Large Eddy Simulation: A Useful Tool for Engineering Fluid Dynamics

C. Fureby
SE 147 25 Tumba, Stockholm, Sweden

Abstract

This paper is dedicated to describe the current state-of-the-art in Large Eddy Simulation (LES) of practical engineering systems. As LES is used in a wide range of applications (aerodynamics, hydrodynamics, combustion etc.) an attempt is made here to provide a compact but still comprehensive description of the LES methodology and an overview of how LES is utilized to provide knowledge about practical engineering systems. Both theoretical aspects of LES, such as subgrid modeling and numerical methods, as well as examples of LES computations in the fields of aerodynamics, hydrodynamics and combustion are presented and discussed. In order to support these applied LES predictions some results for building block flows, for which experimental data is available, are also presented. In addition the issues of verification, validation and uncertainty quantification are also briefly described and discussed. The main conclusion is that LES provides a very useful computational tool for fluid mechanics that can and should be used together with other simulations models and experiments to advance the understanding of fluid flow and to aid the design of engineering systems. With present computational capabilities it is already now possible to gain fundamentally new insight into e.g. car, train and aircraft aerodynamics, ship hydrodynamics and combustion in a range of systems from gas turbines and IC engines, to scramjet engines and White Dwarf stars.

1. Introduction

Large Eddy Simulation (LES) is a mathematical method for turbulent fluid flow used in Computational Fluid Dynamics (CFD). It was first proposed in 1963 by J. Smagorinsky to study atmospheric boundary layer flow, [1], and many of the salient features of LES were first explored by Deardorff, [2]. During the last three decades the use of LES has increased considerably, primarily due to the rapid increase in computational capacity, and is currently used in a variety of applications such as aerodynamics, [3-5], hydrodynamics, [6-7], combustion, propulsion and turbomachinery, [8-12], acoustics, [13-14], geophysics, [15], weather and climate forecasting, [16-17], and astrophysics, [18-19]. LES is based on the compressible, incompressible or reactive Navier-Stokes Equations (NSE), depending on subject area and application, and use a low-pass filtering operation, [20], to eliminate the small-scale flow physics not resolved on the computational grid. This means that the large-scale flow physics is resolved on the computational grid whereas the effects of the unresolved small-scale flow physics must be taken care of by subgrid models. It is commonly agreed, [21], that at least 85% to 90% of the total kinetic energy of the flow should be resolved in order for the small-scale flow physics to be universal enough to be amenable to modeling based on our present understanding and parameterization of Kolmogorov turbulence, [22-24], and its effects on chemical reactions and interfaces, [25-27]. In general this approach allows for better fidelity than alternative approaches such as Reynolds Averaged Navier-Stokes (RANS) methods, [28-29], at a lower computational cost compared to Direct Numerical Simulation, [30-31]. For practical engineering systems the use of LES usually requires large grids, and for wall-bounded flows either wall-resolved LES or wall-modeled LES can be used. In wall resolved LES the grid is successively refined as the wall is approached in order to resolve all dynamically relevant flow scales, whereas in wall modeled LES a wall model is used to represent the effects of the near wall flow scales eliminated by the low-pass filtering, [32-33].

Presently there exist several different LES methodologies such as Detached Eddy Simulation (DES), [34], and its sequels Delayed DES (DDES), [35], and Improved Delayed DES (IDDES), [36], Implicit LES (ILES), [37], and Two Scale LES (TSLES), [38]. For DES, DDES and IDDES a carefully selected unsteady RANS model is employed as a built-in wall model, which in conjunction with a blending function transitions into a conventional LES model outside of the near wall region. This approach leads to tremendous savings in grid size and computational time, whilst delivering reasonable predictions. ILES is based on the observation that the leading order truncation error from finite volume discretization schemes is of the same general form as that of most conventional subgrid models, [39]. Using a carefully selected flux reconstruction function efficient and accurate ILES models result. TSLES is based on a combination of a conventional LES and a one-dimensional DNS in the wall normal direction, resulting in a very efficient simulation model for high Reynolds (Re) number wall bounded flows.

This paper is dedicated to describe the current state-of-the-art in LES (including also DES) of practical engi-
neering systems. As LES is employed in a wide range of applications an attempt is made here to provide a compact but still comprehensive description of the LES methodology and an overview of how LES is used to provide knowledge about practical engineering systems. Both theoretical aspects of LES, such as subgrid modeling and numerical methods, and examples of LES computations, ranging from canonical and building block flows to practical engineering systems, will be presented and discussed. However, due to the broad scope of the paper, most technical details of for example different subgrid models or combustion models will not be provided explicitly but only in the references cited. Verification, validation and uncertainty quantification for LES will also be discussed since it is imperative to at least know how your LES method performs and what the influence is from using different computational grids or different inflow/outflow boundary conditions. At the end of the paper I will try to summarize the paper and provide some future perspectives on how LES will evolve and how LES will be can be used to help investigate or design engineering or physical systems.

