1 Introduction

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Combustion is a socioeconomically important topic in view of its role in civilization for many millenia, with the energy from its reactions used to produce bronze, iron, pottery, and so forth; cook food; produce mechanical power for transportation vehicles; and generate electricity. It is still the case even now, since more than 90% of the world's total primary energy supply (TPES) is met through combustion of fossil and biofuels and waste [1]. Fossil fuels include coal, oil, and natural gas. Shale gas also belongs to this category although its contribution is currently very small. Figure 1.1 shows the share of various fuels for TPES in terms of Mtoe (million tons of oil equivalent). There is 47 GJ of energy per ton of oil, which translates to about 647 EJ of energy for the year 2016 and about 287 EJ for 1973. There is an about 125% increase over this period of 43 years, suggesting a nearly 2.9% increase per year. This is in line with an estimate from the National Academies of Sciences, Engineering, and Medicine of an increase in the global energy consumption of an increase by about 40% in the next two decades [2]. In reality, this rate of energy consumption may increase further because of the recent surge in the "energy-hungry" technologies associated with consumer electronics such as smartphones, smart televisions, and so forth, and also the upcoming technologies such as Internet of things (IoTs), 5G networks required to meet the communication speeds needed for autonomous vehicles such as self-driving cars, and so forth. On the one hand, we all like to have these technologies without asking whether they are needed or not. On the other hand, we decry and worry about the environmental impacts resulting from anthropogenic sources leading to crises such as global warming affecting the weather pattern, agriculture and life on the planet. These two, the energy-hungry modern technologies and mitigation of global warming, are at opposite ends. Bringing them together is a grand challenge, and carefully considered, fully analyzed, and completely evaluated solutions are needed. Otherwise, these technologies may accelerate global warming further. The reports from the Intergovernmental Panel on Climate Change (IPCC) estimate that the global temperature will rise in the next 100 years [3, 4]. If the greenhouse gas (GHG) emissions are low (RCP 2.6[1]), then

[1] Representative Concentration Pathways. These are proposed by IPCC to have a common basis to compare the climate models used across the world. RCP 2.6 suggests that the GHG emissions in gigatons of carbon (GtC) will be close to zero in the year 2100 and the CO_2 concentration in the atmosphere will be about 400 ppm. Under this scenario, the temperature rise because of the radiative loading on the planet ranges from 0.3 to 1.7°C. For the RCP 8.5 scenario, the CO_2 emission is about 30 GtC, giving about 950 ppm of CO_2 concentration in the atmosphere in the year 2100.

the temperature rise will be about 0.3 to 1.7°C and if the GHG emissions are high (RCP 8.5) then the temperature rise could be about 2.6 to 4.8°C. These estimates are relative to 1986–2005 data.

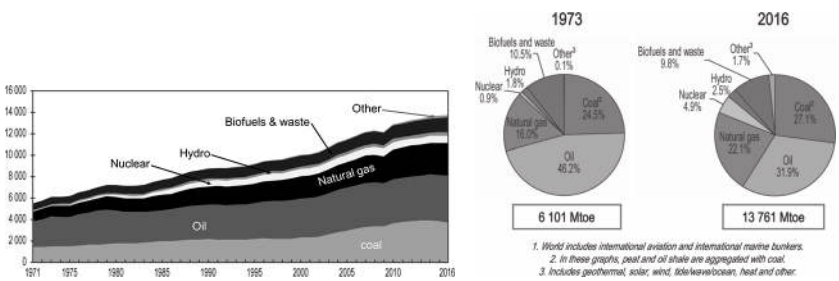

Figure 1.1 World total primary energy supply in Mtoe, million tons of oil equivalent, by fuel type. Adapted from [1], © IEA, 2018.

