Large eddy simulation of turbulence-chemistry interactions in reacting flows

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Abstract. Application of the Large Eddy Simulation (LES) technique provides the formal ability to treat the wide range of multidimensional time and length scales that exist in turbulent reacting flows in a computationally feasible manner. The large energetic-scales are resolved directly. The small “subgrid-scales” are modeled. This allows simulation of the complex multiple-time multiple-length scale coupling between processes in a time-accurate manner. Treating the full range of scales is a critical requirement since turbulent processes are inherently coupled through a cascade of nonlinear interactions. This paper provides a perspective on LES and its application to turbulent combustion. In particular, the combination of LES, high-performance massively-parallel computing, and advanced experimental capabilities in combustion science offer unprecedented opportunities for synergistic high-fidelity investigations. Information from well-defined benchmark flames, using a combination of state-of-the-art experiments and detailed simulations that match the experimental conditions, present new opportunities to understand the central physics of turbulence-chemistry interactions. Understanding these fundamental physical processes, and developing advanced simulation capabilities that efficiently and accurately describe them, are crucial requirements for the development of next generation combustion systems. Results are shown that demonstrate the progression toward more complex systems, with emphasis placed on the fundamental issues of turbulence-chemistry interactions.

1. Introduction

The Large Eddy Simulation (LES) technique has now evolved over three decades, initially on the foundations laid by meteorologists at the National Center for Atmospheric Research [1, 2]. Over these 30 years, progress has been made in a manner largely facilitated by the significant increase in computational speed and capacity. With the advent of massively-parallel computer hardware, LES now provides a means to study coupled combustion, transport, and multiphase processes in parameter spaces that are unattainable using the Direct Numerical Simulation (DNS) technique, with a degree of fidelity that can be far more accurate than conventional methods such as the Reynolds-Averaged Navier-Stokes (RANS) approximation.

Turbulent flow involving heterogeneous chemically-reacting multiphase mixtures arise in many systems of engineering interest. Complicating factors include highly nonlinear chemical kinetics, small-scale velocity and scalar-mixing processes, turbulence-chemistry interactions, compressibility effects (volumetric changes induced by changes in pressure), and variable inertia effects (volumetric changes induced by variable composition or heat addition). Coupling between processes occurs over a wide range of time and length scales, many being smaller than can be resolved in a numerically feasible manner. Further complications arise when multiple phases are present due to the introduction of
dynamically evolving interface boundaries and the complex interfacial exchange processes that occur as a consequence.

Simulating combustion processes encountered in propulsion and power systems pose a particularly complex set of requirements. High-performance, dynamic stability, low pollutant emissions, and low soot formation must be achieved simultaneously in highly confined geometries that generate extremely complex flow patterns. Combustion processes within both the chamber and flow passages are inherently turbulent, and in many cases operating pressures approach or exceed the thermodynamic critical pressure of the fuel and oxidizer. Running at elevated pressures significantly increases the operational Reynolds numbers and broadens the range of space and time scales over which dynamic interactions occur. Additional complications arise as fluid states approach a supercritical condition.

DNS of the broadband processes described above is rarely feasible at practical conditions. Thus, simulating these phenomena almost always begins with some form of formal filtering of the governing conservation equations. The RANS approximation, for example, employs filtering in time to derive the governing conservation equations for the mean state. For this approach all dynamic degrees of freedom smaller than the largest energy containing eddies are averaged and no information exists to describe interactions between the small-scales. LES, on the other hand, has historically employed spatial filtering to split the field variables into time-dependent resolved-scale and subgrid-scale (sgs) components. For this approach the large energetic scales are resolved and sgs quantities are modeled to provide a complete time-accurate representation of dynamic processes over the full range of relevant time and length scales.

2. Approach
Issues related to combustion closures and the treatment of multiphase processes for LES are well known and a variety of approaches have been taken. In fact, the current level of activity is now much greater than can be reviewed in a single paper. Sources that focus on progress, current approaches, and the unresolved issues include the books by Peters [3], Pope [4] and Poinset and Veynante [5]. A recent set of reviews have also been published [6–10]. Here, we augment the discussion by focusing on the fundamental aspects of LES when applied to the conservation equations of mass, momentum, total energy and chemical species for a general class of reacting multiphase flows typically encountered in state-of-the-art propulsion and power systems.

