



Chemical and Environmental Science Archives
(ISSN: 2583-1151)
An International Research Journal

DOI: <https://doi.org/10.47587/CESA.2026.6305>

Review Article

Large Eddy Simulation (LES) of Turbulent Combustion: A Review of Modeling Approaches and Applications

Oseni Temitope Damilola¹, Obojobo Donatus Obukeajeta², Ochuele Dominic Agida³, Moses Adondua Abah³ and Micheal Oladosu Abimbola³

¹Department of Mechanical Engineering, Faculty of Engineering, Kwara State University, Kwara State, Nigeria

²Department of Mechanical Engineering, Faculty of Engineering, Southern Delta University, Ozoro, Delta State, Nigeria

³ResearchHub Nexus Institute, Nigeria

(✉) Corresponding Author: Moses Adondua Abah; m.abah@fuwukari.edu.ng

Received: Aug 20, 2026/ Revised: Sept 20 2026/Accepted: Sept 21, 2026

Abstract

Large Eddy Simulation (LES) has become one of the most powerful computational approaches for investigating turbulent combustion because it resolves the dominant energy-containing turbulent structures while modeling the effects of unresolved subgrid-scale motions. Compared with conventional Reynolds-Averaged Navier–Stokes (RANS) methods, LES provides improved predictive capability for complex, unsteady reacting flows, while remaining computationally more feasible than Direct Numerical Simulation (DNS). Consequently, LES has gained widespread application in the design, optimization, and emission control of modern combustion systems. This review presents a comprehensive overview of modeling approaches and practical applications of LES in turbulent combustion. It first outlines the fundamental principles of LES, including filtered governing equations, turbulence resolution, and the challenges associated with reacting flow simulations. The review then examines major subgrid-scale turbulence models, turbulence chemistry interaction strategies for premixed, non-premixed, and partially premixed combustion, and numerical considerations influencing simulation accuracy and computational efficiency. Current approaches for model validation against experimental measurements and DNS datasets are also discussed, with emphasis on predictive accuracy, uncertainty, and computational cost. Furthermore, the review summarizes representative applications of LES in gas turbines, internal combustion engines, aerospace propulsion, industrial combustion systems, and emerging low-carbon fuel technologies involving hydrogen, ammonia, and biomass. Finally, recent advances in machine learning-assisted LES, hybrid and reduced-order modeling, exascale computing, and digital twin frameworks are highlighted, together with the key scientific and computational challenges that continue to limit widespread industrial implementation. By synthesizing recent developments across modeling methodologies and engineering applications, this review provides a concise reference for researchers and engineers while identifying future directions for improving the accuracy, scalability, and practical adoption of LES in turbulent combustion research.

Keywords: Large Eddy Simulation (LES), Turbulent combustion, Subgrid-scale modeling, Turbulence–chemistry interaction, Computational fluid dynamics (CFD), and Low-carbon combustion.

1. Introduction

Turbulent combustion governs energy conversion in gas turbines, internal combustion engines, aerospace propulsion systems, and numerous industrial combustion devices. The

strong interactions among turbulent fluid motion, chemical reactions, heat transfer, and pollutant formation create highly nonlinear reacting flows that remain challenging to predict accurately. Consequently, computational fluid dynamics (CFD) has become an indispensable tool for understanding combustion physics, improving thermal efficiency, reducing

fuel consumption, and mitigating pollutant emissions. The increasing adoption of hydrogen, ammonia, and biomass-derived fuels has further intensified the need for predictive combustion models capable of accurately resolving complex reacting flow phenomena while supporting the development of cleaner and more sustainable energy technologies (Wang and Yang, 2024). Recent advances in combustion CFD have consequently focused on improving the predictive capability and robustness of turbulence–chemistry interaction models for modern combustion systems (Posch *et al.*, 2025).

Large Eddy Simulation (LES) has emerged as one of the most effective CFD approaches for turbulent combustion because it explicitly resolves the large, energy-containing turbulent structures while modeling only the unresolved subgrid-scale motions (Pitsch, 2006). This scale-resolving strategy provides substantially greater physical fidelity than Reynolds-Averaged Navier–Stokes (RANS) simulations while requiring significantly lower computational resources than Direct Numerical Simulation (DNS) (Poinsot and Veynante, 2011). As computational power and numerical algorithms have advanced, LES has evolved from a predominantly academic research methodology into a practical engineering tool for investigating flame stabilization, combustion instabilities, ignition, extinction, and pollutant formation across diverse combustion systems (Posch *et al.*, 2025). Its ability to capture transient flow structures and complex turbulence–chemistry interactions has made LES particularly valuable for designing next-generation low-emission combustion technologies.

The accuracy of LES predictions depends largely on robust turbulence modeling, reliable turbulence–chemistry interaction formulations, and efficient numerical implementation. Early theoretical developments established the fundamental principles governing turbulent combustion modeling and continue to provide the basis for contemporary LES methodologies (Veynante and Vervisch, 2002). Building upon these foundations, recent studies have introduced advanced filtered tabulated chemistry approaches that significantly improve the representation of premixed turbulent flames while maintaining computational efficiency (Bambauer *et al.*, 2024). Similarly, the Multiple Mapping Conditioning (MMC) framework has enhanced the consistency of turbulence–chemistry interaction modeling for turbulent premixed combustion (Iaroslavtceva *et al.*, 2024). Furthermore, Conditional Source-term Estimation (CSE) has emerged as a promising strategy for representing finite-rate chemistry in turbulent reacting flows while addressing longstanding challenges associated with combustion model accuracy and scalability (Salehi *et al.*, 2024).

Recent LES investigations have demonstrated the growing applicability of advanced combustion models to realistic engineering configurations. LES has been successfully applied to biomass syngas combustion in swirl-stabilized burners, where detailed validation against experimental measurements has shown strong predictive capability for velocity fields, temperature distributions, and species concentrations

(Papafilippou *et al.*, 2024). Such validation studies are essential because they establish confidence in LES predictions for industrial combustion systems operating under complex turbulent and chemically reacting conditions. At the same time, LES-based combustion research has increasingly focused on pollutant formation mechanisms, particularly nitrogen oxide (NO_x) emissions, because accurate emission prediction is critical for meeting stringent environmental regulations and improving combustion system sustainability (Wang and Yang, 2024). These recent developments demonstrate that LES has become a valuable framework for bridging fundamental combustion science with practical engineering applications.

This review aims to provide a concise and comprehensive assessment of Large Eddy Simulation (LES) for turbulent combustion, with emphasis on the major modeling approaches, validation strategies, and engineering applications that have shaped recent progress in the field. The review first outlines the fundamental principles of LES and its role in resolving large turbulent structures in reacting flows. It then examines the principal subgrid-scale turbulence models and turbulence–chemistry interaction formulations used in premixed, non-premixed, and partially premixed combustion. Numerical and computational considerations, including grid resolution, discretization, boundary conditions, and high-performance computing requirements, are also discussed. Furthermore, the review evaluates current approaches for model validation against experimental measurements and DNS datasets, highlighting issues of predictive accuracy, uncertainty, and computational efficiency. Representative applications in gas turbines, internal combustion engines, aerospace propulsion, industrial combustion systems, and low-carbon fuel technologies are summarized. Finally, emerging trends such as machine learning-assisted LES, hybrid and reduced-order modeling, exascale computing, and digital twin frameworks are identified to highlight future research directions and the remaining challenges for widespread industrial implementation of LES in turbulent combustion research.

2. Fundamentals of LES for Turbulent Combustion

A comprehensive understanding of Large Eddy Simulation (LES) requires knowledge of its theoretical foundations, numerical formulation, and role in turbulent combustion modeling. This section outlines the fundamental principles underpinning LES, including the filtered governing equations and the treatment of unresolved turbulent scales. It also compares LES with Reynolds-Averaged Navier–Stokes (RANS) and Direct Numerical Simulation (DNS) to highlight their respective capabilities and limitations. Finally, the section discusses the principal scientific and computational challenges that influence the accuracy, efficiency, and practical application of LES in simulating complex turbulent reacting flows.

