Chapter 8
The Emerging Role of Multiscale Methods in Turbulent Combustion

Tarek Echekki

Abstract Turbulent combustion flows are governed by processes that span the range from atomistic scales to device (e.g. engine) scales and beyond (e.g. oil pool fires, thermo-nuclear flames in type Ia supernovae). The multiscale nature of turbulent combustion flows poses both challenges and opportunities. The challenges arise from the need to predict combustion phenomena that are governed by a broad range of scales. The opportunities arise because of the emergence of the multiscale science that permeates many fields, and which for turbulent combustion, has been motivated by the need to predict phenomena in new and evolving combustion technologies, advances in computational and applied mathematics, and the increasing availibility of computational resources. In this chapter, strategies and requirements for the multiscale modeling and simulation of turbulent combustion flows are discussed. The chapter serves as an introductory chapter to Part III of this book.

8.1 Motivation

A principal challenge in predicting turbulent combustion flows arises from their multiscale nature. In a recent review, Peters [36] highlighted some complexities that arise in the prediction of multiscale phenemena associated with chemistry, flame structure, and flame interactions with turbulence. While Peters' review, a more recent review by the author [12] and the present chapter are timely, concrete ideas about addressing the multisale nature of turbulent combustion flows have been implemented for many decades. In physical sciences, constitutive relations (e.g. viscous stresses for Newtonian fluids) are used to represent processes on the molecular scale in a form applicable to macro-scale formulations (e.g. continuum conservation equations for fluid flow). These relations effectively represent multiscale treatments that eliminate the need to resolve atomistic effects. More specifically in com-

Tarek Echekki
North Carolina State University, Raleigh NC 27695-7910, USA, e-mail: techekk@ncsu.edu

T. Echekki, E. Mastorakos (eds.), *Turbulent Combustion Modeling*,
Fluid Mechanics and Its Applications 95, DOI 10.1007/978-94-007-0412-1_8,

bustion, turbulent combustion paradigms that rest on the principle of separation of scales have been the cornerstone of turbulent combustion models in computational fluid dynamics (CFD) for more than three decades. The eddy-dissipation model (EDM) [27], the eddy break-up model (EBU) [42] and the flamelet model [34] are based on separating the chemical time scales from turbulent time scales or flame length and time scales from the corresponding turbulence scales, respectively.

However, important advances in applied and computational mathematics and resources combined with evolving requirements in novel combustion technologies are enabling the rapid development of various multiscale strategies for the prediction of turbulent combustion flows. These strategies represent important additions, and quite often extensions, to traditional paradigms in turbulent combustion [3].

The present chapter serves three primary objectives: 1) motivate the need for multiscale strategies for the modeling and simulation of turbulent combustion flows, 2) introduce some basic strategies adopted for these flows, and 3) preview the topics covered in Part III of this book, which deal with multiscale approaches for turbulent combustion. The remaining sections of the chapter are organized as follows. In Sec. 8.2, the multiscale nature of turbulent combustion flows is illustrated. In Sec. 8.3, the case is made for the development of multiscale approaches in turbulent combustion based on progress in multiscale science and the need to model evolving combustion technologies. Fundamental considerations for multiscale approaches in turbulent combustion are discussed in Sec. 8.4. A brief survey of multiscale approaches and a preview of related chapters are presented in Sec. 8.5.

8.2 The Multiscale Nature of Turbulent Combustion Flows

Turbulent combustion flows exhibit a broad range of length and time scales, which encompass phenomena from atomistic to device scales. The most elementary processes at the molecular level, which are associated with the electronic structure of molecules and the breaking of chemical bonds, may occur at time scales as short as 10^{-15} s. However, simpler representations of chemical kinetics, such as through the Arrhenius law for the rate constant and the law of mass action, generally reduce the time-scale requirements to a range from approximately 10^{-10} s for the fastest reactions to a few seconds for the slower reactions. Nonetheless, the presence of a wide range of time scales represents an important challenge to the integration of chemistry and the coupling of this chemistry with transport for combustion problems.

Similar disparities are present for length scales. Molecular scales start with ranges of approximately 10^{-10} m. Beyond this, a broad range of scales represents the mechanisms of soot particle formation at molecular scales to hundreds of nanometers for soot particle aggregates [21]. A large gap separates these processes from continuum scales, which start around the scale of 1 μm. Beyond this range, and within the continuum regime, structures within the reaction zones of flames range in thickness from tens of μm (e.g. within the fuel consumption layer of premixed hydrocarbon flames) to a fraction of a millimeter corresponding to a laminar pre-

mixed flame thickness (including the entire reaction zone and a good portion of the preheat zone). Around this upper range of premixed flame thickness, there may be overlap with turbulent scales, starting from the Kolmogorov scale in practical combustion systems. The upper range of the turbulent scales may be comparable to the device scales, which may be of the order of tens of centimeters to meters. Therefore, a broad range of length scales represent the bulk of combustion processes from the atomistic to the device scale.