High-performance massively-parallel computing coupled with advanced experimental capabilities in combustion science offer unprecedented opportunities for synergistic high-fidelity investigations of combustion phenomena. The individual elements provide a strong scientific base. The combined elements provide new paradigm for scientific discovery. The objective of the current research is to systematically focus on select science-based applications where the combination of LES and experiments can have a direct impact on scientific discovery. Information from validated LES solutions, combined with detailed laser-based experiments on well-defined benchmark flames, present new opportunities to understand the central physics of turbulence-chemistry interactions and for the development of accurate predictive models for advanced combustion systems. Our goal is to address leading scientific challenges at the fundamental level in a manner that directly addresses leading engineering issues.

Key components required to achieve this objective are 1) implementation of a unique theoretical-numerical framework, 2) application of unique software and high-performance computational resources, 3) development of advanced models aimed at direct closure of the chemical source terms, 4) rigorous model validation using data acquired from select target experiments, and 5) detailed characterization of complex combustion processes through joint-analysis of data. Here we combine a general treatment of the governing conservation and state equations with state-of-the-art numerical algorithms and massively-parallel programming paradigms. Detailed formulations and recent results are given by Oefelein et al. [11–13]. In the discussion below, we present a systematic progression of case studies that highlight key aspects related to the current state-of-the-art.
3. Theoretical Framework

The approach described above has been enabled through a unique theoretical-numerical framework developed over the last decade. This framework solves the fully coupled conservation equations of mass, momentum, total-energy and species for a general class of chemically reacting flows in complex geometries. The numerical formulation treats the fully-coupled compressible form of the conservation equations, but can be evaluated in the incompressible limit. The theoretical framework handles both multicomponent and mixture-averaged systems, with a generalized treatment of the equation of state, thermodynamics, and transport processes. It can accommodate high-pressure real-gas/liquid phenomena, multiple-scalar mixing processes, finite-rate chemical kinetics and multiphase phenomena in a fully coupled manner.

For LES applications the instantaneous conservation equations are filtered yielding:

- **Mass:**
  \[
  \frac{\partial}{\partial t}(\theta \rho \tilde{u}) + \nabla \cdot (\theta \rho \tilde{u} \tilde{u}) = \dot{\rho}_s.
  \] (1)

- **Momentum:**
  \[
  \frac{\partial}{\partial t}(\theta \rho \tilde{u}) + \nabla \cdot \left[ \theta \left( \rho \tilde{u} \otimes \tilde{u} + \frac{P}{M^2} \mathbf{I} \right) \right] = \nabla \cdot (\theta \tilde{T}) + \tilde{F}_s.
  \] (2)

- **Total Energy:**
  \[
  \frac{\partial}{\partial t}(\theta \rho \tilde{e}_t) + \nabla \cdot \left[ \theta \left( \rho \tilde{e}_t + P \right) \tilde{u} \right] = \nabla \cdot \left[ \theta \left( \tilde{Q}_e + M^2 \tilde{T} \cdot \tilde{u} \right) \right] + \theta \tilde{Q}_e + \tilde{Q}_s.
  \] (3)

- **Species:**
  \[
  \frac{\partial}{\partial t}(\theta \rho \tilde{Y}_i) + \nabla \cdot (\theta \rho \tilde{Y}_i \tilde{u}) = \nabla \cdot (\theta \tilde{S}_i) + \theta \tilde{w}_i + \tilde{\omega}_si.
  \] (4)

The terms \( \theta, \rho_s, \tilde{F}_s, \tilde{Q}_s \) and \( \tilde{\omega}_s \) represent the filtered void fraction and spray source terms that account for interphase exchange of mass, momentum, total energy and species, respectively. The terms \( P, \tilde{T}, \tilde{Q}_e \) and \( \tilde{S}_i \) are respective composite (i.e., molecular plus sgs) stresses and fluxes. The terms \( \tilde{Q}_e \) and \( \tilde{\omega}_i \) are the filtered energy and species source terms.