2.1 LES Principles and Filtered Governing Equations

Large Eddy Simulation (LES) is a scale-resolving computational approach that explicitly resolves the large, energy-containing turbulent eddies while modeling the smaller unresolved scales using subgrid-scale (SGS) models (Pitsch, 2006). By capturing the dominant turbulent structures, LES provides greater physical fidelity than Reynolds-Averaged Navier–Stokes (RANS) simulations while remaining substantially more computationally feasible than Direct Numerical Simulation (DNS) (Poinso and Veynante, 2011). Consequently, LES has become a leading framework for investigating turbulent combustion characterized by complex turbulence–chemistry interactions and transient flame dynamics (Posch *et al.*, 2025). The mathematical basis of LES is the spatial filtering of the governing conservation equations, which separates the flow into resolved and unresolved components. In reacting flows, Favre filtering is commonly adopted to account for density variations and compressibility effects (Pitsch, 2006). The filtering operation introduces

unresolved SGS stresses and scalar fluxes that require closure models to represent their influence on the resolved flow field (Unnikrishnan *et al.*, 2021). Therefore, the predictive accuracy of LES depends strongly on the formulation of SGS models and turbulence–chemistry interaction closures. Recent advances have improved LES through filtered tabulated chemistry, enabling efficient incorporation of detailed chemical kinetics while maintaining computational tractability (Bambauer *et al.*, 2024). Furthermore, advanced SGS formulations incorporating equation-of-state effects have enhanced predictions of transcritical and supercritical combustion by improving the representation of variable-density and thermodynamic phenomena (Zhou *et al.*, 2023). Nevertheless, simulation accuracy remains sensitive to grid resolution, numerical discretization, and model consistency. Ongoing efforts to develop physically consistent turbulence, chemistry, and numerical coupling strategies continue to improve the robustness and applicability of LES across a wide range of turbulent combustion systems (Salehi *et al.*, 2024).

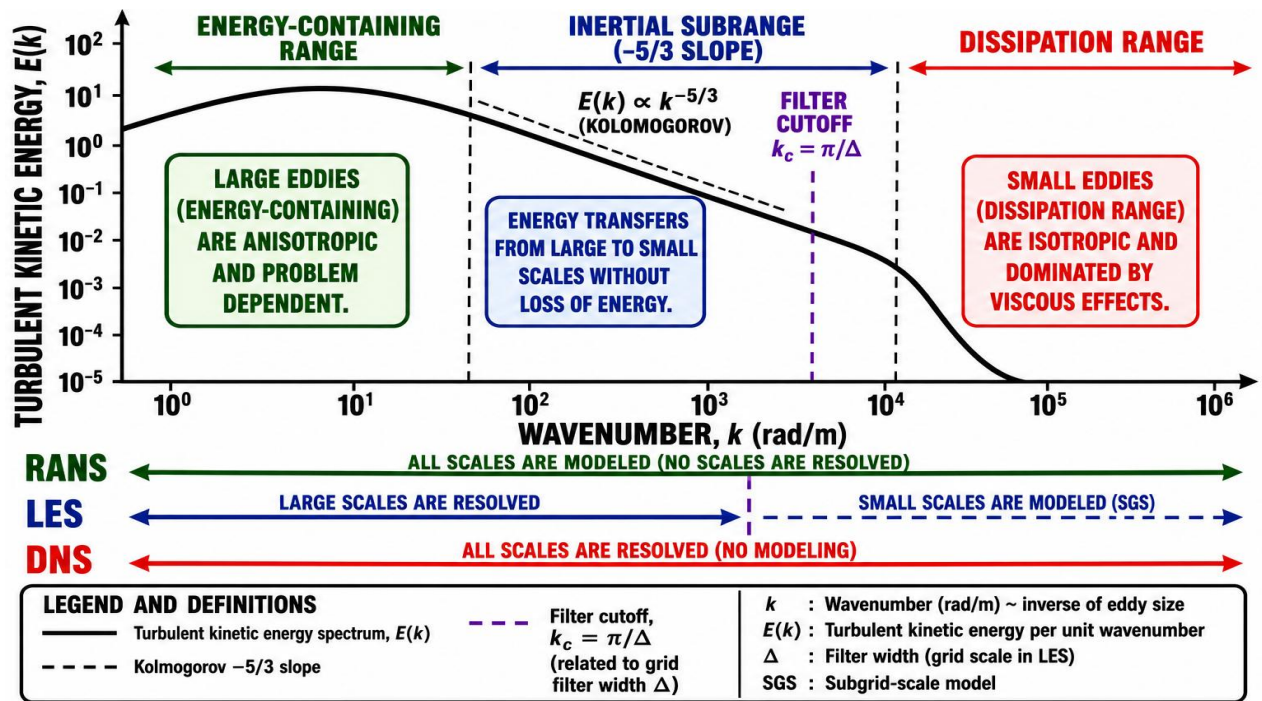


Figure 1. Turbulent kinetic energy spectrum illustrating turbulence scale resolution in RANS, LES, and DNS. The turbulent kinetic energy spectrum illustrates how turbulent kinetic energy is distributed across eddy scales. RANS models the entire turbulence spectrum, LES resolves the large energy-containing eddies while modeling the unresolved subgrid-scale motions, and DNS resolves all turbulent scales. The filter cutoff defines the transition between resolved and modeled scales in LES Source: Modified from Tay-Wo-Chong (2012)

2.2 Comparison with RANS and DNS

Computational simulation of turbulent combustion is primarily based on three approaches: Reynolds-Averaged Navier–Stokes (RANS), Large Eddy Simulation (LES), and Direct Numerical

Simulation (DNS), which differ in turbulence resolution and computational cost. RANS models all turbulent fluctuations through time- or ensemble-averaged governing equations, making it computationally efficient for engineering applications (Poinso and Veynante, 2011). However, averaging suppresses transient flow structures, limiting its ability to accurately predict flame dynamics, combustion

instabilities, and turbulence–chemistry interactions in highly unsteady reacting flows (Posch *et al.*, 2025). In contrast, DNS resolves the complete spectrum of turbulent and chemical scales without turbulence modeling, providing the highest level of physical fidelity (Pitsch, 2006). It has substantially advanced the understanding of flame structure, turbulent mixing, and chemical kinetics while providing benchmark datasets for model development and validation (Salehi *et al.*, 2024). Nevertheless, its computational cost increases rapidly with Reynolds number and chemical complexity, restricting its application to canonical configurations and fundamental studies (Poinot and Veynante, 2011). LES provides a practical compromise by resolving the large, energy-containing turbulent eddies while modeling only the unresolved subgrid-scale motions (Pitsch, 2006). Compared

with RANS, LES more accurately captures transient coherent structures, vortex dynamics, and flame behavior, yet remains significantly less computationally demanding than DNS (Posch *et al.*, 2025). Its predictive capability has been further enhanced through filtered tabulated chemistry for premixed combustion (Bambauer *et al.*, 2024) and consistent Multiple Mapping Conditioning (MMC)-LES formulations for improved turbulence–chemistry interaction (Iaroslavtceva *et al.*, 2024). Consequently, LES has become the preferred framework for investigating combustion instability, pollutant formation, and low-carbon fuel combustion, offering an optimal balance between computational efficiency and predictive accuracy (Wang and Yang, 2024).

Table 1. Comparison of RANS, LES, and DNS for turbulent combustion simulations

Features	RANS	LES	DNS
Turbulence resolution	Fully modeled	Large eddies resolved; SGS modeled	Fully resolved
Computational cost	Low	Moderate–High	Extremely high
Predictive accuracy	Moderate	High	Very high
Transient flow prediction	Limited	Excellent	Excellent
Turbulence–chemistry interaction	Averaged	Explicitly resolved at large scales	Fully resolved
Industrial applicability	High	Increasingly adopted	Limited
Typical applications	Design optimization	Research and engineering analysis	Fundamental studies

2.3 Key Challenges in Turbulent Combustion Simulation

Accurate simulation of turbulent combustion remains challenging because turbulence, chemical kinetics, molecular transport, heat transfer, and thermodynamic processes interact across a broad range of spatial and temporal scales. These nonlinear interactions govern flame stabilization, ignition, extinction, combustion efficiency, and pollutant formation, making their accurate representation essential for predictive simulations, particularly under transient operating conditions and with alternative fuels (Veynante and Vervisch, 2002; Wang and Yang, 2024). A major challenge in LES is the closure of unresolved subgrid-scale (SGS) processes. Although LES resolves the dominant turbulent structures, unresolved scalar mixing and chemical reactions must be modeled, and inaccurate closures can compromise predictions of flame propagation, heat release, and species transport. Consequently, improving turbulence–chemistry interaction models remains a research priority. Recent advances in

Conditional Source-term Estimation (CSE) have enhanced the representation of finite-rate chemistry (Salehi *et al.*, 2024), while consistent Multiple Mapping Conditioning (MMC)-LES formulations have improved predictions of turbulent premixed flames by strengthening turbulence–chemistry coupling (Iaroslavtceva *et al.*, 2024). Computational cost and numerical accuracy also constrain the application of LES to realistic combustion systems. High-fidelity simulations require fine grid resolution, robust numerical schemes, and efficient treatment of detailed chemical kinetics, particularly for high-Reynolds-number and complex geometries. These challenges are further intensified under transcritical and supercritical conditions, where variable thermodynamic properties necessitate advanced equation-of-state-aware SGS models (Unnikrishnan *et al.*, 2021; Zhou *et al.*, 2023). Equally important is rigorous validation against experimental measurements and DNS datasets to quantify predictive uncertainty and improve model reliability. Recent validation studies on biomass syngas combustion demonstrate the importance of experimental benchmarking for enhancing LES accuracy and extending its industrial applicability (Papafiliippou *et al.*, 2024; Posch *et al.*, 2025).