To reduce the rate of GHG emission and thereby the rate of global warming, energy production using renewable and sustainable sources is gaining popularity and has become widespread since the past decade. The renewable sources include hydro, solar, wind, and tidal. Including nuclear power among renewables is debatable. There are arguments to include it in the list of renewables for the following two reasons: (1) uranium deposits could provide energy for as long as the relationship between Earth and the sun is expected to last (about 5 billion years) [5] and (2) it does not emit GHGs while satisfying the increasing demand for energy in the world [6, 7]. The arguments to exclude it from the list of renewable energies are based on safety issues and the concept of clean energy. Figure 1.1 shows the nuclear energy had an about 5% share of the world TPES in 2016 whereas the contribution of renewables, excluding hydropower and biofuels, was only 1.7%. However, there is a substantial increase from 0.1% in 1973 for the renewables because of the advancement in the associated technologies in the past couple of decades. Both rooftop and commercial solar photovoltaic (PV) systems have become popular but the capital cost projections reported in [8] (see their figure 4.1), about £1000 per kilowatt for 2019, seems to be about half of the actual cost in the year. Also, the efficiency of the solar panel is only about 22%, which is improving with time.

If one considers the levelized cost of electricity (LCOE)[2] from utility-scale power generation using renewable technologies in the period from 2010 to 2017 then it becomes clear that these technologies are becoming competitive with the traditional power technologies using fossil fuels, with a cost ranging from about 0.05 to 0.18 USD per kilowatt-hour [9]. This comparison is shown in Fig. 1.2 for various renewable technologies. Biomass, geothermal, hydro, and onshore wind technologies are becoming highly competitive with prices ranging from 0.05 to 0.07 USD per kilowatt-hour. Both PV and concentrating solar power (CSP) technologies are becoming less expensive

[2] This is projected life cycle cost and is calculated as the ratio of costs for (investment + operation + maintenance + fuel) to the electricity energy generated.

and their LCOE is projected to range between 0.04 and 0.06 USD per kilowatt-hour for the year 2022 [9]. It is also possible that the LCOE for renewables will undercut that of fossil fuel-fired technologies. These trends and projections are encouraging, giving us hope to mitigate the global warming issues in due course. Nevertheless, one must recognize that there is no "free lunch" – because there are economical and environmental implications and costs associated with the renewable technologies as well. The typical *payback* period that is quoted for these technologies, for example 5 to 7 years for solar PV, is based purely on the initial investment cost for the system but one needs to consider the payback period for the environmental impact. For example, one can ask how long does it take to offset the GHG emissions produced in creating and constructing the renewable systems?

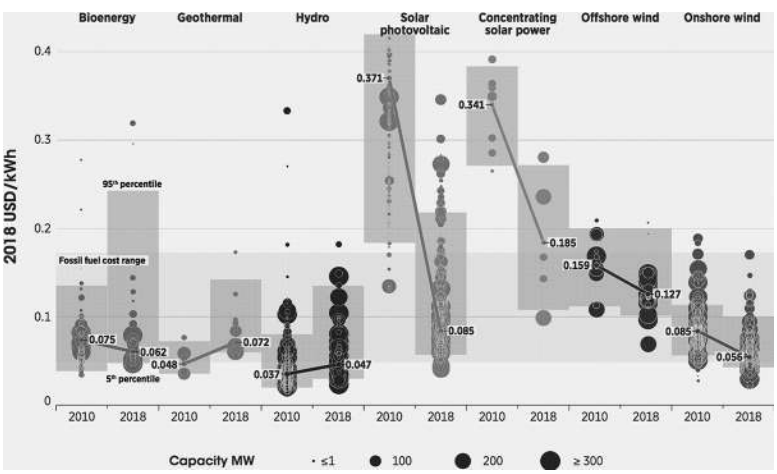

Figure 1.2 Global levelized cost of electricity for utility-scale renewable power technologies for the period from 2010 to 2018. Reproduced from [9], © IRENA, 2018. The diameter of the circle represents the size of the plant and the global averaged cost is shown by the line.

Careful considerations of these implications bring up two questions [10]: (1) Is there sufficient energy production, required as per the TPES data in Fig. 1.1, using renewable technologies to meet the total world primary energy demand? (2) What are the environmental impacts in terms of kilograms of CO_2 equivalents per megawatt-hour of electricity produced using the renewable technologies? The data shown in Fig. 1.3 provide some answers to the first question. The second question is somewhat controversial and needs a careful and honest full life cycle analysis/assessment (LCA) for each alternative technology.