3.1. Subgrid-Scale Closure

The current sgs closure is obtained using the dynamic Smagorinsky model by combining the models proposed by Erlebacher et al. [14] and Speziale [15] with the dynamic modeling procedure [16–20]. Details are given by Oefelein [13] and thus will be omitted here. A key aspect associated with this approach is the fact that there are no tuned constants employed anywhere in the closure. The overall model includes the Leonard and cross-term stresses and provides a Favre averaged generalization of the Smagorinsky eddy viscosity model [21] coupled with gradient diffusion models that account for sgs mass and energy transport.

3.2. Thermodynamic and Transport Properties

Thermophysical processes in state-of-the-art systems typically occur at elevated pressures that approach or exceed the thermodynamic critical point of the fluid. Under these conditions, the ideal gas equation state can become invalid, especially in the vicinity of injected fuel and oxidizer streams and in cooler regions of the flow. To account for thermodynamic nonidealities and transport anomalies under these circumstances, a generalized scheme has been developed that provides a complete description of fluid mixture properties over a wide range of pressures and temperatures. The extended corresponding states model [22, 23] is employed in a manner that incorporates equation of state implementations as simple as the ideal gas law, and as complex as the Benedict-Webb-Rubin (BWR), Soave-Redlich-Kwong (SRK)
and Peng-Robinson (PR) equations. Implementation of these classes of state equations provide a highly accurate description of the \( p-v-T \) behavior inherent in dense multicomponent gas/liquid mixtures.

Having established an analytical representation for real mixture \( p-v-T \) behavior, thermodynamic properties are obtained in two steps. First, respective component properties are combined at a fixed reference temperature using the extended corresponding states methodology to obtain the mixture state at a given reference pressure. A pressure correction is then applied using departure functions of the form given by Reid et al. [24, Chapter 5]. These functions provide exact relations and make full use of the real mixture \( p-v-T \) path dependencies dictated by the equation of state. Standard state properties are obtained using the databases developed by Gordon and McBride [25] and Kee et al. [26]. Molecular transport properties are evaluated in an analogous manner. The viscosity and thermal conductivity are obtained using the methodologies developed by Ely and Hanley [27, 28]. The mass and thermal diffusion coefficients are obtained using the methodologies outlined by Bird et al. [29], Hirschfelder et al. [30], and Takahashi [31].

### 3.3. Progress and Unresolved Issues

Progress and unresolved issues related to combustion modeling have been systematically documented over the past several years [6–10]. The key issue for reacting flows is that no portion of the filtered chemical source terms can be resolved. Most models developed to-date have been carried over from RANS and extended in a way that makes use of the additional information available from LES. Closure schemes for nonpremixed flames include laminar flamelet models [32–36], the conditional moment closure (CMC) model [37–41], probability density function (PDF) transport models [42–49], the linear eddy model (LEM) [50–58], and its successor the one dimensional turbulence (ODT) [59] model. More recently, a new class of reconstruction sgs models have been proposed [60, 61] that combine the purely mathematical approximate deconvolution procedure with physical information from an assumed scalar spectrum to match specific scalar moments.

Our combustion modeling approach facilitates direct treatment of turbulence-chemistry interactions and multiple-scalar mixing processes without the use of tuned model constants. The systematic development and validation of this approach is currently a major focal point. Unlike conventional models, chemistry is treated directly within the LES formalism. The filtered energy and chemical source terms are closed by selecting an appropriate chemical kinetics mechanism and employing a stochastic moment-based reconstruction methodology that provides a modeled representation of the local instantaneous scalar field. Model coefficients are evaluated locally in closed form as a function of time and space using the dynamic modeling procedure. In the limit as the grid resolution and time-step approach the smallest relevant scales, contributions from the subgrid-scale models approach zero and the limit of DNS is achieved. This limiting behavior is highly desirable and offers a systematic method toward DNS of a given target experiment without having to make oversimplified canonical geometric and phenomenological approximations.