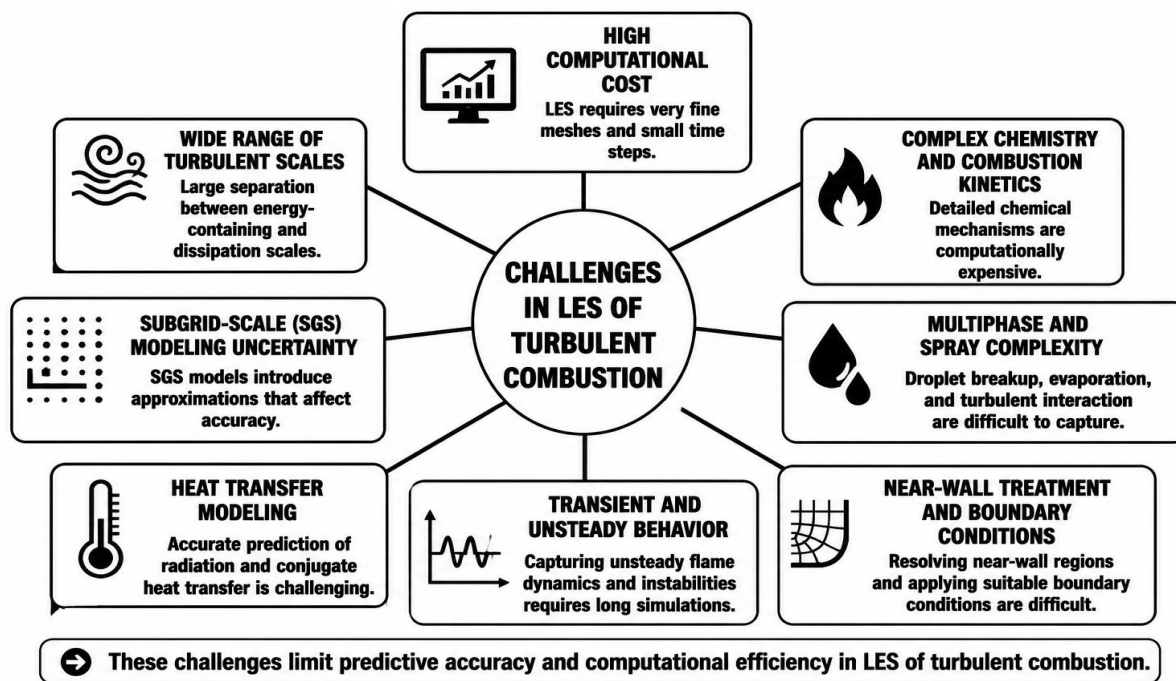


Figure 2. Key challenges affecting the predictive performance of Large Eddy Simulation (LES) in turbulent combustion. The figure summarizes the major scientific and computational challenges that influence the predictive accuracy of LES for turbulent combustion. These include subgrid-scale (SGS) modeling, turbulence–chemistry interaction, computational cost, numerical resolution, complex chemical kinetics, near-wall treatment, and model validation. Addressing these challenges is essential for improving the reliability and industrial applicability of LES

Source: [Unnikrishnan *et al.* \(2021\)](#)

3. Modeling Approaches in LES of Turbulent Combustion

The predictive capability of Large Eddy Simulation (LES) depends on the effective integration of turbulence modelling, combustion modelling, and numerical implementation ([Pitsch, 2006](#); [Poinot and Veynante, 2011](#)). Over the past two decades, significant advances in subgrid-scale (SGS) turbulence models, turbulence–chemistry interaction (TCI) formulations, and computational techniques have substantially improved the accuracy and applicability of LES for a wide range of turbulent combustion systems ([Salehi *et al.*, 2024](#); [Posch *et al.*, 2025](#)). This section reviews the principal modelling approaches underpinning contemporary LES, highlighting their theoretical foundations, strengths, limitations, and suitability for different combustion regimes and engineering applications ([Bambauer *et al.*, 2024](#); [Iaroslavtceva *et al.*, 2024](#)).

3.1 Subgrid-Scale (SGS) Turbulence Models

Subgrid-scale (SGS) turbulence models are fundamental to Large Eddy Simulation (LES) because they represent the influence of unresolved turbulent motions on the resolved

flow field. Their formulation largely determines the accuracy of momentum transfer, scalar mixing, and turbulence–chemistry interactions, thereby influencing the overall

predictive performance of LES. Over the years, SGS modelling has evolved from classical eddy-viscosity closures to more advanced structural and mixed formulations that improve physical realism while maintaining computational efficiency ([Pitsch, 2006](#); [Posch *et al.*, 2025](#)). The following subsections review the principal SGS modelling approaches and their applications in turbulent combustion.

3.1.1 Eddy-Viscosity Models

Eddy-viscosity models remain the most widely used SGS closures in LES because of their simplicity, numerical robustness, and computational efficiency. These models approximate unresolved turbulent stresses by relating them to the resolved strain rate through an eddy-viscosity hypothesis. The classical Smagorinsky model established the foundation for SGS modelling, although its use of a constant model coefficient often leads to excessive dissipation in transitional and near-wall flows. Dynamic formulations improve predictive accuracy by computing model coefficients locally, while the Wall-Adapting Local Eddy-viscosity (WALE) model provides superior near-wall performance without empirical damping functions. Consequently, dynamic Smagorinsky and WALE models are widely adopted in practical LES of turbulent combustion owing to their improved adaptability across complex reacting flows ([Pitsch, 2006](#); [Unnikrishnan *et al.*, 2021](#); [Posch *et al.*, 2025](#)).

3.1.2 Structural and Mixed SGS Models

Unlike eddy-viscosity formulations, structural SGS models seek to reconstruct the influence of unresolved turbulent structures rather than representing them solely through enhanced dissipation. Mixed models combine structural and eddy-viscosity concepts to improve the prediction of momentum transfer, scalar mixing, and turbulence–chemistry interactions while maintaining numerical stability. Recent developments have extended these approaches to combustion-aware SGS stress models that explicitly account for the effects

of heat release on turbulence evolution. For example, Wang *et al.* (2024) demonstrated that a combustion-informed SGS stress model improved the prediction of turbulent stresses and showed superior agreement with high-fidelity reference data during both a priori and a posteriori assessments. These advances indicate that physics-informed SGS closures provide greater accuracy for highly anisotropic and variable-density reacting flows than conventional eddy-viscosity models.

Table 2. Comparison of representative subgrid-scale (SGS) turbulence models for LES

SGS model	Principles	Strength	Limitations
Smagorinsky	Constant eddy-viscosity	Simple and robust	Over-dissipative; weak near walls
Dynamic Smagorinsky	Dynamic model coefficient	Improved local accuracy	Higher computational cost
WALE	Wall-adapting eddy-viscosity	Accurate near-wall prediction	Limited for highly anisotropic flows
Structural	Reconstructs unresolved structures	Better flow physics	Reduced numerical stability
Mixed	Combines structural and eddy-viscosity models	Balanced accuracy and stability	Increased model complexity
Combustion-aware SGS	Incorporates combustion effects into SGS closure	Improved reacting-flow prediction	Limited validation

Abbreviations: LES = Large Eddy Simulation, SGS = Subgrid-Scale, WALE = Wall-Adapting Local Eddy-viscosity. Source: Pitsch (2006); Unnikrishnan *et al.* (2021); Wang *et al.* (2024), and Posch *et al.* (2025).

3.2 Turbulence–Chemistry Interaction Models

Turbulence–chemistry interaction (TCI) modelling is fundamental to LES because unresolved turbulent mixing strongly influences chemical reactions, flame propagation, ignition, extinction, and pollutant formation. Although LES resolves the dominant turbulent structures, subgrid-scale scalar mixing and reaction processes require appropriate combustion closures to accurately represent their effects on the resolved flow field (Pitsch, 2006; Poinot and Veynante, 2011). A wide range of TCI models has been developed to accommodate different combustion regimes and levels of chemical complexity. These include flamelet-based approaches, filtered tabulated chemistry, flame surface density (FSD) and artificially thickened flame (ATF) models, finite-rate chemistry, and transported PDF/FDF formulations. The suitability of each approach depends on the combustion mode, fuel characteristics, computational cost, and desired predictive accuracy (Fiorina *et al.*, 2010; Salehi *et al.*, 2024). The following subsections discuss these modelling strategies for premixed, non-premixed, and partially premixed combustion, as well as finite-rate chemistry and PDF/FDF approaches.