While the above so-called chemical flames appear untameable, thermonuclear flames, such as the ones encountered in type Ia supernovae exhibit even broader ranges of length and time scales [41, 49]. These flames exhibit much stronger nonlinearity in their nuclear source terms (carbon burning rate during ignition is proportional to the temperature to the 23rd power [49]), turbulence length scales spanning over eleven decades, and flame thicknesses, which are comparable to those of chemical flames [49].

Although, the basic processes of combustion may be described using established physical laws, their direct simulation is beyond today's and near-future computational capabilities. Current estimates of computing resources needed to resolve length scales place an upper limit of three decades of length scales for tera-scale computing and four decades of length scales for peta-scale [29]. Even if computer memory can accommodate large problems, time integration remains an important challenge, and many computations of turbulent reacting flows remain CPU-time-limited. Therefore, multiscale strategies are needed to capture the contribution of processes ranging from atomistic to device scales.

It is possible to carry out computations that are designed for a particular range of scales. For example, quantum dynamics calculations may be used to resolve the necessary electronic structure of molecules to determine kinetic rate parameters and heats of formations of molecules. Molecular dynamic simulations and kinetic Monte-Carlo simulations may be used to model soot processes [21] or to determine molecular transport properties. Fine- and coarse-grained continuum simulations, respectively, may be used to capture particular flame-turbulence interations or to model an actual device. Bootstrapping results from the different computations, which are specialized for different ranges of scales can be done through different strategies depending on the degree of coupling between scales. Here, we must distinguish between two types of coupling [12]: 1) physical coupling, which is associated with the presence of cause-and-effect between two processes occurring at different ranges of scales, and 2) scale coupling, which is associated with the presence of overlap between the length or time scales or both between two processes.

Many important applications in combustion involve a one-way coupling between processes operating at disparate scales. For these applications, various analytical and computational methods are available. Examples of such methods include:

- **Constitutive relations**: In reacting flows, the most common constitutive laws often represent models for atomistic processes in continuum governing equations. An obvious example is the relation between the rate-of-strain and viscous stresses in flows for Newtonian fluids. Another example of relevance to combustion includes the formulation of expressions for species reaction rates based on the Ar-

rhenius law and the law of mass action. Constitutive relations may be based on phenomenological laws (e.g. proportionality between two quantities and scaling relations) or may be derived from more rigorous analysis (e.g. the kinetic theory of gases).

- **Time-scale reduction**: In addition to constitutive relations, various methods of time-scale reduction may be adopted to represent fast processes, which are not coupled with transport, under the assumption of separation of scales and one-way coupling between processes. For example, chemistry reduction using dynamical systems approaches such as computational singular perturbation (CSP) [25] or the intrinsic low-dimensional manifold (ILDM) approach [38] can be used to tabulate the contribution of the 'fast' time scales and integrate primarily the remaining range of 'slow' scales. However, in contrast with traditional constitutive relations for chemistry and molecular transport, these latter approaches (e.g. CSP and ILDM) may depend on the mixture characteristics, the burning modes (e.g. premixed or diffusion flames) or the combustion regime (e.g. flamelet, distributed reaction).

Examples of problems that involve two-way physical coupling and scale separation includes the formation of soot in fires. In this problem, soot is a major contributor to radiative heat loss from the flame zone, and plays a critical role in determining the flame temperature. In turn, the temperature profiles within the flame also contribute to the formation of soot and its transport. Despite the presence of soot-flame coupling, multiscale strategies are enabled by scale separation. Instead of constitutive relations, which address single terms in the governing equations, moment transport equations may be adopted, which features models for transport (e.g. thermophoeresis) and sink and source terms (e.g. condensation, surface growth).

Other examples, which involve separation of scales and strong coupling between the scales, include flame-turbulence interactions in the flamelet regime and thermoacoustic coupling in a combustion chamber. When an account of the physical coupling is needed to represent physics at all scales, more robust formulations are needed that identify the dynamics of contributions across the scales.

Despite the prevalence of problems in combustion that exhibit scale separation, there is a growing need to address problems with strong physical and scale coupling. This need is addressed in the next section.

8.3 The Case for Multiscale Strategies in Turbulent Combustion

In recent years, important paradigm shifts have occurred in two relevant fronts associated with turbulent combustion flows. The first is associated with the emergence of novel combustion technologies that have pushed the envelope on the types of combustion regimes and modes encountered in practical devices. This shift also entails new requirements for the combustion performance and its prediction associated with combustion efficiency, flexibility of the combustion fuels and operating conditions, the mitigation of pollutants' emissions and safety [29]. The second shift is

associated with the emergence of the field of multiscale science as an important discipline in applied and computational mathematics and its increasing implementation in physical sciences. This emergence is fueled by increasing computational resources and technological innovations in various physical sciences (e.g. nanotechnologies, material science).

8.3.1 Emerging Combustion Technologies

New combustion technologies have been proposed in recent decades to address the clean and efficient burning of a growing range of combustion fuels [29]. These new technologies, invariably, push the envelope on the operational regimes of practical combustion devices. Two examples of combustion technologies illustrate these trends.