### 4. Numerical Framework

Case studies presented in subsequent sections were performed using a single unified numerical framework. The formulation treats the fully-coupled compressible conservation equations but can be evaluated in the incompressible limit. Thus, incompressibility is treated as a limiting extreme of the more general compressible equation set given by Eqs. (1)–(4). A unique dual-time multistage scheme is employed with a generalized (pseudo-time) preconditioning methodology that treats convective, diffusive, geometric, and source term anomalies in an optimal manner. The spatial scheme employs a staggered methodology in generalized curvilinear coordinates that provides non-dissipative spectrally clean damping characteristics and discrete conservation of mass, momentum, and total-energy. This is a critically important feature for LES. The differencing methodology includes appropriate switches to handle shocks, detonations, flame-fronts and/or contact discontinuities. The baseline method provides a fully implicit time advancement using a fully explicit multistage scheme in pseudo-time. The implicit
5. Unified Treatment of Key Processes
Activities to date have focused on verification and validation of the theoretical-numerical framework with two mutually dependent objectives. The first was to develop a single unified model base suitable for performing high-fidelity LES of the complex phenomena associated with state-of-the-art propulsion and power systems. The second was to develop a high-performance massively-parallel software platform to support the implementation of large-scale simulations. The combined package provides a unique capability that incorporates the stringent algorithmic requirements of LES within a framework designed to optimally treat coupled reacting flow phenomena at practical conditions. These phenomena include 1) wall-bounded shear-dominated three-dimensional flow, 2) geometrically dominated high Reynolds number turbulence, 3) high-pressure mixed-mode combustion dynamics, 4) strongly coupled thermodynamics, transport and chemical kinetics, and 5) injection and breakup of hydrocarbon and cryogenic propellants at near-critical and supercritical conditions. Processes are typically acoustically active and evolve over a large Mach operating range. The discussion below is intended to highlight key accomplishments related to the establishment of the overall framework. Detailed descriptions and quantitative comparisons with various datasets are given by Oefelein et al. [11–13].

5.1. Low-Mach-Number, High-Reynolds-Number Turbulence
Combustion processes are dominated by both upstream injection characteristics and the downstream pressure distribution at the combustor exit. Injection of fuel and oxidizer into the chamber always involves strongly-coupled fluid dynamic interactions in regions of high-shear. Fluid entering the chamber is initially dominated by wall induced turbulent boundary layer interactions. Upon expansion into the
chamber, a transition occurs to a condition dominated by spatially evolving shear-layer interactions. These interactions have a strong influence on the local turbulent flame structure. Thus, it is imperative that the initial flow evolution be treated rigorously. To demonstrate the level of accuracy achieved using the wall-resolved approach, we have performed a validation study by comparing results from an \( \text{LES} \) to the \( \text{DNS} \) data provided by Moser, Kim and Mansour [62]. Moser et al. have performed \( \text{DNS} \) calculations of a turbulent channel flow up to a Reynolds number based on the friction velocity of \( \text{Re}_\tau = 590 \). The \( \text{LES} \) calculations were performed on a grid that was \( 100^3 \). No-slip boundary conditions were applied at the upper and lower walls. Periodic conditions were applied in the streamwise and spanwise directions.

Figure 2 shows a representative result for a Reynolds number based on the friction velocity of \( \text{Re}_\tau = 590 \). This Reynolds number is the highest considered by Moser et al. and coincides with values that typically exist in simple laboratory-scale injector ducts at atmospheric pressure. Shown are contours of the instantaneous (dimensionless) magnitude of vorticity. Contour ranges are set to highlight both the structure of the core flow and the longitudinal vortical streaking near the wall. The dimensionless magnitude is observed to vary from 0 to 1 in the core flow, and approaches values of 30 near the wall. The longitudinal, cross-stream and near-wall structure is indicative of the well-known horseshoe vortex dynamics that occurs in turbulent boundary layers. The results shown here are unique in that the solution was obtained by solving the full-compressible conservation equations in the incompressible limit using a time-step based on the convective velocity. In addition to demonstrating an ability to run the full compressible equation set efficiently, these data provide baseline resolution requirements for \( \text{LES} \) of fully-developed turbulence in a duct.