The projections shown in Fig. 1.3 suggest that there will be about 1 TW of electricity power produced using solar and wind technologies in the year 2020. Using a conservative estimate of about 12 hours per day of operation gives about 4380 TWh of energy, which is equivalent to 376.8 Mtoe. The data collected from 2010 to 2018 reported in [11] suggest that there will be about 1.5 TW of electricity produced using other renewable technologies, which gives 3 Mtoe if one takes 24 hours (again a

conservative estimate) of operation per day. The data in Fig. 1.1 and the projected 3% rise yield TPES required in the year 2020 of about 15,412.32 Mtoe. These estimates show that the supply of renewables is only about 2.5% of the world TPES. Hence, the answer to our first question is clear.

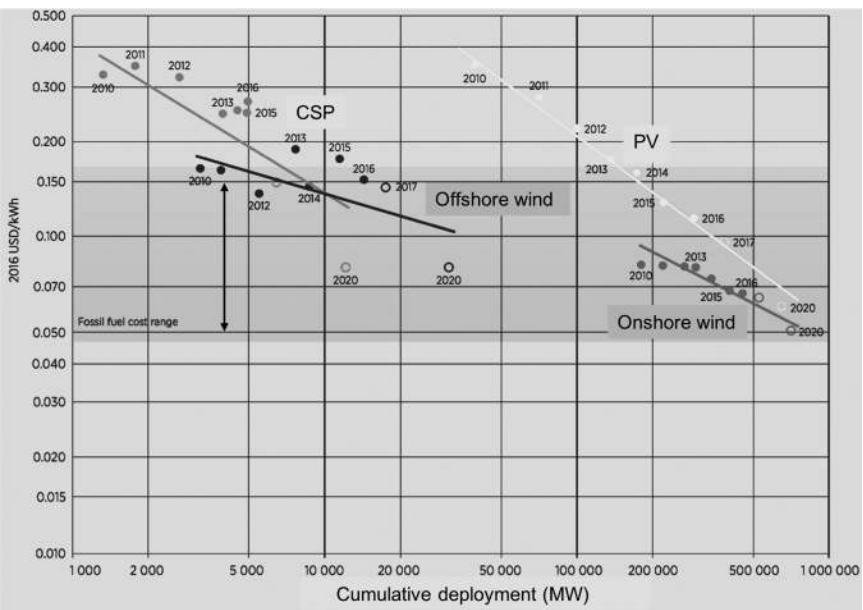

Figure 1.3 Variation of global averaged LCOE for solar, CSP and PV, and wind, onshore and offshore, technologies. Reproduced from [9], © IRENA, 2018.

To find a meaningful answer to the second question, one needs a careful LCA for all renewable technologies. This assessment must include the energy spent and GHGs emitted in *upstream*, operation, and *downstream* stages of the technology [12]. The upstream stage includes raw material extraction, manufacturing of construction materials, components of the power plant, and construction of the power plant. This stage includes the fuel cycle – extraction of fuel materials, their processing or conversion, and their delivery to the power plant side. The contribution from the fuel cycle stage is zero for most of the renewable technologies except for biofuels, biomass, and biowaste technologies. The operation stage includes combustion (for conventional technologies), plant operation, and maintenance. The downstream stage involves dismantling and decommissioning of the plant and disposal and recycling of the equipment and components. This type of assessment can help to determine energy and environmental burdens from *cradle to grave* and facilitate more consistent comparisons of energy technologies for making investment and policy decisions [12]. However, it must be recognized that the LCA can be quite difficult because of the scatter in the required data available in the literature. The scatter arises from the assumptions and approximations invoked, method of analysis employed, and so forth. Hence, it is a common