3.2.1 Premixed Combustion

In premixed combustion, fuel and oxidizer are mixed before ignition, making flame propagation primarily dependent on the interaction between turbulence and the flame front. LES modelling therefore focuses on accurately representing unresolved flame wrinkling, flame stretch, and heat release while preserving computational efficiency. Flamelet-based approaches remain the most widely adopted because the flame thickness is typically much smaller than the resolved turbulent scales, allowing detailed chemical kinetics to be incorporated through simplified combustion manifolds (Pitsch, 2006; Poinot and Veynante, 2011). Among these approaches, Filtered Tabulated Chemistry (FTC) has become a robust framework for premixed LES by coupling filtered reaction chemistry with precomputed lookup tables, thereby improving predictions of flame structure and species transport without the computational burden of solving detailed reaction mechanisms directly (Fiorina *et al.*, 2010). Building on this concept, filtered tabulated chemistry has demonstrated high predictive accuracy for turbulent premixed flames while maintaining consistency between turbulence and combustion modelling (Bambauer *et al.*, 2024). Recent advances have further improved premixed LES through Multiple Mapping Conditioning (MMC), which enhances the representation of unresolved scalar fluctuations and finite-rate chemistry, leading to better agreement with experimental observations (Iaroslavtceva *et al.*, 2024). Alternative models, including Flame Surface Density (FSD) and Artificially Thickened Flame (ATF) formulations, improve the representation of

unresolved flame wrinkling when the computational grid cannot fully resolve the flame front. Their performance depends on combustion regime and turbulence intensity, but they remain effective for practical premixed and partially premixed flames (Lomada *et al.*, 2024). Recent DNS-based studies have also shown that appropriate selection of reaction progress variables significantly improves model accuracy, particularly for hydrogen-rich and syngas combustion where preferential diffusion strongly influences flame behaviour (Wehrmann *et al.*, 2024). Collectively, these developments have made flamelet-based and tabulated chemistry approaches the preferred modelling strategies for LES of premixed turbulent combustion because they provide an effective balance between physical fidelity and computational efficiency.

3.2.2 Non-Premixed Combustion

In non-premixed combustion, fuel and oxidizer enter the combustor separately, and combustion is controlled primarily by turbulent mixing rather than flame propagation. Consequently, turbulence–chemistry interaction models must accurately represent scalar mixing and local reaction rates while accounting for unresolved subgrid-scale fluctuations. Flamelet-based formulations remain the dominant approach because they describe combustion in terms of the mixture fraction and scalar dissipation rate, enabling efficient incorporation of detailed chemical kinetics into LES (Pitsch, 2006; Poinso and Veynante, 2011). To improve predictive accuracy, modern LES increasingly combines flamelet models with advanced statistical closures. Transported scalar methods, including Conditional Source-term Estimation (CSE), enhance the representation of finite-rate chemistry by incorporating conditional statistics of reactive scalars, thereby improving predictions of heat release and species formation across a wide range of combustion conditions (Salehi *et al.*, 2024). Validation against Direct Numerical Simulation (DNS) has further strengthened confidence in these approaches by identifying their strengths and limitations under different mixing regimes (Zhou, 2024). Recent applications demonstrate the effectiveness of these modelling strategies in practical combustion systems. LES studies of diffusion flames in space propulsion have shown that improved subgrid turbulent flux models enhance predictions of scalar transport and flame stability under highly turbulent conditions (Martinez-Sanchis *et al.*, 2024). Similarly, validation of LES for biomass syngas combustion has confirmed that appropriate turbulence–chemistry interaction models can accurately reproduce temperature fields, species distributions, and flow dynamics when supported by reliable experimental data (Papafilippou *et al.*, 2024). These advances have established flamelet-based and conditional statistical approaches as the principal modelling strategies for LES of turbulent non-premixed combustion.

3.2.3 Partially Premixed Combustion

Partially premixed combustion combines characteristics of both premixed and non-premixed flames, producing complex flame structures in which combustion is governed simultaneously by flame propagation and turbulent mixing. This dual behaviour makes turbulence–chemistry interaction modelling particularly challenging, as combustion models must accurately capture local variations in mixture composition, flame topology, and reaction rates under changing operating conditions (Poinso and Veynante, 2011; Posch *et al.*, 2025). Hybrid combustion models have therefore become the preferred approach for LES of partially premixed flames. Flame Surface Density (FSD) and Artificially Thickened Flame (ATF) models effectively represent unresolved flame wrinkling while maintaining computational efficiency, particularly when the flame front cannot be fully resolved by the computational grid. Comparative studies have demonstrated that both approaches provide reliable predictions of flame structure and heat release, although their performance depends on turbulence intensity and combustion regime (Lomada *et al.*, 2024). Likewise, flamelet-based progress-variable formulations have shown improved predictive capability for partially premixed hydrogen–methane flames by accurately capturing the combined effects of turbulent mixing and chemical reactions (Singh & Roy, 2024). Recent developments increasingly integrate hybrid flamelet formulations with detailed chemistry and adaptive turbulence closures to improve robustness across fuel-flexible combustion systems. These advances have expanded the applicability of LES to practical combustors operating with alternative fuels, where partially premixed combustion is frequently encountered (Bambauer *et al.*, 2024; Posch *et al.*, 2025).

3.2.4 Finite-Rate Chemistry and PDF/FDF Approaches

Finite-rate chemistry models explicitly solve chemical reaction kinetics without assuming infinitely fast reactions, making them particularly suitable for combustion regimes involving ignition, extinction, pollutant formation, and alternative fuels where chemical timescales strongly influence flame behaviour. Although these models provide high physical fidelity, their computational cost increases substantially with reaction mechanism complexity, limiting their routine application in large-scale LES (Poinso and Veynante, 2011; Impagnatiello *et al.*, 2024). To improve computational efficiency while preserving predictive accuracy, Probability Density Function (PDF) and Filtered Density Function (FDF) approaches describe the statistical distribution of reactive scalars instead of directly modelling nonlinear chemical source terms. These methods naturally account for turbulence–chemistry interactions and finite-rate effects, making them well suited for highly turbulent reacting flows. Recent advances in Conditional Source-term Estimation (CSE) have further strengthened PDF/FDF-based formulations by improving the representation of unresolved scalar fluctuations and conditional reaction rates, thereby enhancing predictive

performance across diverse combustion regimes (Salehi *et al.*, 2024). Consequently, finite-rate chemistry and PDF/FDF approaches remain indispensable for LES applications

requiring accurate treatment of complex chemical kinetics while balancing computational efficiency and model fidelity.

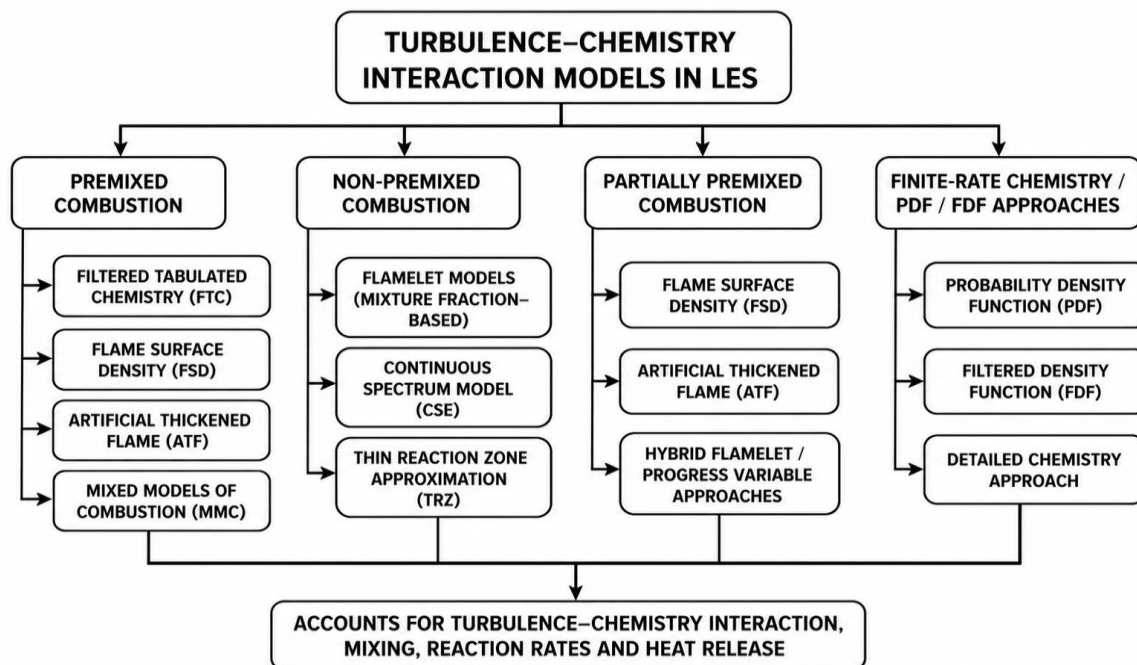


Figure 3. Turbulence–chemistry interaction modeling approaches in Large Eddy Simulation (LES) of turbulent combustion. The figure summarizes the principal turbulence–chemistry interaction (TCI) modeling approaches used in LES, classifying them according to combustion regime and chemical treatment. It highlights the major frameworks employed for premixed, non-premixed, partially premixed, and finite-rate reacting flows, providing an overview of their application in predicting turbulent combustion behavior

Source: Modified from Pitsch (2006) and Salehi *et al.* (2024).