- In reciprocating internal combustion engines, there is a classical distinction between two competing technologies: diesel and spark-ignited engines, with the first more efficient and the second associated with cleaner burning. Alternative technologies have been proposed in recent years to overcome the limitations of each engine; these technologies include gasoline direct injection (GDI) engines, diesel low-temperature combustion (LTC) and homogeneous charge compression ignition (HCCI) engines [7, 29]. In HCCI engines, combustion is initiated by the compression ignition of nearly homogeneous mixtures of fuel and air, resulting in diesel-like efficiencies and lower emissions of NO_x particulate matter through better control of the charge and mixture conditions at combustion. Various control strategies may be adopted, which impact the competition between the rates of mixing and chemistry [7, 45]. When these rates are competitive, a separation of the chemical and transport scales is not feasible, and strategies to couple both effects are needed. Moreover, since the mixture homogeneity may evolve as chemistry evolves, different modes of combustion (with varying degrees of partial premixing) may be encountered during the HCCI combustion process [7].
- In gas turbine engines, strategies to lower emissions and increasing efficiency have been developed as well [5]. One strategy includes burning at lean or ultra-lean fuel-air mixture conditions. However, these conditions also may contribute to the onset of different, and often coupled, combustion instabilities [19]. Important manifestations of these instabilities may include the non-equilibrium effects of extinction and re-ignition events. Capturing non-equilibrium effects provide important challenges to the state-of-the-art turbulent combustion models.

Common among the above-stated problems are requirements of fuel flexibility as a broader range of combustion fuels are considered, including in addition to the standard fuels, heavy hydrocarbons (e.g. oil sands, oil shale) and renewable fuels (e.g. ethanol, biodiesel) [29]. With the above considerations, the traditional paradigms of turbulent combustion based on the assumption of separation of scales may not be applicable when mixing time scales are competitive with chemical time scales

or where well-established and stable combustion fronts (i.e. flames) determine the combustion process. More importantly, within the context of moment-based methods in turbulent combustion, three additional challenges emerge:

1. The choice and the number of appropriate transported moments is very critical to capture the desired physics. Generally, to capture more physics, such as extinction and re-ignition, more moments are needed.
2. Closure for non-linear terms in the moment transport equations is very critical as well, especially when different outcomes of the problem may be encountered (e.g. burning and non-burning solutions).
3. The prediction or the assumption of particular statistical distribution (e.g. joint scalars' probability density functions) becomes an additional challenge as well.

Moment-based models have been successful in predicting problems in combustion applications; however, they remain limited by their underlying assumptions, which may be related to the combustion mode (e.g. premixed vs. non-premixed), the combustion regime (e.g. flamelet vs. distributed reaction) or dominant chemistry. These assumptions determine the choice of transported moments, the implementation of closure in the moment equation and the reconstruction of the spatial statistical distributions for these moments. Significant progress has been achieved in all fronts as illustrated by results discussed in the various chapters of this book.

Multiscale strategies within the continuum regime may be used to replace potential empiricism in the closure for unclosed terms in the moment governing equations, construct more robust statistical distributions for the moments, or replace all moments altogether.

8.3.2 Emerging Multiscale Science

Multiscale science permeates many disciplines in the physical (e.g. solid and fluid mechanics, biological systems, chemistry), mathematical and computational sciences. It is concerned with problems and phenomena where an account for a broad range of scales is needed. Renewed interest in multiscale science is motivated in part by growth in computational resources, which in turn fuel interest in computing larger problems in the physical sciences. This growth has enabled scientists and engineers to go beyond scale-specific applications and tools (e.g. quantum dynamics vs. continuum-based calculations) to address the solution of larger problems and couple different scales within the same problem. Invariably, the attempts within the various disciplines are different because of modeling requirements and the extent to which scales are coupled.

Important developments in multiscale science reflect growth in a number of important areas:

- The development of robust mathematical frameworks and scale coupling strategies designed to accurately represent the contribution of all relevant scales and their coupling. A mathematical framework is distinct from the individual

model(s) used for the different scales and in different applications. Therefore, they may be applicable to a broad range of problems. The choice of a particular framework depends on a number of factors, which include the extent of coupling (physical and scale) between the different phenomena and the type of inter-dependence between the scales. Therefore, a principal goal of the mathematical frameworks is to reduce the mathematical complexity of multiscale problems associated with their high-dimensionality, high degrees of freedom and the complex inter-dependence between phenomena at different ranges of scales. Two mathematical frameworks appear to be very promising for the study of turbulent combustion flows: the heterogeneous multiscale method (HMM) [9], and variational multiscale method (VMS) [20]. Chapter 18 illustrates the implementation of the HMM for the coupling of multiple scale solutions associated with turbulent flame propagation in turbulence. Although the implementation of VMS for non-reacting turbulent flows has been extensively studied, only recently an extension of VMS for variable-density flows has been formulated [18].

