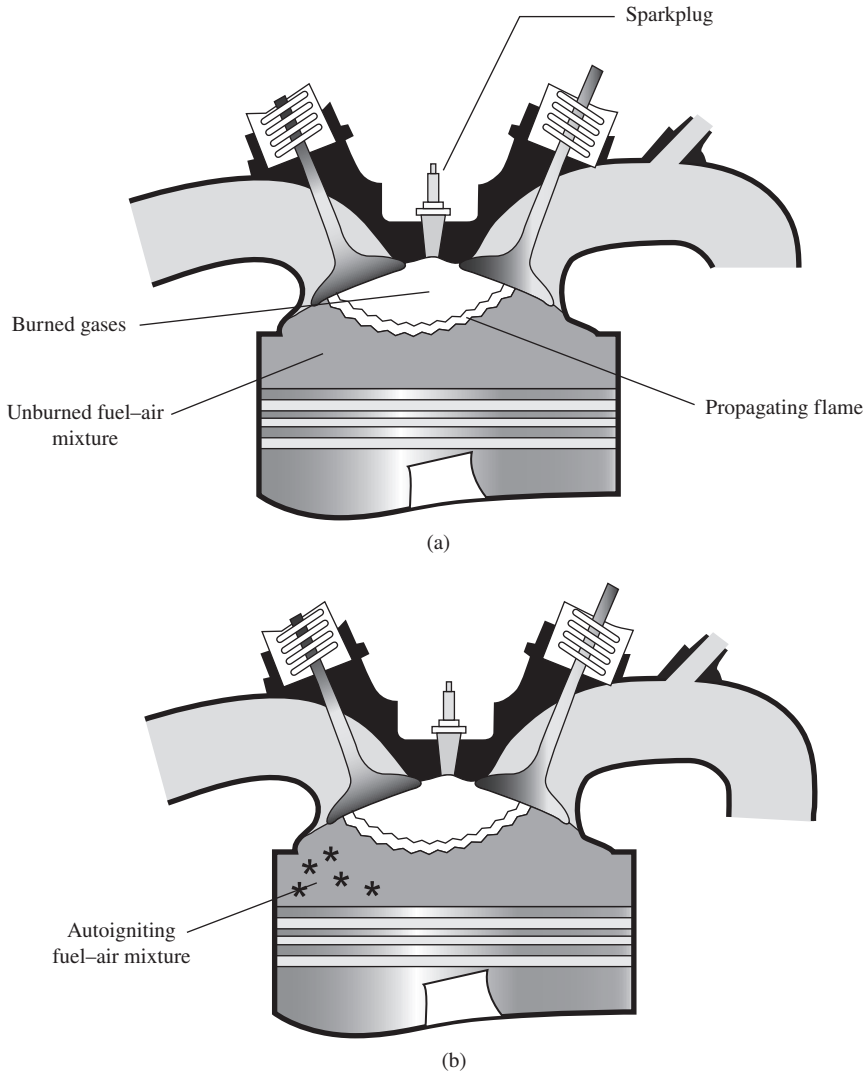


Figure 1.12 (a) Flame and (b) nonflame modes of combustion in a spark-ignition engine. Autoignition of the mixture ahead of the propagating flame is responsible for engine knock.

"diffusion" applies strictly to the molecular diffusion of chemical species, i.e., fuel molecules diffuse toward the flame from one direction while oxidizer molecules diffuse toward the flame from the opposite direction, and products of combustion diffuse away from the flame. In turbulent nonpremixed flames, turbulent convection mixes the fuel and air together on a macroscopic basis. Molecular mixing at the small scales, i.e., molecular diffusion, then completes the mixing process so that chemical reactions can take place.

APPROACH TO OUR STUDY

We begin our study of combustion by investigating the key underlying physical processes, or sciences, which form the fundamental framework of combustion science: **thermochemistry** in Chapter 2; **molecular transport of mass (and heat)** in Chapter 3; **chemical kinetics** in Chapters 4 and 5; and, in Chapters 6 and 7, the coupling of all of these with **fluid mechanics.** In subsequent chapters, we apply these fundamentals to develop an understanding of laminar premixed flames (Chapter 8) and laminar diffusion flames (Chapters 9 and 10). In these laminar flames, it is relatively easy to see how basic conservation principles can be applied. Most practical combustion devices operate with turbulent flows, however, and the application of theoretical concepts to these is much more difficult. Chapters 11, 12, and 13 deal with turbulence, turbulent flames, and their practical applications. The final chapters concern the combustion of solids, as exemplified by carbon combustion (Chapter 14); pollutant emissions (Chapter 15); detonations (Chapter 16); fuels (Chapter 17); and low-net-carbon combustion (Chapter 18).

A major goal of this book is to provide a treatment of combustion that is sufficiently simple so that students with no prior introduction to the subject can appreciate both the fundamental and practical aspects. It is hoped, however, that as a result, some may be motivated to learn more about this fascinating field, either through more advanced study, or as practicing engineers.

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