practice to employ a procedure called harmonisation to reduce the variability in the required data (GHG emissions or energy spent) and details can be found in [13, 14]. The estimates of GHG emissions in grams of CO_2 equivalent per kilowatt-hour of electricity energy produced using both renewable and nonrenewable technologies. There are some differences in the data from these two studies but there is a general agreement in the trend. The maximum values reported in [15] seem to correspond to the median values reported in [12], shown in Fig. 1.4b and 1.4a respectively. Switching from coal to natural gas reduces the GHG emissions by nearly 50%, which is well known today. The emission levels of waste treatment and biomass technologies are comparable to those of natural gas because these technologies involve combustion in one form or another. However, the emission level shown in Fig. 1.4a for the biopower from the IPCC report [12] is substantially different (lower) compared to the estimate in [15] shown in Fig. 1.4b. A similar observation is also made for PV systems between these two studies. The data in Fig. 1.4b show that the life cycle GHG emissions for PV systems about 60% of those for natural gas technology. It seems that there is still a great deal of variation and disparity in these types of data coming from various studies and thus one needs to be cautious in drawing conclusions. One can hope that these differences are likely to decline with time as more careful investigations in the future will provide further data. Nevertheless, one can see that renewable technologies can help to mitigate global warming. However, the current trend and projected capacities of these technologies are inadequate to meet the world total primary energy demand (shown by the TPES data in Fig. 1.1), as discussed earlier. It is probable that fossil fuel–derived energy is required for constructing renewable technologies. So, a utopian solution would be to reduce energy usage by every individual, which would require social engineering and drastic energy policies but these are impractical for political and personal reasons.

A heavily accelerated introduction of renewables to replace fossil-fuel technologies may sound like a plausible solution but the GHG emissions from the upstream stage of LCA and various activities (e.g., mining to meet the huge demand for resources, the required energy coming from fossil fuel sources) associated with this stage may cause irreversible changes to the planet. Alternatively, a gradual (an appropriate question to ask here would be at what rate?) shift toward renewables while improving the technologies for nonrenewable may be a more pragmatic way forward. Combustion-based technologies are likely to play a central role for applications such as transports requiring high energy densities but the form and type of combustion are likely to change for future applications.

Electric vehicles (EVs) are projected to have zero emission but this depends on where the boundary for the analysis is drawn. The LCA of this technology shows that one has to drive an EV of Nissan LEAF size for about 35,000 km (about 3 years) to offset the CO_2 emissions coming from just the battery pack production part in the upstream stage of the LCA. It is important to note that the GHG emissions coming from the production of a vehicle or the electricity required to charge the battery pack for 35,000 km of driving are not included. Also, this amount of CO_2 is equivalent to producing 6400 liters of gasoline and the amount of energy spent to produce the