- The development of efficient numerical tools and computational frameworks: Computational tools may include parallel solvers for partial differential equations, linear-algebra suites, multiresolution utilities for the decomposition of the solution vector or data analysis, adaptive mesh refinement tools and other relevant applications. The various computational tools may be common among different disciplines. Therefore, potentially a large pool of users may contribute to their developments. However, certain rules must be put in place to ensure the tools' portability across computational platforms and applications. Chapter 17 illustrates a computational framework that enables a collaborative environment for various tools' development based on the common-component architecture paradigm. The chapter also illustrates the implementation of such a framework for combustion problems.

8.4 Multiscale Considerations for Turbulent Combustion

As stated earlier, mathematical and computational frameworks for the development of multiscale approaches may be shared among different disciplines. However, the choice of which frameworks to adopt and the individual models that represent physics at the different scales is different for each discipline. What drives the choice are the characteristics of the problem, which include: 1) the extent of coupling physical and scale coupling between the different phenomena at different scales, and 2) the choice of the models that are approriate to capture physics at the different scales. This latter consideration is very unique, as it dictates strategies for reduction of order or dimensionality of the problem and the type of closure needed to capture unresolved physics. In the following sections, basic requirements for multiscale approaches and choices of the physical models are discussed. Some of these requirements and associated multiscale approaches may be extended to a broader range of problems beyong turbulent combustion flows [26].

8.4.1 Basic Requirements for Multiscale Approaches in Turbulent Combustion

Important aspects of the multiscale nature of turbulent combustion flows have already dictated the choice of traditional paradigms in turbulent combustion. The first aspect is the prevalence of flames which can propagate and be wrinkled by turbulent flows. These flames represent interfaces between reactants and products, fuels and oxidizers, as well as zones of localized reaction and heat release. In numerous applications, these flames can be thin; and therefore, strategies to couple detailed reactions zones at the interface with fluid dynamics form one potential multiscale approach in turbulent combustion. Indeed, flame-embedding (see Chapter 12) represents one such strategy. Mathematical multiscale frameworks for flame embedding are concerned with the implementation of coupling strategies between the flame solutions and the flow field. Illustrations of such coupling using the heterogeneous multiscale method (HMM) are given in Chapter 18. When flames are present, potential strategies to reduce the physical dimension of the flame solutions are enabled due to the strong gradients along the flame normal.

A second aspect of the multiscale nature of turbulent combustion flows is the clear separation between atomistic scales and continuum scales. Therefore, robust constitutive equations for reaction and molecular transport in the continuum governing equations are a viable substitute to hybrid atomistic-continuum simulations. Nonetheless, there is great effort to be expanded in both scale regimes to develop chemical rate and transport data from atomistic simulations and device-scale simulations from the continuum equations.

Finally, given the non-linear nature of the governing equations, the presence of many coupled variables representing both flow and scalar quantities, and the coupling between fine and coarse scales in combustion, analytical methods (e.g. homogenization, asymptotic methods, renormalization group methods) by themselves are not sufficient to solve or separate scales in turbulent combustion flows. Instead, these tools can be coupled with numerical techniques to develop robust multiscale frameworks for these flows.

At this stage, it is useful to re-iterate the basic desirable attributes for multiscale approaches in turbulent combustion. These approaches are subject to the following constraints:

- All time and length scales are resolved at least within the context of continuum-based transport equations and including a closed-form treatment of chemistry and molecular transport processes using constitutive relations.
- The models must preserve structure (e.g. flames) involving the coupling of reaction and diffusion transport.
- No statistical distribution shapes may be assumed for the reactive scalars; and this distribution must be reconstructed, if needed, as part of the multiscale solution.

8.4.2 General Frameworks for the Governing Equations for Multiscale Models of Turbulent Combustion

The description of the turbulent flow of a multicomponent reacting mixture is prescribed through a set of conservation laws for mass, momentum and composition and auxiliary equations. The most common representation of these laws in the continuum regime are extensions of the Navier-Stokes equations (Eq. 2.2).

In Chapter 2, different mathematical forms of these governing equations in the continuum regime are presented. They include the instantaneous forms used in direct numerical simulations (DNS) and forms involving ensemble/time averaging (i.e. RANS formulations) and spatial averaging (or filtering) (i.e. LES). Averaging, invariably, results in unclosed terms in the governing equations, which must be modeled.

Within the context of multiscale frameworks, only the instantaneous and the LES governing equations enable scale separation. In LES, coarse scales are resolved; while, the smaller scales have to be modeled. In contrast, RANS averaging impacts all scales, and closure compensates for information that is 'lost' across all the scales. Therefore, based on the instantaneous and the LES formulations, two principal classes of multiscale strategies emerge. The first is based on the concept of 'mesh adaptivity' and involve the use of the same set of governing equations and the adoption of a hierarchical grid structure. The level of resolution within this grid structure depends on the spatial and temporal resolution requirements within different zones of the computational domain. The second strategy is based on hybrid combinations of a fine- and a coarse-grained solutions and may adopt a LES implementation for the coarse-grained solution. For the fine-grained solution, different strategies for reducing the model complexity at the small scales may be adopted.