2. The Large Eddy Simulation Formalism

The incompressible, compressible and reactive equations are the balance equations of mass, momentum and energy, [40], describing advection, diffusion and chemical reactions (when appropriate). LES is based on a separation of scales, which is achieved via spatial low-pass filtering. Physical processes occurring on scales larger than the filter width, $\Delta$, are resolved, whereas physics occurring on scales smaller than $\Delta$ are modeled by subgrid models. For an incompressible linear viscous fluid the LES equations becomes, [20],

$$\partial_t \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot (2\nu \mathbf{D}) - \mathbf{b}, \quad \nabla \cdot \mathbf{v} = 0,$$

in which $\mathbf{v}$, $\mathbf{p}$, $\mathbf{D} = \nabla \mathbf{v} \cdot \nabla \mathbf{v}$ and $\mathbf{v}$ are the filtered velocity, pressure, rate-of-strain tensor and kinematic viscosity, respectively, whilst $\mathbf{b} = \nabla \mathbf{v} \cdot \nabla \mathbf{v}$ is the subgrid stress tensor, representing the unresolved transport of momentum, [20, 41]. For a compressible linear viscous fluid with Fourier heat conduction and obeying the ideal gas law the LES equations becomes, [42],

$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla \rho + \nabla \cdot (2\nu \mathbf{D} - \mathbf{b}^{\nu} - \mathbf{b}^{\kappa})$$

$$\partial_t \mathbf{v} + \nabla \cdot (\mathbf{v} \mathbf{v}) = -\nabla \mathbf{p} + \nabla \cdot (2\nu \mathbf{D} - \mathbf{b}^{\nu} - \mathbf{b}^{\kappa}) - \mathbf{b},$$

in which, $\rho$, $\mathbf{v}$, $\mathbf{P}$ and $\mathbf{D} = \nabla \mathbf{v} \cdot \nabla \mathbf{v}$ are the filtered density, velocity, temperature and rate-of-strain tensor, respectively. The thermal equation of state is usually that of an ideal gas, $\mathbf{p} = \rho R \mathbf{T}$, in which $R$ is the gas constant. The fluid is described by the dynamic viscosity $\mu$, and the thermal diffusivity $\kappa = \mu/\rho$, with $\rho$ being the Prandtl number. The caloric equation of state is typically formulated in terms of the internal energy so that $E = \int_0^\rho c_i dT + \frac{1}{2} \mathbf{v}^2 + \mathbf{k}$, in which $c_i$ is the specific heat (at constant volume) and $\mathbf{k}$ the subgrid kinetic energy. Following the notations for the incompressible LES model in (1) the subgrid stress and flux terms are $\mathbf{b}^{\nu} = \tilde{\mathbf{p}}(\tilde{\mathbf{v}} \cdot \tilde{\mathbf{v}})$ and $\mathbf{b}^{\kappa} = \tilde{\mathbf{p}}(-\tilde{\mathbf{E}} \cdot \tilde{\mathbf{v}})_L$, respectively. For a linear viscous gaseous mixture, having Fourier heat conduction and Fickian diffusion, the LES equations becomes, [9],

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla \mathbf{p} + \nabla \cdot (2\nu \mathbf{D} - \mathbf{b}^{\nu} - \mathbf{b}^{\kappa})$$