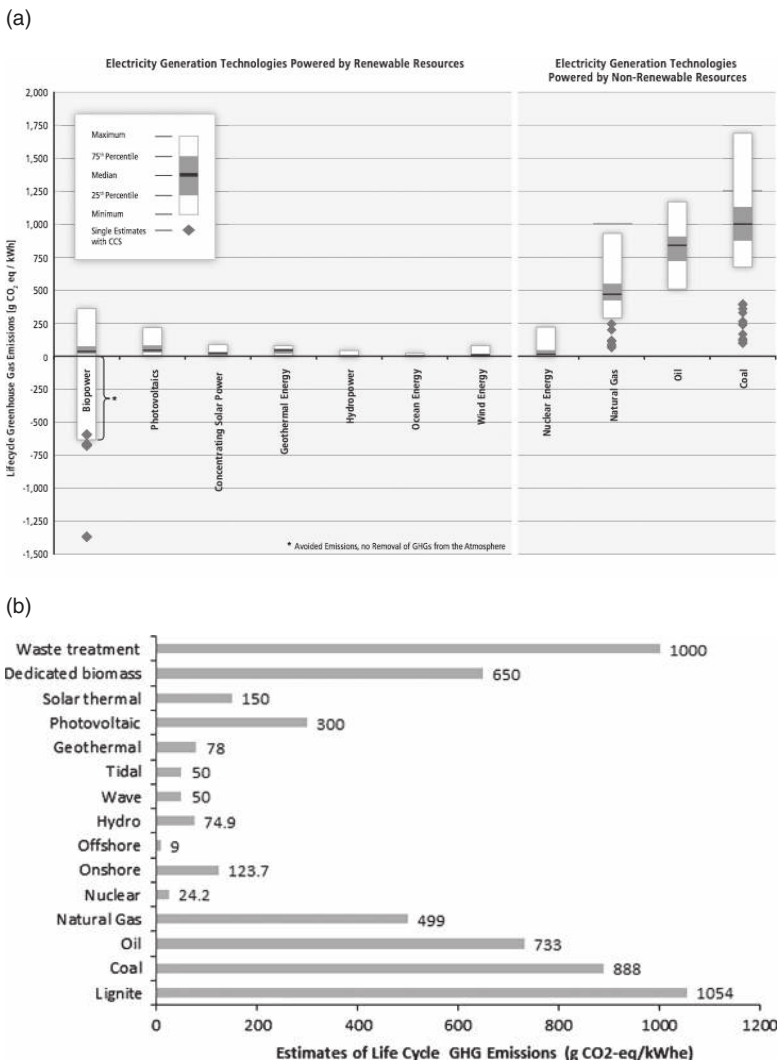

Figure 1.4 Estimates of GHG emissions in g CO_2-eq/kWh for various electricity generation methods. (a) A broad range with median reported in [12]. ©Cambridge University Press, 2011. (b) Maximum levels as reported in [15]. Reproduced with permission, © Elsevier, 2014.

battery pack is equivalent to 8500 liters of gasoline delivered to the tank. The details of this analysis, known as *cave to case* (CtC), can be found in [16].

1.1 Role of Combustion Technology

Global warming is truly a global problem and hence a globally agreed upon solution is going to be more effective than countrywise measures. Thus, concerted efforts across various nations (more aptly continents) are required so that GHG emissions across

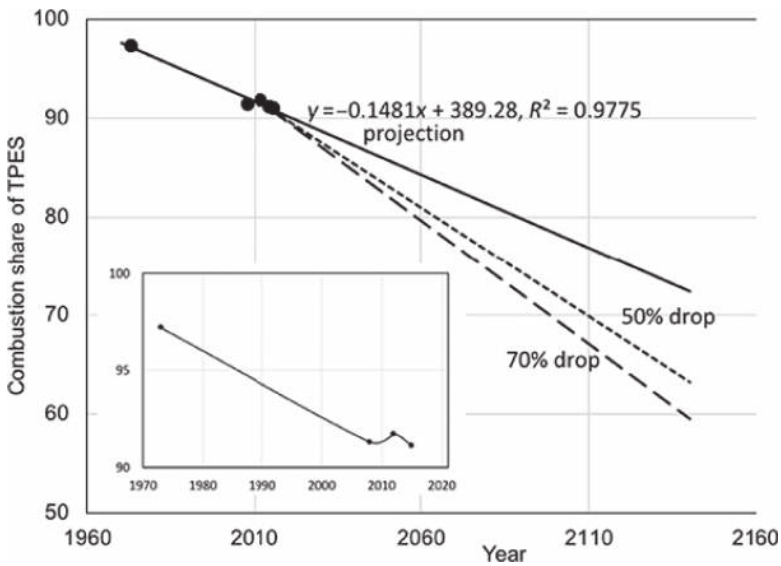

Figure 1.5 Combustion share of world TPES and its future projections.