3.3 Numerical and Computational Considerations

The predictive capability of LES depends not only on turbulence and combustion models but also on the numerical methods used to solve the governing equations. Grid resolution, spatial discretization, boundary condition specification, and computational resources directly influence simulation accuracy, numerical stability, and computational cost. Optimizing these factors is therefore essential for achieving reliable and efficient LES of turbulent combustion systems (Unnikrishnan *et al.*, 2021; Posch *et al.*, 2025).

3.3.1 Grid Resolution and Discretization

Grid resolution and numerical discretization are fundamental determinants of LES accuracy because they govern the separation between resolved turbulent structures and unresolved subgrid-scale motions. An adequately refined grid is required to capture the dominant energy-containing eddies

and flame dynamics, whereas insufficient resolution increases numerical dissipation and shifts excessive turbulence to the

SGS model, reducing predictive accuracy (Pitsch, 2006; Posch *et al.*, 2025). The choice of discretization scheme is equally important. High-order spatial discretization methods are generally preferred because they minimize numerical diffusion and improve the representation of unsteady flow structures, scalar transport, and flame propagation. Recent studies have emphasized that grid design should remain consistent with SGS turbulence and combustion models to avoid numerical inconsistencies, particularly in high-pressure and variable-density reacting flows (Unnikrishnan *et al.*, 2021; Zhou *et al.*, 2023). Consequently, systematic grid-independence assessment and appropriate discretization strategies remain essential for obtaining reliable and physically consistent LES predictions across practical combustion applications.

3.3.2 Boundary Conditions

Accurate boundary condition specification is essential in LES of turbulent combustion because inlet turbulence characteristics, wall interactions, and outlet treatments strongly influence flow development, flame stabilization, and pollutant prediction. Unlike steady simulations, LES requires boundary conditions that realistically represent unsteady

fluctuations and turbulence structures entering or leaving the computational domain (Posch *et al.*, 2025). In practical combustor simulations, synthetic turbulence generation and experimentally derived inlet profiles are frequently employed to reproduce realistic inflow conditions. Inadequate representation of inlet turbulence can lead to inaccurate mixing rates, flame dynamics, and heat-release predictions. Similarly, wall boundary treatment remains challenging because near-wall turbulence scales are often unresolved, requiring appropriate modelling approaches to balance accuracy and computational cost (Unnikrishnan *et al.*, 2021). Recent LES studies of practical combustion systems have demonstrated that careful selection and validation of boundary conditions are critical for achieving agreement with experimental measurements and improving confidence in model predictions (Impagnatiello *et al.*, 2024; Papafilippou *et al.*, 2024).

3.3.3 High-Performance Computing

High-performance computing (HPC) has become indispensable for LES because resolving large turbulent structures and incorporating advanced combustion models require substantial computational resources. The increasing availability of massively parallel computing architectures has enabled larger computational domains, finer grid resolutions, and more detailed chemical mechanisms, thereby extending LES to realistic engineering-scale combustion systems (Posch *et al.*, 2025). Recent advances in parallel algorithms, domain decomposition, and GPU-accelerated computing have further improved the efficiency and scalability of LES. These developments support the integration of computationally intensive approaches, including combustion-aware SGS models, detailed chemistry, and data-driven turbulence closures, without prohibitive computational costs (Kim *et al.*, 2024; Wang *et al.*, 2024). As exascale computing continues to evolve, HPC will remain a key enabler for high-fidelity LES of next-generation combustion technologies, including low-carbon fuel systems and advanced propulsion applications.

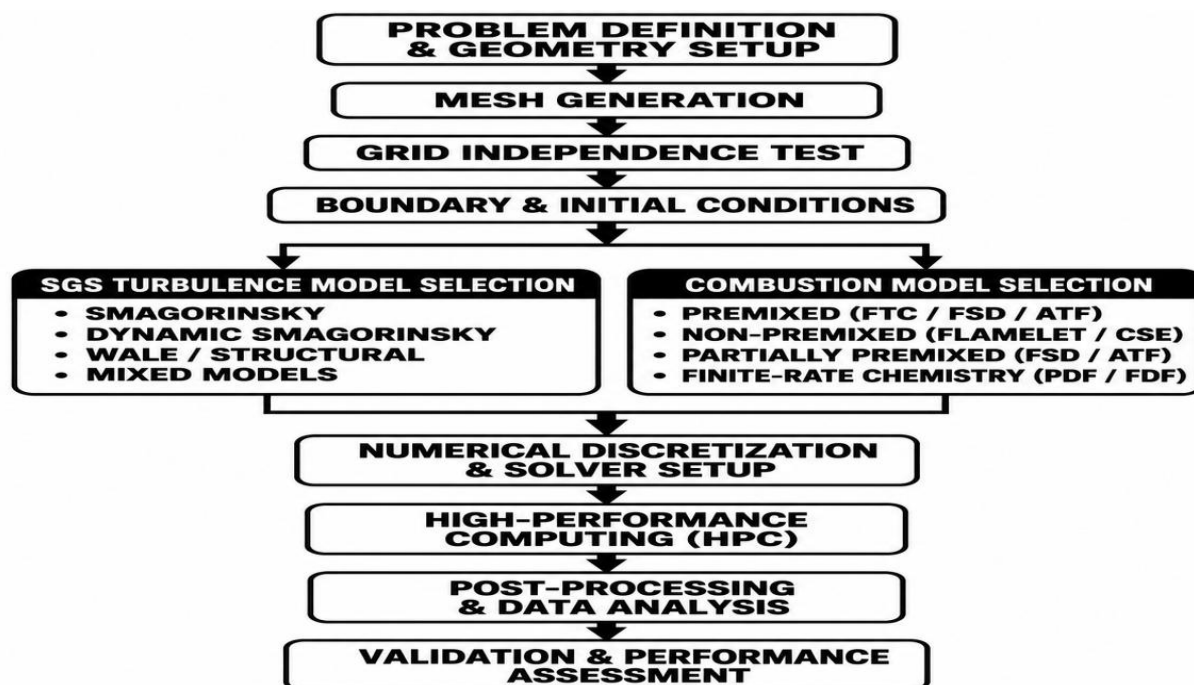


Figure 4. Numerical workflow for Large Eddy Simulation (LES) of turbulent combustion. The workflow summarizes the major computational stages in LES of turbulent combustion, including geometry and mesh generation, boundary condition specification, turbulence and combustion model selection, numerical discretization, high-performance computing, and validation. These interconnected steps collectively determine the accuracy, stability, and computational efficiency of LES predictions. Source: Modified from Pitsch (2006)

4. Model Validation and Performance Assessment

Model validation and performance assessment are essential for establishing the reliability and predictive capability of Large Eddy Simulation (LES) in turbulent combustion. Validation against experimental measurements and Direct Numerical Simulation (DNS) datasets enables systematic evaluation of

turbulence, combustion, and turbulence–chemistry interaction models, while performance assessment examines simulation accuracy, uncertainty, and computational efficiency. Together, these approaches provide the basis for determining the applicability of LES to both fundamental investigations and practical engineering combustion systems (Pitsch, 2006; Posch *et al.*, 2025).

4.1 Experimental and DNS Validation

Rigorous validation is essential to establish the predictive reliability of Large Eddy Simulation (LES) for turbulent combustion. Experimental measurements and Direct Numerical Simulation (DNS) datasets provide complementary benchmarks for assessing the accuracy of turbulence, combustion, and turbulence–chemistry interaction models. While experiments offer realistic operating conditions and measurable quantities such as velocity, temperature, species concentrations, and flame structure, DNS provides highly resolved flow-field data that enable detailed evaluation of subgrid-scale (SGS) closures and combustion models (Pitsch, 2006; Domingo and Vervisch, 2022). Experimental validation remains the primary approach for demonstrating the applicability of LES to practical combustion systems. Agreement with measured flame stabilization, heat release, pollutant formation, and flow characteristics provides confidence in model predictions and identifies deficiencies requiring further refinement. Recent investigations have shown that LES can accurately reproduce combustion dynamics in premixed and biomass syngas burners when appropriate turbulence and chemistry models are employed and carefully validated against experimental observations (Åkerblom and Fureby, 2024; Papaflippou *et al.*, 2024). Similarly, validation studies have demonstrated improved predictive capability of advanced turbulence–chemistry interaction formulations, including consistent Multiple Mapping Conditioning (MMC), for turbulent premixed flames (Iaroslavtceva *et al.*, 2024). DNS complements experimental validation by providing high-fidelity benchmark datasets that are free from turbulence-model assumptions. These datasets have become indispensable for evaluating SGS models, investigating flame–turbulence interactions, and validating finite-rate chemistry formulations under controlled conditions. Recent DNS-based assessments have further strengthened the development of turbulent combustion models by identifying model limitations and guiding improvements in LES closures across different combustion regimes (Jozefik *et al.*, 2024; Zhou, 2024). Together, experimental measurements and DNS

benchmarks constitute the foundation for robust validation and continued advancement of predictive LES methodologies.