It is important to note that within the context of LES, various extensions of the traditional LES approach may be adopted for turbulent combustion flows. Multilevel strategies may be derived within various contexts, such as homogenization approaches [15] and the variational multiscale method [20].

An alternative strategy to the extended Navier-Stokes formulations is the Boltzmann-Maxwell equation, which models the temporal and spatial evoution of one-particle distribution function. The lattice-Boltzmann method (LBM) is a computationally efficient method to solve the Boltzmann-Maxwell equations. In contrast to the well-established conservations laws based on the Navier-Stokes equations, the LBM approach is more recent. Yet, it is becoming an increasingly popular alternative to the Navier-Stokes approach for the solution of complex fluids. LBM can be used to effectively straddle sub-continuum and continuum phenomena; therefore, it may be viewed primarily as a mesoscale approach. Moreover, LBM can naturally accomodate a variety of boundary conditions, including prescribed conditions across fluid phases. The LBM is discussed in detail in Chapter 19.

8.5 Multiscale Approaches in Turbulent Combustion and Preview of Relevant Chapters

The sections below summarizes different strategies to model turbulent combustion flows. Although restricted to only one component of turbulent combustion models, chemistry acceleration is included and an entire chapter (Chapter 9) is dedicated to this topic. The present multiscale strategies in turbulent combustion may be associated closely with either established multiscale numerical/mathematical frameworks or traditional paradigms in turbulent combustion as discussed below. The various approaches can be classified as follows:

1. Time-step acceleration and mesh adaptive methods
2. Flame embedding methods
3. Hybrid LES and low-dimensional models

A brief discussion of the various approaches is provided below:

8.5.1 Time-Step Acceleration

Chemistry integration represents a critical bottle-neck in the time-integration of reactive scalar equations. The disparity of time scales between the fastest and the slowest reactions or time-steps required to resolve transport is at the heart of the stiffness problems in chemical mechanisms. Strategies to accelerate the time-integration of chemistry are based on a combination of different approaches. They include:

- **Chemical mechanism reduction** This step addresses the reduction of the size of the representative species and reactions. Chemistry reduction may involve, as a first step, the development of a skeletal mechanism that contains the most relevant species and elementary reactions. In a second step, a more aggressive reduction strategy may be adopted to develop a global mechanism with even fewer species and global steps. This second step may render the reduction process applicable to a more limited range of problems. More importantly, it does not guarantee that the resulting global mechanism removes the original mechanism stiffness. Important progress has been achieved to address mechanism reduction from the classical strategies of the quasi-steady state (QSS) and the partial equilibrium (PE) approximations, to more systematic model reduction strategies, such as the ones based on the ILDM and the CSP approaches. Chapter 9 provides an extensive review of chemistry reduction strategies.
- **Numerical stiff and mildly-stiff integrators** In the past, stiff chemistry integration have been addressed through implicit integrators, such as VODE [4] and DASSL [37]. However, more recently, explicit as well as implicit-explicit integrators have been developed that are used to efficiently and accurately integrate stiff and mildly stiff ordinary and partial differential equations. There is inherently a trade-off between the computational cost, numerical accuracy and the

coupling requirements with transport operators that must be taken into consideration.

- **Chemistry tabulation, storage and retrieval approaches** Another important strategy for chemistry acceleration is the development of storage and retrival strategies for tabulation results of chemistry integration. Efficient strategies for tabulation, storage and retrieval are available, including the in situ adaptive tabulation (ISAT) algorithm [39], the piece-wise reusable implementation of solution mapping (PRISM) [43] and artificial neural networks (ANN) [6].

8.5.2 Mesh Adaptive Methods

As outlined earlier, one principal consideration for multiscale approaches in turbulent combustion is that combustion and important scalar and velocity gradients may be associated with well-defined regions in the flow (e.g. flames). Mesh adaptivity is based on adapting the spatial resolution (and accordingly, the temporal resolution) to capture fine details of the flow and the scalar field when needed and coarsen when not needed. Mesh adaptive methods can be implemented within the context of both instantaneous and statistical models (e.g. LES).

Chapters 13 and 14 illustrate two adaptive mesh strategies. The first is based on the adaptive mesh refinement (AMR) approach [2] (Chapter 13). In this approach, a recursive refinement of the mesh is implemented until resolution requirements are met within a region of the flow. The second approach is based on the multiresolution wavelet approach [40] (Chapter 14). This approach is based on a decomposition of the solution into spatially- and temporally-varying multiresolution modes (e.g. wavelet modes) to capture the solution at different multiresolution levels.

8.5.3 Flame Embedding Approaches

Flame embedding strategies may represent an extension of the flamelet paradigm [34]; although, some of the ideas of flame-embedding have been proposed earlier [17]. A principal outcome of the flamelet paradigm is the separation of the flame scales from the energetic flow scales, enabling a degree of decoupling of the flamelet and the flow solutions. Therefore, three important implementation elements associated with flame embedding are needed: 1) a solution of the flowfield, 2) a flame solution, and 3) flame tracking.