5.2. Premixed Flame Phenomena

As an extension of research currently underway in the Combustion Research Facility \( \text{CRF} \) Turbulent Combustion Laboratory, we have begun to develop a joint numerical-experimental program that combines high-fidelity \( \text{LES} \) and detailed experimental diagnostics, with emphasis placed on turbulent swirl-stabilized lean premixed flames. The baseline configuration is the laboratory-scale dump-combustor shown in Fig. 3. This burner has been designed to generically emulate high Reynolds number fluid dynamic, thermodynamic, thermo-chemical, and transport processes that occur in typical gas-turbine combustors. The design has been optimized to provide non-ambiguous boundary conditions required for the validation of high-fidelity \( \text{LES} \) simulations while making optimal use of the advanced laboratory and diagnostic capabilities developed at the \( \text{CRF} \). The burner consists of an annular injector...
attached to a cylindrical chamber and nozzle assembly. The annular injector is designed to provide an acoustically clean, swirling, fully-developed turbulent profile with a uniform equivalence ratio, flow rate, and diminished wake effects due to the swirler. The cylindrical chamber is designed to provide clean, diagnostically accessible swirling flames without complicating factors such as wall impingement effects. Included in the figure are the results from a preliminary LES calculation that identically matches the experimental geometry. The instantaneous velocity field is shown on the left. The time averaged velocity is shown on the right. This figure qualitatively illustrates the complex structure of the flow, which includes both primary and secondary recirculation zones, an unsteady stagnation point and an annular separation region along the wall. These features dominate the local flame structure, performance, and emission characteristics and must be included in any meaningful study of such devices.

5.3. Sprays and Multiphase Flow
To build on the criteria established in the previous section we now focus on the next level of complexity. Sommerfeld et al. [63–65] provide a detailed series of one-component phase-Doppler-anemometer (PDA) measurements from a swirling particle-laden flow in a dump combustor configuration very similar to that shown in Fig. 3. These data provide two excellent benchmark cases for validation of LES in a turbulent swirling-flow environment, under highly controlled conditions, and with well-defined boundary conditions. They provide a way to systematically validate LES models for unsteady dilute spray dynamics without having to simultaneously treat the more complex issues related to atomization, secondary breakup, and coupling between the gas and particulate phases under highly loaded conditions. Establishing this level of validation is a key progressive step toward treating these more daunting issues.

A representative LES solution is shown in Fig. 4. Here the instantaneous particle distribution in the region of interest is superimposed on the corresponding turbulent velocity field in the y-x and z-y planes at the axial locations of $x/R = 0.78, 1.6, 2.7$ and $3.5$. These four radial cross-sections correspond to the axial stations where PDA measurements were made. This figure clearly highlights the asymmetric precessing nature of the flow. At any instant in time there are approximately 2.5-million particles being tracked in the region of interest. Tracking this number of particles is significant since
it verifies the feasibility of employing large numbers of physical particles and eliminates the need to implement more limiting model approximations for cases such as this. In all cases, the agreement between the measured and modeled results was excellent. With this confidence in place, we are able to extract additional information from the calculations that cannot be measured experimentally to gain further insights relevant to modeling sprays. This includes key turbulence scales, the particle Reynolds number for different particle sizes, and the predicted deformation characteristics that a liquid drop would exhibit under the observed conditions.