4.2 Accuracy, Uncertainty, and Computational Efficiency

The performance of LES is determined by its ability to balance predictive accuracy with computational cost. Simulation accuracy depends on the combined effects of SGS turbulence models, turbulence–chemistry interaction formulations, numerical discretization, grid resolution, and boundary conditions. Inadequate treatment of any of these components can increase uncertainty in predictions of flame propagation, ignition, extinction, and pollutant formation (Unnikrishnan *et al.*, 2021; Posch *et al.*, 2025). Quantifying uncertainty has therefore become an important aspect of LES model evaluation. Sources of uncertainty include model assumptions, numerical errors, parameter selection, and experimental measurement variability. Systematic sensitivity analyses, grid-independence studies, and comparisons with experimental and DNS data are widely employed to assess model robustness and establish confidence in simulation results (Domingo and Vervisch, 2022; Ahmed *et al.*, 2024). Such practices are particularly important for advanced combustion systems operating under high-pressure or fuel-flexible conditions, where turbulence–chemistry interactions become increasingly complex. Despite its higher computational demand compared with Reynolds-Averaged Navier–Stokes (RANS) methods, LES offers substantially greater physical fidelity while remaining far more practical than DNS for engineering-scale applications. Continued advances in high-performance computing, parallel algorithms, and efficient combustion models have significantly reduced computational limitations, enabling LES to simulate increasingly complex reacting flows with improved accuracy and scalability (Salehi *et al.*, 2024; Posch *et al.*, 2025). Consequently, LES has emerged as the preferred compromise between computational efficiency and predictive capability for modern turbulent combustion research and engineering design.

Table 3. Representative validation studies of LES for turbulent combustion.

Reference	Combustion system	Validation method	Outcomes
Papaflippou <i>et al.</i> (2024)	Biomass syngas burner	Experimental	Accurate prediction of temperature and species fields
Iaroslavtceva <i>et al.</i> (2024)	Premixed flame	DNS/Experimental	Improved turbulence–chemistry interaction prediction
Åkerblom and Fureby (2024)	Spray combustor	Experimental	Good agreement with flame characteristics
Jozefik <i>et al.</i> (2024)	Methane–air combustion	DNS	Benchmark for model assessment
Zhou (2024)	Turbulent combustion models	DNS review	Identified strengths and limitations of validation strategies

5. Applications of LES in Turbulent Combustion

Large Eddy Simulation (LES) has evolved from a research-oriented technique into a practical tool for analyzing and optimizing a wide range of turbulent combustion systems. Its ability to resolve unsteady flow structures and accurately represent turbulence–chemistry interactions has enabled improved prediction of combustion performance, stability, and emissions across diverse engineering applications. This section highlights the major applications of LES in gas turbines, internal combustion engines, aerospace propulsion, industrial combustion systems, and emerging low-carbon fuel technologies (Pitsch, 2006; Posch *et al.*, 2025).

5.1 Gas Turbines

Large Eddy Simulation (LES) has become an indispensable tool for investigating turbulent combustion in modern gas turbines because it accurately resolves unsteady flow structures, flame dynamics, and turbulence–chemistry interactions that strongly influence combustion stability, efficiency, and emissions (Pitsch, 2006; Shankar *et al.*, 2024). Compared with Reynolds-Averaged Navier–Stokes (RANS) methods, LES provides improved prediction of vortex–flame interactions, thermoacoustic instabilities, and pollutant formation, making it particularly valuable for the design of low-emission combustors (Poinsot and Veynante, 2011; Kondor, 2025). Recent applications have increasingly focused on alternative fuels, particularly hydrogen and ammonia, to support the transition toward carbon-neutral power generation. LES has been successfully employed to evaluate flame stabilization, combustion dynamics, fuel flexibility, and nitrogen oxide (NO_x) emissions under varying operating conditions, providing insights that are difficult to obtain experimentally (Pashchenko, 2024; Zhao and Tian, 2025). Furthermore, fuel-flexible combustor concepts capable of operating with hydrogen, ammonia, and methane blends have demonstrated the potential of LES to optimize combustion performance while maintaining low emissions (Patel *et al.*, 2025). Despite these advances, predictive accuracy remains dependent on robust turbulence–chemistry interaction models and high computational resources, particularly for multi-fuel and high-pressure combustion systems. Continued

improvements in combustion modelling and high-performance computing are expected to further strengthen the role of LES in the development of next-generation gas turbines with enhanced efficiency, fuel flexibility, and environmental performance (Posch *et al.*, 2025).

5.2 Internal Combustion Engines

Large Eddy Simulation (LES) has become an effective tool for investigating in-cylinder combustion processes in internal combustion engines, where highly unsteady flow fields, turbulence–chemistry interactions, and cyclic variability strongly influence engine performance and emissions (Posch *et al.*, 2025). By resolving the dominant turbulent structures,

LES provides more accurate predictions of ignition, flame propagation, heat release, and pollutant formation than conventional RANS approaches, thereby supporting the optimization of combustion strategies and engine design (Pitsch, 2006; Poinsot and Veynante, 2011). Recent studies have extended LES to low-carbon engine technologies, particularly hydrogen- and ammonia-fueled engines, to evaluate combustion stability, efficiency, and emission characteristics under diverse operating conditions (Eyisse *et al.*, 2025). These simulations have improved understanding of fuel-specific combustion behaviour and facilitated the development of cleaner, fuel-flexible engine concepts. As computational capabilities continue to advance, LES is expected to play an increasingly important role in designing high-efficiency, low-emission internal combustion engines powered by conventional and sustainable fuels (Eyisse *et al.*, 2025; Posch *et al.*, 2025).

5.3 Aerospace Propulsion

Large Eddy Simulation (LES) is increasingly employed in aerospace propulsion to improve the prediction of combustion processes in aero-engines and rocket propulsion systems, where complex turbulence–chemistry interactions, high-pressure operation, and combustion instabilities present significant modelling challenges (Pitsch, 2006; Boretti, 2024). By resolving transient flow structures and flame dynamics, LES provides valuable insights into ignition, flame stabilization, heat release, and thermoacoustic behaviour, thereby supporting the design of safer and more efficient propulsion systems. Recent applications have focused on hydrogen- and ammonia-fuelled propulsion technologies to reduce carbon emissions while maintaining high combustion performance. LES has been used to evaluate fuel flexibility, combustion stability, and emission characteristics, providing critical guidance for the development of next-generation sustainable aerospace engines (Boretti, 2024; Zhao and Tian, 2025). Continued advances in turbulence modelling and computational resources are expected to further expand the role of LES in the design and optimization of future aerospace propulsion systems.

5.4 Industrial Combustion Systems

Large Eddy Simulation (LES) has been widely applied to industrial combustion systems, including furnaces, boilers, burners, and process heaters, where accurate prediction of turbulent mixing, flame stabilization, heat transfer, and pollutant formation is essential for efficient and reliable operation (Pitsch, 2006; Poinsot and Veynante, 2011). Compared with conventional turbulence models, LES provides improved resolution of transient flow structures and combustion dynamics, enabling more reliable optimization of burner design and operating conditions. Recent studies have demonstrated the capability of LES to accurately predict biomass syngas combustion and swirl-stabilized flame behaviour when validated against experimental measurements, highlighting its value for industrial-scale combustion analysis

(Papafilippou *et al.*, 2024). In addition, LES has been increasingly applied to ammonia-based industrial combustion systems to evaluate combustion efficiency and emission characteristics, supporting the transition toward cleaner industrial energy technologies (Alnajideen *et al.*, 2024). These advances reinforce the growing role of LES as a predictive tool for developing high-efficiency, low-emission industrial combustion systems.