Through the decoupling of the flow and flamelet solutions, different strategies may be adopted to resolve the flow (e.g. vortex methods) and the reactive scalar within the flame. For the flame, two principal approaches may be identified, which correspond to 1) flame-normal embedding, and 2) flamelet tabulation. Chapter 12 discusses primarily flame-normal strategies where 1D flames are solved along the flame surface normal with prescribed input parameters from the flowfield (e.g. strain

rate). Another strategy is based on the transport of a representative scalar for flame tracking and the tabulation of the remaining reactive scalars, such as approaches based on the flamelet-generated manifold (FGM) [44] and the flame-prologation of ILDM (FPI) schemes [13].

Flame embedding strategies can be implemented within the context of the instantaneous equations or statistical models. In these latter models, flamelet solutions with sufficient variability in time and space are used to build statistical models of the flame response in turbulence. Examples of such strategies include the use of the LEMLES approach based on the linear-eddy model (LEM) (see Chapter 10); although, the same strategies may be adopted using the ODTLES approach based on the one-dimensional turbulence (ODT) model (see Chapter 11). More recently, Fureby [15] proposed a homogenization-based LES (hLES) approach, which converts the governing equations into a cascade of equations at different scales. Fureby [15] implemented a flame-embedding strategies using one-dimensional forms of the equations at different scales.

Tabulation strategies represent alternative approaches to *in situ* flame calculations. These approaches represent an extension of the strategies adopted with FGM and FPI. Here, we cite the recent work of Vreman et al. [47] and Fiorina et al. [14]. In both studies, it is proposed that filtered reaction rate solutions of reactive scalars are constructed by filtering of one-dimensional flame solutions.

8.5.4 Hybrid LES-Low-Dimensional Models

Potentially more versatile methods may involve a hybrid formulation involving LES combined with a low-dimensional model for subgrid scale (SGS) physics. Statistical flame-embedding approaches represent an important sub-class of hybrid methods; however, the more general hybrid strategies do not require fine-grained flame solutions to be attached to flame normals or tabulated via transported reactive scalars. Hybrid methods are primarily designed to construct statistical information, such as subgrid scale source terms or filtered scalar quantities. Because a hybrid scheme that spans the range of scales of interest is ultimately costly, strategies for dimensional reduction are needed. The different hybrid strategies adopted for such hybrid LES schemes generally involve either a stochastic or a dynamical-systems formulation incorporated with a reduced physical dimension or a lower order of the solution vector. Among the frameworks adopted for turbulent combustion, we cite:

- Low-dimensional stochastic models, including the linear-eddy model (LEM) [23] (Chapter 10) and the one-dimensional turbulence (ODT) model [24] (Chapter 11).
- Transported probability and filtered density functions with structure-based mixing models (e.g. the PSP approach by Meyer and Jenny [30]).
- The homogenization-based LES (hLES) approach [15].
- The chaotic map approach by McDonough and co-workers [28, 31].

Low-dimensional stochastic models, including the LEM and ODT models, involve the embedding of one-dimensional domains within the 3D computational domain. The 1D transport equations for each LEM or ODT domain feature the usual terms in the governing equations for momentum (in the case of ODT) and scalars, albeit in 1D. The resolution requirements are DNS-like and the computational saving is derived principally from the reduced dimension.

The chaotic map model [28, 31] is based on a fundamentally different strategy from that adopted using 1D stochastic models. The model is based on an estimation procedure for the reactive scalars based on a definition of a chaotic dynamical system. In the chaotic map approach, residual terms of reactive scalars (i.e. instantaneous subtracted filtered values) are represented at each discrete grid point as the product of an amplitude factor, which is derived from classical theories of isotropic turbulence, an anisotropy correction factor, and components of a discrete dynamical system (DDS), whose governing equations are derived from the original reactive scalars transport equations [28, 31]. An additional component of the derivation is the discretization of the solution vector for the reactive scalars into a Fourier series in which only leading coefficients are retained and ordinary differential equations for the Fourier coefficients are solved.

8.6 Concluding Remarks

The direct resolution of all scales in turbulent combustion flows is practically impossible given their multiscale nature. In this chapter, some of the basic challenges and opportunities towards the development of multiscale strategies for turbulent combustion flows are discussed. A principal goal of these strategies is to provide viable alternatives to the traditional closure problem in turbulent combustion, when these latter models fail or are limited in their predictions. The emergence of such strategies is dictated by technological requirements for combustion, advances in computational sciences and the increasing availability of powerful computational resources. A principal challenge to tackle is associated with the representation of chemisty as a critical bottleneck in the temporal integration of solutions of reacting flows. Multiscale approaches for turbulent combustions are based on two general strategies based on either mesh-adaptivity or model-adaptivity. Adaptive mesh refinement (Chapter 13) and wavelet-based methods (Chapter 14) represent promising examples of multiscale approaches based on mesh-adaptivity. Model-adaptive approaches primarily adopt the coupling of fine-scale reduced dimension or order solution and coarse-scale solutions, such as LES. Chapters 10, 11 and 12 illustrate different applications of such model-adaptive methods.