in which, $\tilde{\mathbf{p}}$, $\tilde{\mathbf{v}}$, $\tilde{\mathbf{T}}$, $\tilde{\mathbf{E}}$ and $\tilde{\mathbf{D}} = \nabla \mathbf{v} \cdot \nabla \mathbf{v}$ are the filtered density, velocity, temperature and rate-of-strain tensor, respectively. The thermal equation of state is often that of a mixture of ideal gases, for which the filtered pressure is $\mathbf{p} = \rho R \mathbf{T}$, with $R$ being the composition dependent gas constant. The mixture is usually described by the viscosity $\mu$, and the species and thermal diffusivities, $D_{ij} = \mu_{ij}/\rho$, respectively, with $\rho$, $\mu_{ij}$ being the Schmidt and Prandtl numbers. The caloric equation of state is typically formulated in terms of enthalpies to ease the handling of reactions so that $E = \Sigma_i (h_i^e + f_i^e c_i \mathbf{v}) - \rho \mathbf{p} + \frac{1}{2} \mathbf{v}^2 + \mathbf{k}$, in which $h_i^e$ are the formation enthalpies, $c_i$ the specific heats (at constant pressure) and $\mathbf{k}$ the subgrid kinetic energy. The chemical kinetics enters (3) via the filtered species reaction rates $\tilde{\omega}_i = M_i P_i \tilde{w}_i$, in which $\tilde{w}_i = A_i T^m_i e^{-E_i/RT} (\tilde{P}_i \mathbf{Y})^{\lambda_i}$ are the reaction rates, $P_i$ the stoichiometric coefficients and $A_i$, $m_i$, $n_i$ and $b_i$ the Arrhenius parameters. The non-linearity of $\tilde{w}_i$ prevents any attempt at formulating simple models for $\tilde{w}_i$, [9, 29], and other types of models for $\tilde{w}_i$ are exploited. Following the notations used for the compressible LES model (2) the subgrid stress and flux terms are $\mathbf{b}^{\nu} = \tilde{\mathbf{p}}(\tilde{\mathbf{v}} \cdot \tilde{\mathbf{v}})$, $\mathbf{b}^{\kappa} = \tilde{\mathbf{p}}(-\tilde{\mathbf{E}} \cdot \tilde{\mathbf{v}})_L$ and $\mathbf{b} = \tilde{\mathbf{p}}(-\tilde{\mathbf{E}} \cdot \tilde{\mathbf{v}})$, respectively.

2.1. Subgrid Flow Models

To close the filtered LES equations (1), (2) or (3) a subgrid model is required that attempts to describe the effects of the unresolved flow on the resolved flow, using the resolved variables, [20]. In LES, conventional subgrid models can be characterized as either functional or structural, [20], depending on if they are intended to mimic the kinetic energy cascade from large to small scales or if they are intended to mimic the structure of the subgrid stress tensor. In addition to conventional LES models we will also discuss ILES and DES modeling. Note that the models described hereafter are formulated for reactive flow as it is the most general situation.

Functional models are the most widely used class of subgrid models and are most conveniently, [20], formulated as $\mathbf{b} = -2\mu \mathbf{D}_{\mathbf{p}}$, $b_{\mathbf{w}}(\mu_S/\rho_S) \tilde{\mathbf{Y}}$ and $b_{\mathbf{w}}(\mu/\rho) \mathbf{v} \cdot \tilde{\mathbf{v}}$, with $\mathbf{D}_{\mathbf{p}}$ being the deviatoric part of $\mathbf{D}$, $\mu$ the dynamic subgrid viscosity, $\rho_S$ and $\rho_S$ the turbulent Schmidt and Prandtl
numbers, respectively. This class of models include the well-known Smagorinsky model (SMG), \cite{43-44}. \[ \mu_s = \tau_p c_1^2 A^3 \frac{\partial^2 u}{\partial y^2}, \]
and \[ \kappa c_1^2 A^3 \frac{\partial^2 v}{\partial y^2}, \]
in which the model coefficients \( c_1 \) and \( c_2 \) can be prescribed as in \cite{43} (\( c_2 = 0.02 \) and \( c_2 = 0.07 \)) or computed as in \cite{44}. Another frequently employed functional model is the Wall-Adapting Local Eddy-viscosity model, (WALE), \cite{45}, \[ \mu_s = \tau_p c_1^2 A^3 \frac{\partial^2 v}{\partial y^2}, \]
with \( \tau_p (\mathbf{G}_w \mathbf{G}_w)^{\frac{1}{2}} (\mathbf{D}D) \) and \( \mathbf{G}_w \mathbf{G}_w \) in which \( \mathbf{G}_w \mathbf{G}_w \) is the shear stress tensor and \( c_2 \) a model coefficient calculated to 0.5 in \cite{45} by comparison with data from \cite{46}. This model, however, lacks a model for \( k \) that often is needed for modeling the subgrid turbulence chemistry interactions. Yet another functional model is the One- Equation Eddy Viscosity Model (OEEVM), \cite{47-48}, that is founded on the assumption that \( \mu_s \) is related to \( k \) energy by \[ \mu_s = \tau_p c_1^2 A^3 \frac{\partial^2 v}{\partial y^2}. \]
The subgrid kinetic energy may then be obtained from the following model transport equation,
\[
\frac{\partial (\rho k)}{\partial t} + \nabla \cdot (\rho \mathbf{v} \rho k) = 2 \mu_s \frac{\partial^2 k}{\partial y^2} + \nu (\rho \nabla \rho k - \tau_p \rho k \frac{\partial^2 \rho}{\partial y^2}), \tag{4}
\]
in which \( \epsilon = \rho c_1^2 A^3 \frac{\partial^2 v}{\partial y^2} \) is the dissipation. The coefficients \( c_1 \) and \( c_2 \) can be assumed constant as in \cite{47} (\( c_2 = 0.07 \) and \( c_1 = 1.05 \)), or can be evaluated dynamically as in the Localized Dynamic k-equation Model (LDKM) of Kim & Memon, \cite{48}.