5.5 Low-Carbon Fuels (Hydrogen, Ammonia, and Biomass)

The transition to low-carbon fuels has significantly expanded the application of Large Eddy Simulation (LES) in turbulent combustion research. LES has been extensively used to investigate hydrogen, ammonia, and biomass combustion because these fuels exhibit distinct flame characteristics, ignition behaviour, and emission pathways that are difficult to resolve using conventional turbulence models (Pashchenko,

2024; Shankar *et al.*, 2024). Its ability to capture transient turbulence–chemistry interactions provides valuable insight into flame stability, combustion efficiency, and pollutant formation under practical operating conditions. Hydrogen combustion presents challenges related to high flame speed and flashback, whereas ammonia combustion requires careful control of ignition and nitrogen oxide (NO_x) emissions. Biomass-derived syngas introduces additional complexity because of its variable composition and fuel flexibility. Recent LES studies have improved understanding of these phenomena and supported the optimization of combustor designs for cleaner and more efficient energy conversion (Papafilippou *et al.*, 2024; Zhao and Tian, 2025). As the global energy sector advances toward carbon neutrality, LES is expected to remain a key computational tool for accelerating the development and deployment of sustainable combustion technologies (Kondor, 2025; Patel *et al.*, 2025).

Table 4. Representative applications of Large Eddy Simulation (LES) in turbulent combustion

Application	LES contribution	Key challenges
Gas turbines	Predicts flame dynamics, thermoacoustics, and emissions	Multi-fuel combustion; computational cost
Internal combustion engines	Resolves in-cylinder flow, ignition, and combustion	Cyclic variability; detailed chemistry
Aerospace propulsion	Captures high-pressure flame behaviour and instabilities	Extreme operating conditions
Industrial combustion systems	Optimizes mixing, heat transfer, and emissions	Complex geometries; experimental validation
Low-carbon fuels	Evaluates H ₂ , NH ₃ , and biomass combustion performance	Fuel-specific kinetics and NO _x control

Abbreviations: LES = Large Eddy Simulation, H₂ = Hydrogen, NH₃ = Ammonia, NO_x = Nitrogen oxides.

Source: Alnajideen *et al.* (2024); Shankar *et al.* (2024) and Posch *et al.* (2025)

6. Emerging Trends and Future Perspectives

Rapid advances in computational science, data-driven modelling, and high-performance computing are reshaping the future of Large Eddy Simulation (LES) for turbulent combustion. Emerging approaches aim to improve predictive accuracy, reduce computational cost, and enable real-time simulation of increasingly complex combustion systems. This section highlights recent developments in machine learning-assisted LES, hybrid and reduced-order modelling, exascale computing and digital twins, and the key research challenges that will influence the next generation of turbulent combustion modelling (Parente and Swaminathan, 2024; Deng *et al.*, 2025).

6.1 Machine Learning-Assisted LES

Machine learning (ML) is increasingly being integrated into Large Eddy Simulation (LES) to enhance turbulence modelling, combustion prediction, and computational efficiency. By learning complex relationships from high-fidelity datasets, ML algorithms can improve subgrid-scale closures, accelerate chemical kinetics, and reduce modelling uncertainties while preserving physical fidelity (Girimaji, 2024; Deng *et al.*, 2025). These capabilities are particularly valuable for turbulent combustion, where conventional models often struggle to represent highly nonlinear turbulence–chemistry interactions. Recent advances have focused on physics-informed machine learning and scientific ML frameworks that combine data-driven techniques with governing physical principles, improving model generalizability and robustness (Deng *et al.*, 2025). In gas turbine applications, ML-assisted combustion models have demonstrated considerable potential for optimizing flame stability, emission prediction, and computational performance, highlighting their growing role in next-generation LES frameworks (Mo *et al.*, 2025). Although challenges related to data quality, interpretability, and model transferability remain,

machine learning is expected to become an integral component of future predictive combustion simulations.

6.2 Hybrid and Reduced-Order Modeling

Hybrid and reduced-order modeling approaches are emerging as effective strategies for improving the computational efficiency of Large Eddy Simulation (LES) while maintaining predictive accuracy. Hybrid methods combine LES with complementary techniques, such as Reynolds-Averaged Navier–Stokes (RANS), to balance computational cost and physical fidelity across different flow regions. Reduced-order models, meanwhile, employ data-driven and mathematical techniques to represent complex flow dynamics with substantially fewer computational degrees of freedom (Kramer *et al.*, 2024). Recent advances in operator inference and nonlinear reduced-order modelling have demonstrated the potential to accelerate combustion simulations without compromising the essential physics of turbulent reacting flows (Kramer *et al.*, 2024). Combined with scientific machine learning, these approaches offer promising pathways for rapid design optimization, uncertainty quantification, and real-time engineering analysis, extending the practical applicability of LES to increasingly complex combustion systems (Deng *et al.*, 2025).

6.3 Exascale Computing and Digital Twins

Advances in exascale computing and digital twin technologies are expected to significantly expand the capabilities of Large Eddy Simulation (LES) for turbulent combustion. Exascale computing enables high-fidelity simulations of complex reacting flows with larger computational domains, finer grid resolutions, and more detailed chemical kinetics, thereby improving predictive accuracy for practical combustion systems (Le *et al.*, 2024). These capabilities are increasingly supported by scalable algorithms and modern high-performance computing architectures. Digital twins further extend the application of LES by integrating real-time simulation, sensor data, and data-driven models to enable continuous monitoring, optimization, and predictive maintenance of combustion systems (Parente and Swaminathan, 2024). The combination of exascale computing and digital twins is expected to accelerate the design of cleaner, more efficient, and fuel-flexible combustion technologies while supporting intelligent decision-making in industrial and aerospace applications.

6.4 Outstanding Challenges and Future Research Directions

Despite substantial progress, several challenges continue to limit the broader application of Large Eddy Simulation (LES) in turbulent combustion. Improving the accuracy and generalizability of subgrid-scale and turbulence–chemistry interaction models, reducing computational cost, and enhancing predictive capability for high-pressure, multi-fuel, and multiphase combustion remain key research priorities

(Girimaji, 2024; Posch *et al.*, 2025). Robust validation using high-quality experimental and Direct Numerical Simulation (DNS) datasets is also essential for improving model reliability across diverse operating conditions. Future research is expected to emphasize the integration of physics-informed machine learning, reduced-order modelling, exascale computing, and digital twin technologies to enable faster and more accurate combustion simulations (Parente and Swaminathan, 2024; Deng *et al.*, 2025). Continued advances in these areas will strengthen the role of LES as a predictive tool for designing efficient, low-emission, and fuel-flexible combustion systems capable of meeting future energy and environmental demands.

7. Conclusion

Large Eddy Simulation (LES) has emerged as a powerful approach for predicting turbulent combustion by balancing physical accuracy with computational efficiency. Advances in turbulence modeling, turbulence–chemistry interaction, and numerical methods have expanded its application across diverse combustion systems, including gas turbines, internal combustion engines, aerospace propulsion, industrial burners, and low-carbon fuels. Although challenges related to model accuracy, computational cost, and validation remain, ongoing developments in machine learning, reduced-order modeling, and high-performance computing are expected to further enhance the predictive capability and industrial applicability of LES. Consequently, LES will continue to play a pivotal role in advancing efficient, low-emission, and sustainable combustion technologies.

Acknowledgement

We thank all the researchers who contributed to the success of this research work.

Conflict of Interest

The authors declared that there are no conflicts of interest.

Funding

No funding was received for this research work.

References

- Ahmed, U., Ghai, S.K. and Chakraborty, N. (2024). Assessment of Laws of the Wall During Flame–Wall Interaction of Premixed Flames Within Turbulent Boundary Layers. *Flow Turbulence Combust.* 112:1161–1190. <https://doi.org/10.1007/s10494-024-00541-7>
- Åkerblom, A. and Fureby, C. (2024). LES Modeling of the DLR Generic Single-Cup Spray Combustor: Validation and the Impact of Combustion