Acknowledgement

Dr. T. Echekki acknowledges support from the Air Force Office of Scientific Research through grants F49620-03-1-0023 monitored by Dr. Julian Tishkoff and FA9550-09-1-0492 monitored by Dr. Fariba Fahroo and the National Science Foundation through grant DMS-0915150 monitored by Dr. Junping Wang.

References

1. Bell, J.B., Day, M.S., Grcar, J.F., Lijewski, M.J., Driscoll, J.F., Filatyev, S.A.: Numerical simulation of laboratory-scale turbulent slot flame. Proc. Combust. Inst. **31**, 1299–1307 (2009)
2. Berger, M., Oliger, J.: Adaptive mesh refinement for hyperbolic partial differential equations. J. Comput. Phys. **53**, 484–512 (1984)
3. Bilger, R.W., Pope, S.B., Bray, K.N.C., Driscoll, J.F.: Paradigms in turbulent combustion, Proc. Combust. Inst. **30**, 21–42 (2005)
4. Brown, P.N., Byrne, G.D., Hindmarsh, A.C.: VODE: A variable coefficient ODE solver. SIAM J. Sci. Stat. Comput. **10**, 1038–1051 (1989)
5. Correa, S.M.: Power generation and aeropropulsion gas turbines: From combustion science to combustion technology. Proc. Combust. Inst. **27**, 1793–1807 (1998)
6. Christo, F.C., Masri, A.R., Nebot, E.M.: An integrated PDF/neural network approach for simulating turbulent reacting systems, Proc. Combust. Inst. **26**, 43–48 (1996)
7. Dec, J.E.: Advanced compression-ignition engines – understanding the in-cylinder processes. Proc. Combust. Inst. **32**, 2727–2742 (2009)
8. Dubois, T., Jauberteau, F., Teman, R.: Dynamic Multilevel Methods and the Numerical Simulation of Turbulence. Cambridge University Press (1999)
9. E, W., Engquist, B.: The heterogeneous multiscale method. Comm. Math. Sci. **1**, 1062–1070 (2003)
10. E, W., Engquist, B.: Multiscale modeling and computation. Notices AMS **50**, 1062–1070 (2003)
11. E, W., Engquist, B., Huang, Z.: Heterogeneous multiscale method: A general methodology for multiscale modelign. Phys. Rev. B **67**, 092101 (2003)
12. Echekki, T.: Multiscale methods in turbulent combustion: strategies and computational challenges. Comput. Sci. Disc. **2**, 013001 (2009)
13. Fiorina, B., Baron, R., Gicquel, O., Thevenin, D., Carpentier, S., Darabiha, N.: Modelling non-adiabatic partially premixed flames using flame-prolongation of ILDM. Combust. Theory Model. **7**, 449–470 (2003)
14. Fiorina, B., Vicquelin, R., Auzillon, P., Darabiha, N., Gicquel, O., Veynante, D.: A filtered tabulated chemistry model for LES of premixed combustion, Combust. Flame. **157**, 465–475 (2010)
15. Fureby, C.: Homogenization based LES for turbulent combustion. Flow Turbul. Combust. **84**, 459–480 (2010)
16. Galpin, J., Naudin, A., Vervisch, L., Angelberger, C., Colin, O., Domingo, P.: Large-eddy simulation of a fuel-lean premixed turbulent swirl-burner. Combust. Flame **155**, 247–266 (2008)
17. Ghoniem, A.F., Chorin, A.J., Oppenheim, A.K.: Numerical modeling of turbulent combustion in premixed gases. Proc. Combust. Inst. **18**, 1375–1385 (1981)
18. Gravemeier, V., Wall, W.A.: Residual-based variational multiscale methods for laminar, transitional and turbulent variable-density flow at low Mach number. Int. J. Num. Meth. Fluids, DOI:10.1002/fld.2242 (2009)
19. Huang, Y., Yang, V.: Dynamics and stability of lean-premixed swirl-stabilized combustion. Prog. Energy Combust. Sci. **35**, 293–364 (2009)