5.4. High-Pressure (Supercritical) Mixing and Combustion

Use of cryogenic propellants in liquid-rocket engines at chamber pressures that exceed the thermodynamic critical point of the propellants has been well established as a combination that provides high efficiency for a variety of launch vehicle applications. The chamber pressure in these engines exceeds 100 atm, which is significantly higher than the thermodynamic critical pressure of both propellants. Using the joint numerical-experimental approach outlined above, we have established one of the first quantitative characterizations of the flame structure and associated property variations in liquid-oxygen–hydrogen (LOX–H₂) flames at supercritical pressure. Figures 5 and 6 show results from a joint analysis conducted in collaboration with the NASA Marshall Space Flight Center and the German Aerospace Center (DLR). Emphasis was placed on shear-coaxial injection processes in the laboratory-scale uni-element rocket configuration developed and studied experimentally at DLR. Shown are a photograph and diagram of the experimental configuration and results from a multiscale analysis, extracted from the LES results, that has provided key insights. Shear-coaxial injection processes in liquid rocket engines exhibit two distinct modes of combustion. At subcritical pressures the liquid jets atomize. Dynamic forces and surface tension promote the formation of a heterogeneous spray and lifted spray flames form in a manner consistent with the modes of combustion exhibited by local drop clusters. When chamber pressures approach or exceed the critical pressure of a particular propellant, however, injected liquid jets undergo a transcritical change of state as interfacial fluid temperatures rise above the critical temperature of the local mixture. For this situation, diminished inter-molecular forces promote diffusion dominated mixing prior to atomization. Respective jets vaporize in the presence of exceedingly large thermophysical gradients and diffusion flames evolve as a consequence that are anchored by small but intensive recirculation zones just downstream of the LOX-post. Results have quantified the distinct nature of the shear-layer region. Though continuous, gradients in the flame zone approach the behavior of a contact discontinuity. A three order of magnitude change in density over an extremely small spatial interval was clearly evident. The depletion of all of the oxygen in the flame, the flame structure, and
Figure 5: Laboratory-scale uni-element rocket configuration developed at the German Aerospace Center (DLR) in Lampoldshausen: (a) photograph and schematic of the experimental apparatus, (b) corresponding flow visualization of shear-coaxial LOX–H₂ injection, mixing and combustion at supercritical pressure.

Figure 6: Turbulent kinetic energy field from an LES of the (DLR) configuration shown in Fig. 5 at identical conditions and subsequent multiscale analysis showing the flow-flame structure and flame-holding mechanism in critical regions.
the fuel-rich characteristics on the hydrogen side of the flame were also apparent. The coupled effects of these phenomena produce a mode of combustion near stoichiometric conditions and a wake that effectively separates the hydrogen and oxygen streams as the flow evolves downstream. Near-field flame extinction due to low Mach number dilatation was also observed under certain conditions. The unique aspect of these calculations are due to the fact that the Reynolds number is an order of magnitude higher than is typically observed at atmospheric conditions and the extreme nature of the thermodynamic nonidealities and transport anomalies.

5.5. Transient Propagation of Detonation Waves

Figure 7 provides an example of the front-tracking capability designed within the staggered finite-volume LES framework described above. In addition to the treatment of shocks, the front-tracking methodology has been designed and optimized for detonations, contact discontinuities, and flame-fronts. The figure shows plots of the pressure, temperature, density, and flame-structure of a detonation wave propagating in a cylindrical tube 200 mm wide, with a diameter of 20 mm. The tube was charged with a stoichiometric mixture of hydrogen and oxygen. The detonation was initiated by igniting the head-end with equilibrium products at 30 atm and 3000 K. The initial conditions are: \( p = 1 \text{ atm} \), \( T = 300 \text{ K} \) and \( u = 0 \). Finite-rate hydrogen-oxygen kinetics are employed using the nine species \( \text{H}_2, \text{O}_2, \text{OH}, \text{H}_2\text{O}, \text{H}, \text{O}, \text{HO}_2, \text{H}_2\text{O}_2, \text{N}_2 \), 19-step mechanism developed by Westbrook and Dryer [66] and Yetter et al. [67]. This example demonstrates a capability to handle complex chemistry and thermophysical coupling at supersonic conditions. The classical structure and key features of the detonation wave are listed in the caption.

6. Future Directions

With the current state-of-the-art capability in place we can effectively combine the unique strengths of LES and experiments in an optimal manner. This will allow us to effectively focus on issues related to advanced modeling and bridge the gap between basic research and engineering applications. Current efforts represent a direct extension of joint activities currently being pursued as part of the International Workshop on Measurement and Computation of Turbulent Nonpremixed Flames (TNF) [68]. These activities involve significant domestic and international collaborations. We are currently performing a detailed calculation of the Sandia TNF flame series, with emphasis placed on 1) investigating the fine-scale structure of mixture fraction and scalar dissipation fields in turbulent flames, 2) studying the
instantaneous three-dimensional flame dynamics and orientation, and 3) investigating the influence of scalar dissipation on species mass fractions and temperature. Establishing a validated matrix of optimally selected studies will have a direct impact on scientific discovery at both the fundamental and applied levels. By following this approach we have a program that is focused on fundamental science in a manner that will directly impact a variety of propulsion and power systems.

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