- Chemistry. *Flow Turbulence Combust.* 112:557–585. <https://doi.org/10.1007/s10494-023-00512-4>
- Alnajideen, M., Shi, H., Northrop, W., et al. (2024). Ammonia combustion and emissions in practical applications: A review. *Carbon Neutrality.* 3: 13. <https://doi.org/10.1007/s43979-024-00088-6>
- Bambauer, M., Pfitzner, M. and Klein, M. (2024). LES of Premixed Turbulent Combustion Using Filtered Tabulated Chemistry. *Flow Turbulence Combust.* 113: 1111–1143. <https://doi.org/10.1007/s10494-024-00563-1>
- Boretti, A. (2024). Towards hydrogen gas turbine engines aviation: A review of production, infrastructure, storage, aircraft design and combustion technologies. *International Journal of Hydrogen Energy.* 88: 279-288. <https://doi.org/10.1016/j.ijhydene.2024.09.121>
- Deng, S., Wang, L., Kim, S. and Koenig, B. C. (2025). Scientific machine learning in combustion for discovery, simulation, and control. *Proceedings of the Combustion Institute.* 41: 105796. <https://doi.org/10.1016/j.proci.2025.105796>
- Domingo, P. and Vervisch, L. (2022). Recent developments in DNS of turbulent combustion. *Proceedings of the Combustion Institute.* 39(1):35–66. <https://doi.org/10.1016/j.proci.2022.06.030>
- Eyisse, E. F., Nadimi, E. and Wu, D. (2025). Ammonia Combustion: Internal Combustion Engines and Gas Turbines. *Energies.* 18(1):29. <https://doi.org/10.3390/en18010029>
- Fiorina, B., Vicquelin, R., Auzillon, P., Darabiha, N., Gicquel, O. and Veynante, D. (2010). A filtered tabulated chemistry model for LES of premixed combustion. *Combustion and Flame.* 157(3): 465–475. <https://doi.org/10.1016/j.combustflame.2009.09.015>
- Girimaji, S. S. (2024). Turbulence closure modeling with machine learning: A foundational physics perspective. *New Journal of Physics.* 26:071201. <https://doi.org/10.1088/1367-2630/ad6689>
- Iaroslavtceva, N., Kronenburg, A. and Gärtner, J. W. (2024). A consistent MMC-LES approach for turbulent premixed flames. *Proceedings of the Combustion Institute.* 40(1–4): 105226. <https://doi.org/10.1016/j.proci.2024.105226>
- Impagnatiello, M., Malé, Q. and Noiray, N. (2024). Numerical study of ignition and combustion of hydrogen-enriched methane in a sequential combustor. *Flow, Turbulence and Combustion.* 112: 1249–1273. <https://doi.org/10.1007/s10494-024-00540-8>
- Jozefik, Z., Harvazinski, M. E., Sankaran, V., Dammati, S. S., Poludnenko, A. Y., Lu, T. et al. (2024). Modeling of high-speed, methane–air, turbulent combustion, Part I: One-dimensional turbulence modeling with comparison to DNS. *Combustion and Flame.* 263:113379. <https://doi.org/10.1016/j.combustflame.2024.113379>
- Kim, M., Park, J. and Choi, H. (2024). Large-eddy simulation of flow over a circular cylinder with a neural network-based subgrid-scale model. *Journal of Fluid Mechanics.* 984:A6. <https://doi.org/10.1017/jfm.2024.154>
- Kondor, I. P. (2025). Sustainable Fuels for Gas Turbines—A Review. *Sustainability.* 17(13):6166. <https://doi.org/10.3390/su17136166>
- Kramer, B., Peherstorfer, B. and Willcox, K. (2024). Learning nonlinear reduced models from data with Operator Inference. *Annual Review of Fluid Mechanics.* 56:521–548. <https://doi.org/10.1146/annurev-fluid-121021-025220>
- Le, J., Yang, M., Guo, M., Tian, Y. and Zhang, H. (2024). Progress and prospects of artificial intelligence development and applications in supersonic flow and combustion. *Progress in Aerospace Sciences.* 151:101046. <https://doi.org/10.1016/j.paerosci.2024.101046>
- Lomada, S., Pfitzner, M. and Klein, M. (2024). Flame Surface Density and Artificially Thickened Flame Combustion Models Applied to a Turbulent Partially-Premixed Flame. *Flow Turbulence Combust.* 112:729–750. <https://doi.org/10.1007/s10494-023-00477-4>
- Martinez-Sanchis, D., Sternin, A., Banik, S., Haidn, O. and Tajmar, M. (2024). Subgrid Turbulent Flux Models for Large Eddy Simulations of Diffusion Flames in Space Propulsion. *Fluids.* 9(6): 124. <https://doi.org/10.3390/fluids9060124>
- Mo, D., Lin, Y., Liu, Y. et al. (2025). A review of recent advances in the application of machine learning algorithms for gas turbine combustion. *Propul. Energy.* 1:20. <https://doi.org/10.1007/s44270-025-00022-w>
- Papafilippou, N., Pignatelli, F., Subash, A.A. et al. (2024). LES of Biomass Syngas Combustion in a Swirl Stabilised Burner: Model Validation and Predictions. *Flow Turbulence Combust.* 113: 1189–1214. <https://doi.org/10.1007/s10494-024-00558-y>
- Parente, A. and Swaminathan, N. (2024). Data-driven models and digital twins for sustainable combustion technologies. *iScience.* 27(4):109349. <https://doi.org/10.1016/j.isci.2024.109349>
- Pashchenko, D. (2024). Ammonia fired gas turbines: Recent advances and future perspectives. *Energy.* 290:130275. <https://doi.org/10.1016/j.energy.2024.130275>
- Patel, S. J., Noble, D. R., Emerson, B., and Lieuwen, T. (2025). "Back to the Future: Revisiting Nonpremixed Designs for Fuel Flexible (H₂/NH₃/CH₄), Low NO_x Combustion." *ASME. J. Eng. Gas Turbines Power.* 147(11): 111008. <https://doi.org/10.1115/1.4068587>
- Pitsch, H. (2006). Large-eddy simulation of turbulent combustion. *Annual Review of Fluid Mechanics.* 38: 453–482.

- <https://doi.org/10.1146/annurev.fluid.38.050304.092133>
- Poinsot, T. and Veynante, D. (2011). Theoretical and numerical combustion (4th ed.).
- Posch, S., Gößnitzer, C., Lang, M., Novella, R., Steiner, H. and Wimmer, A. (2025). Turbulent combustion modeling for internal combustion engine CFD: A review. *Progress in Energy and Combustion Science*. 106:101200. <https://doi.org/10.1016/j.pecs.2024.101200>
- Salehi, M. M., Devaud, C. and Bushe, W. K. (2024). Advances and challenges of the Conditional Source-term Estimation model for turbulent reacting flows. *Progress in Energy and Combustion Science*. 104:101172. <https://doi.org/10.1016/j.pecs.2024.101172>
- Shankar, A., Parammasivam, K. M. and Surya Narayanan, S. (2024). "A review on computational studies on hydrogen combustion for gas turbine applications". *Aircraft Engineering and Aerospace Technology: An International Journal*. 96(9):1225–1233. doi: <https://doi.org/10.1108/AEAT-12-2023-0312>
- Singh, P. P. and Roy, R. N. (2024). Evaluation of flow and flame characteristics of turbulent bluff-body CH₄-H₂ flame using LES-FPV approach. *Journal of Turbulence*. 25(4–6). <https://doi.org/10.1080/14685248.2024.2352490>
- Tay-Wo-Chong, L. (2012). Numerical simulation of the dynamics of turbulent swirling flames (Doctoral dissertation). Technical University of Munich
- Unnikrishnan, U., Huo, H., Wang, X. and Yang, V. (2021). Subgrid scale modeling considerations for large eddy simulation of supercritical turbulent mixing and combustion. *Physics of Fluids*. 33(7): 075110. <https://doi.org/10.1063/5.0055751>
- Veynante, D. and Vervisch, L. (2002). Turbulent combustion modeling. *Progress in Energy and Combustion Science*. 28(3): 193–266. [https://doi.org/10.1016/S0360-1285\(01\)00017-X](https://doi.org/10.1016/S0360-1285(01)00017-X)
- Wang, Y., Luo, K., Xiao, H., Jin, T., Xing, J. and Fan, J. (2024). A novel subgrid-scale stress model considering the influence of combustion on turbulence: A priori and a posteriori assessment. *Physics of Fluids*. 36(8): 085161. <https://doi.org/10.1063/5.0222050>
- Wang, Z. and Yang, X. (2024). NO_x Formation Mechanism and Emission Prediction in Turbulent Combustion: A Review. *Applied Sciences*. 14(14): 6104. <https://doi.org/10.3390/app14146104>
- Wehrmann, V. S., Chakraborty, N., Klein, M., *et al.* (2024). Choice of reaction progress variable under preferential diffusion effects in turbulent syngas combustion based on detailed chemistry direct numerical simulations. *Scientific Reports*. 14: 14861. <https://doi.org/10.1038/s41598-024-64552-0>
- Zhao, Y. and Tian, Y. (2025). Recent progress and prospects of ammonia combustion for gas turbines. *Chinese Journal of Aeronautics*. 38(10). <https://doi.org/10.1016/j.cja.2025.103619>
- Zhou, L. (2024). A review for the progress in validation of the SOM turbulent combustion model by DNS. *International Communications in Heat and Mass Transfer*. 159: 108099. <https://doi.org/10.1016/j.icheatmasstransfer.2024.108099>
- Zhou, M., Ding, S. and Wang, S. (2023). Review of subgrid models of the equation of state in the large eddy simulation of transcritical and supercritical flows and combustion. *Journal of Tsinghua University (Science and Technology)*. 63(4): 473–486. <https://doi.org/10.16511/j.cnki.qhdxxb.2023.25.013>

How to cite this article

Damilola, O. T., Obukeajeta, O. D., Agida, O. D., Abah, M. A., & Abimbola, M. O. (2026). Large Eddy Simulation (LES) of turbulent combustion: A review of modeling approaches and applications. *Chemical and Environmental Science Archives*, 6(3), 77–91. <https://doi.org/10.47587/CESA.2026.6305>

This work is licensed under a [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/)