20. Hughes, T.J.R., Mazzei, L., Jansen, K.E.: Large eddy simulation and the variational multiscale method. Comput. Vis. Sci. **3**, 47–59 (2000)
21. Izvekov, S., Violi, A.: A coarse-grained molecular dynamics study of carbon nanoparticle aggregation. J. Chem. Theory Comput. **2**, 504–512 (2006)
22. Keller, J.J.L.: Thermoacoustic oscillations in combustion-chambers of gas-turbines. AIAA J. **33**, 2280–2287 (1995)
23. Kerstein, A.R.: Linear-eddy modeling of turbulent transport. II: Application to shear layer mixing. Combust. Flame **75**, 397–413 (1989)
24. Kerstein, A.R.: One-dimensional turbulence: Model formulation and application to homogeneous turbulence. J. Fluid Mech. **392**, 277–334 (1999)
25. Lam, S.H., Goussis, D.A.: Understanding complex chemical kinetics with the computational singular perturbations. Proc. Combust. Inst. **22**, 931–941 (1988)
26. Law, C.K. Combustion at a crossroads: Status and prospects. Proc. Combust. Inst. **31**, 1–29 (2006)
27. Magnussen, B.F., Hjertager, B.H.: On mathematical modeling of turbulent combustion with special emphasis on soot formation and combustion. Proc. Combust. Inst. **16**, 719–729 (1976)
28. McDonough, J.M., Huang, M.T.: A low-dimensional model of turbulence-chemical kinetics interactions. Proc. Third Int. Symp. Scale Model (10–13 September 2000, Nagoya, Japan) Paper ISSM3-E8 (2000)
29. McIlroy, A., McRae, G., Sick, V., Siebers, D.L., Westbrook, C.K., Smith, P.J., Taatjes, C., Trouvé, A., Wagner, A.E., Rohlfing, E., Manley, D., Tully, F., Hilderbrandt, R., Green, W., Marceau, D., O'Neal, J., Lyday, M., Cebulski, F., Garcia, T.R., Strong, D., Basic research needs for clean and efficient combustion of 21st century transportation fuels. Department of Energy Office of Science Report (2006)
30. Meyer, D.W., Jenny, P.: A mixing model for turbulent flows based on parameterized scalar profiles. Phys. Fluids **18**, 035105 (2006)
31. Mukerji, S., McDonough, J.M., Mengu, M.P., Manickavasagam, S., Chung, S.: Chaotic map models of soot fluctuations in turbulent diffusion flames. Int. J. Heat Mass Transfer **41**, 4095–4112 (1998)
32. Perrier, P., Pironneau, O.: Coupling large with small turbulent structures by theory of homogenization. Comptes Rendus Hebd. Seances Acad. Sci. Ser. A. **286**, 635–638 (1978)
33. Perrier, P., Pironneau, O.: Subgrid turbulence modeling by homogenization. Math. Model. **2**, 295–317 (1981)
34. Peters, N.: Local quenching due to flame stretch and non-premixed turbulent combustion. Combust. Sci. Technol. **30**, 1–17 (1983)
35. Peters, N.: Turbulent Combustion, Cambridge University Press, 2000
36. Peters, N.: Multiscale combustion and turbulence. Proc. Combust. Inst. **32**, 1–25 (2009)
37. Petzold, L.R., A description of dassl: A differential/algebraic system solver, SAND82-8637, Sandia National Laboratories (1982)
38. Pope, S.B., Maas, U.: Implementation of simplified chemical kinetics based on intrinsic low-dimensional manifolds. Proc. Combust. Inst. **24**, 103–112(1992)
39. Pope, S.B.: Computationally efficient implementation of combustion chemistry using in situ adaptive tabulation, Combust. Theory Model. **1**, 41–63 (1997)
40. Prosser, R., Cant, R.S.: On the use of wavelets in computational combustion. J. Comput. Phys. **147**, 337–61 (1998)
41. Röpke, F.K., Bruckschen, R.: Thermonuclear supernovae: a multi-scale astrophysical problem challenging numerical simulation and visualization. New J. Phys. **10**, 125009 (2008)
42. Spalding, D.B.: Mixing and chemical reaction in steady confined turbulent flames. Proc. Combust. Inst. **13**, 649–657 (1971)
43. Tonse, S.R., Moriary, N.W., Brown, N.J., Frenklach, M.: PRISM: piece reusable implementation of solution mapping. An economical strategy for chemical kinetics. Isr. J. Chem. **39**, 97–106 (1999)
44. van Oijen, J.A., de Goey, L.P.H.: Modelling of premixed laminar flames using flamelet-generated manifolds. Combust. Sci. Technol. **161**, 113–138 (2000)

45. Yao, M., Zheng, Z., Liu, H.: Progress and recent trends in homogeneous charge compression ignition (HCCI) engines. Prog. Energy Combust. Sci. **35**, 398–437 (2009)
46. Veynante, D., Fiorina, B., Domingo, P., Vervisch, L.: Using self-similar properties of turbulent premixed flames to downsize chemical tables in high-performance numerical simulations, Combust. Theory Model. **12**, 1055–1088 (2008)
47. Vreman, A.W., van Oijen, J.A., de Goey, L.P.H., Bastiaans, R.J.M.: Subgrid scale modeling in large eddy simulation of turbulent combustion using premixed flamelet chemistry. Flow Turbul. Combust. **82**, 511–535 (2009)
48. Westbrook, C.K., Mizobuchi, Y., Poinsot, T.J., Smith, P.J., Warnatz, J.: Computational combustion. Proc. Combust. Inst. **30**, 125–157 (2005)
49. Woosley, S.E., Almgren, A., Bell, J.B., Glatzmaier, G., Kasen, D., Kerstein, A.R., Ma, H., Nugent, P., Röpke, F., Sankaran, V., Zingale, M.: Type Ia supernovae. J. Phys.: Conf. Ser. **78**, 012081 (2007)