the planet are reduced. While a complete shift toward renewable energies sounds attractive, it does not seem to be plausible in a short timescale set by various governments across the globe. These accelerative shifts, although desired in view of global warming mitigation, may likely accelerate global warming because the additional energy required to increase the TPES share of renewables (related to manufacturing and construction of these systems) has to come from nonrenewables. Thus, one needs a balanced approach to meet the ever increasing energy demands without aggravating global warming. Combustion technologies play an important role in this respect, which is clear from the results in Fig. 1.5 showing future projections of the potential combustion share of world TPES under three different scenarios [17]. The inset is the actual data from the International Energy Agency [1] showing a gradual decrease in the share of combustion. A small rise in 2012 is attributable to the increase in coal combustion in some countries around the world in that year. If one naively projects these data by assuming that the progress in renewable technologies to replace combustion to meet the energy demand is steady and organic following the current trends then the combustion share is likely to be more than 70% even by the year 2110 (the solid line). The slope of this curve is related to the progress and advancement of alternative energy technologies. If one keeps an optimistic view for these technologies progressing at an about 50% faster pace compared to the current trend then the combustion share falls just below 70% by 2110. This share decreases to 67% by the year 2110 even if one assumes optimistically that the alternative technologies progress at a 70% faster pace. It seems that a radical paradigm shift is required for a significant reduction of the combustion share. Whether this is practical or not is an open question. A pragmatic approach to mitigate the impact of combustion on

the environment is to seek alternative combustion concepts and technologies that can significantly reduce GHG emissions and can act as retrofits to the existing fossil and biofuel systems involving combustion. Fuel-lean and MILD (moderate, intense or low dilution) combustion concepts emerge as potential solutions, since they have potentials to deliver both low emissions and high efficiency. However, using them for practical applications brings their own challenges, as pointed out in the book edited by Swaminathan and Bray [18].

1.2 Setting the Stage

The discussion in the previous section identified that combustion science and technology will play an important role in meeting our future energy demand. The question is how can one minimize the impacts of combustion (of not only fossil fuels but also other fuels such as biomasses, biofuels, solid waste, etc.) on the environment, since combustion will emit oxides of carbon, hydrogen, nitrogen, and other elements present in the fuel. Many of these oxides are known to be hazardous and detrimental to the environment and also to life. For example, the aldehydes coming from biofuel combustion are toxic to both life and the environment. Hence, the challenging question in front of us is, *how can we control and minimize the formation of these oxides and chemicals in combustion processes?* Also, how do we use hydrocarbon fuels in the most efficient and environmentally responsible way to meet our ever-growing demand for energy? These questions will remain even if one moves away from the carbon economy completely or into a carbon-neutral economy in view of sustainability. Advancing combustion science is imperative to find answers to these challenging questions and it is not quite right to say that the intricacies in this field are well understood. If that is the case then we should be able to build "green combustion systems" (with high efficiency and low impact on the environment) and one knows that we are quite far from this!

Turbulent combustion in many practical systems is complicated for a number of reasons such as complex geometries, multiple phases involved and energy exchange among these phases, operating conditions involving elevated temperature and pressure, and also radiative heat exchange between hot gases and the walls of the system. The reactivity and chemical pathways at elevated temperature and pressure conditions can yield unexpected behaviors compared to normal temperature and pressure conditions as noted in [19]. For example, the laminar flame speed can increase with pressure for elevated temperature while it is expected to decrease with pressure based on studies conducted at normal temperature. The chemical pathways and their attributes and significance can change at elevated temperature and pressure, leading to unexpected behavior. Hence one needs to be cautious in extending our knowledge and wisdom to new operating conditions.

Radiative heat transfer is dealt with elaborately in many textbooks on heat transfer. So, this topic is discussed only briefly when and where required in this book and other complexities are covered to good extent. Liquid fuels have to be atomized and

vaporized first whereas solid fuels undergo pyrolysis, producing combustible gases. Therefore, combustion typically occurs in the gas phase in almost all practical systems. The final phase of solid fuel combustion involves a heterogeneous reaction on the char surface because of oxygen transported to the surface through diffusion processes. Nevertheless, the fraction of heat release from the char oxidation is relatively small compared to that from the gas phase combustion. Also, the minerals in the solid fuels end up as ash in various forms. Handling all these complexities with scientific rigor is very challenging and typically some empirical approximations are made. A similar approach of employing empirical relations is also used for descriptions of liquid spray and atomization processes.

Turbulent combustion of gases is classically investigated by separating turbulence and combustion by assuming that the relevant combustion timescales are shorter than those for turbulence. This led to the development of the *flamelet* modeling approach, which has been discussed elaborately in many textbooks, for example, [20, 21]. Although the aforementioned separation is artificial, this approach is shown to work well for many practical applications. However, alternative theories are required to predict pollutants and their formation, since their timescales are not small enough to separate them from those for turbulence. So, many approaches such as transported probability density function and conditional moment closure were proposed in past studies and these approaches are being developed further to improve their performances. The flamelet and nonflamelet approaches have been developed for both non-premixed and premixed combustion, which are two classical limits studied extensively. Combustion in modern practical systems such as gas turbine engines and direct injection internal combustion engines belongs to neither of these two limits but falls within partially premixed combustion. This mode is more complex compared to the two classical modes because it involves a wide range of equivalence ratios and the fuel–air mixing and combustion proceed together. These aspects create further complexities, creating a close coupling among turbulence, mixing, and combustion. Thus, one needs to be cautious and careful while extending the learnings from the two classical modes of combustion to the partially premixed combustion. Also, combustion with vitiated air having low oxygen is employed for stationary gas turbines to reduce nitrogen oxides (NOx) emissions. Recent investigations using direct numerical simulation (DNS) methodology showed that the combustion with vitiated air has its own distinctive features while sharing some attributes of classical combustion modes. The propulsion devices for high-speed air transport applications involve combustion in a supersonic stream and it is likely that supersonic combustion may share some of the distinctive features of vitiated air combustion.

Three numerical approaches, namely DNS, large eddy simulation (LES), and Reynolds-averaged Navier–Stokes (RANS) calculation, are used to study turbulent combustion. These approaches involve different levels of detail, approximations, and modeling. The complete set of conservation equations is solved with no models using high-order numerical schemes in the DNS approach and further details are discussed in Section 1.6. In the LES approach discussed in Section 1.7, the contributions and effects of small scales, which are known as subgrid scales, are filtered out and

modeled. The combustion and associated chemical reactions are typically small-scale phenomena and thus they need to be modeled. Appropriately averaged conservation equations are solved in the RANS approach discussed briefly in Section 1.8. These averaged equations need quite a large number of models and approximations, which are discussed elaborately in many past works; for example, see the books edited by Libby and Williams [22, 23] and the works in [18]. Thus, we aim to provide a discussion in view of LES of turbulent combustion, with related modeling, and physical insights. The importance of laser diagnostics cannot be understated in providing valuable information to improve our physical understanding of turbulent combustion and reliable statistics for model validations and developments. It is imperative that there be closer interactions among experimentalists, modelers, and theoreticians working in the field of combustion and related areas to find answers to the challenging questions such as those identified in the preceding text and to recognize the role of combustion in meeting the ever-increasing energy demand with minimal environmental impact.

1.3 Governing Equations

In this section, governing equations for combustion of gaseous fuels are discussed. These equations require additional source terms or interphase boundary conditions when combustion of liquid and solid fuels is considered. Details of the source terms or interphase boundary conditions in liquid and solid fuel combustion will be discussed in Chapters 8 and 9 respectively.

Combustion of gaseous fuels involves multiple constituents, say N_s different species. Some of these species will be consumed and some will be produced in chemical reactions. The turbulent combustion process is governed by three basic conservation laws: the conservation of mass, momentum, and energy. Transport equations for the species mass fraction, momentum, and energy can be derived from these basic conservation laws, as discussed in the text that follows.

Since different species in the system have different molecular weights, different species generally have different macroscopic velocities. This velocity is different from the microscopic velocity of each individual molecule. The macroscopic velocity of species α ($\alpha = 1, 2, 3, \ldots, N_s$) is an averaged quantity of many molecules and it is not directly related to the temperature as is the microscopic (molecule) velocity.

Let us write the velocity of species α as $\mathbf{u}_\alpha$. One may define a mass-weighted average velocity for the mixture as $\mathbf{u}$, viz.,

$$\mathbf{u} = \sum_{\alpha=1}^{N_s} Y_\alpha \mathbf{u}_\alpha, \tag{1.1}$$

where Y_α is the mass fraction of species α. The difference between velocity of species α and the mass-weighted average velocity of the mixture is known as the diffusion velocity of species α,