Most subgrid viscosity models are designed for low Ma number flows and fail when strong shocks are present. In regions of shocks the dilatation, \( \nabla \cdot \mathbf{v} \), is large and to extend the use of these models to high Ma number flows with shocks Cabot & Cook, \cite{49}, developed a subgrid viscosity model for shock-turbulence interactions. This subgrid model is based on the shock-capturing approach of Neumann & Richtmyer, \cite{50}, and the classical SMG model, and take the form \[ \mathbf{B} = -\beta_E (\nabla \cdot \mathbf{v}) - \mathbf{D}_h, \]
with \( \beta_E \) being the subgrid bulk viscosity. Cabot & Cook, \cite{49}, propose to use \[ \beta_E = C_1 \tau_p A^3 V_n \nabla \cdot \mathbf{D}, \]
and \[ \beta_s = C_2 \tau_p A^3 V_n \nabla \cdot \mathbf{D}, \]
for \( r = 2, 4, 6 \). The use of the bulk viscosity term is the key to capturing shocks without destroying vorticity as \( \beta_s \) can be made large (to smooth shocks) without harming small-scale turbulence in regions where \( \nabla \cdot \mathbf{v} = 0 \). By setting \( r > 0 \) the subgrid viscosity keys directly on the ringing, rather than indirectly on gradients, thus eliminating the need for ad hoc limiters and dynamic procedures to turn off \( \mu_s \) in special cases and uniform shear.

Structural models incorporate a wide range of subgrid flow models, see \cite{20} for a comprehensive survey, aiming at describing the structure of the subgrid stress tensor and flux vectors instead of the effects of these terms on the resolved flow. The most straightforward structural model is probably the Scale Similarity (SS) model of Bardina et al., \cite{51}, in which the subgrid stress tensor is modeled as \[ \mathbf{B} = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}, \]
and accordingly would the subgrid mass and energy flux vectors be estimated as \[ \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}, \]
and \[ \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}. \]
respectively. The drawback with this model, although showing very high correlations with experimental data, \cite{52}, is that it is not dissipative enough to represent the effects of the small-scale turbulence. Instead, it was observed that by combing

the scale similarity model with an eddy viscosity model, \cite{53}, a more accurate and robust subgrid flow model was obtained. This so-called Mixed Model (MM) can be formulated as, \[ \mathbf{B} = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}. \]

In LES the raw (or unfiltered) incompressible, compressible or reactive flow equations are solved using non-oscillatory finite volume methods, \cite{37, 54}. LES was found to be accurate and robust in particular when based on monotonicity preserving convection schemes, such as Flux Corrected Transport (FCT), \cite{55}. Using Modified Equations Analysis (MEA) Fureby & Grinstein, \cite{56}, were able to derive expressions for the implicit (or build-in) subgrid models in a finite volume framework using a hybrid flux formulation. More specifically, can the implicit subgrid models be expressed as \[ \mathbf{B} = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}. \]

In LES the raw (or unfiltered) incompressible, compressible or reactive flow equations are solved using non-oscillatory finite volume methods, \cite{37, 54}. LES was found to be accurate and robust in particular when based on monotonicity preserving convection schemes, such as Flux Corrected Transport (FCT), \cite{55}. Using Modified Equations Analysis (MEA) Fureby & Grinstein, \cite{56}, were able to derive expressions for the implicit (or build-in) subgrid models in a finite volume framework using a hybrid flux formulation. More specifically, can the implicit subgrid models be expressed as

\[ \mathbf{B} = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}. \]

In LES the raw (or unfiltered) incompressible, compressible or reactive flow equations are solved using non-oscillatory finite volume methods, \cite{37, 54}. LES was found to be accurate and robust in particular when based on monotonicity preserving convection schemes, such as Flux Corrected Transport (FCT), \cite{55}. Using Modified Equations Analysis (MEA) Fureby & Grinstein, \cite{56}, were able to derive expressions for the implicit (or build-in) subgrid models in a finite volume framework using a hybrid flux formulation. More specifically, can the implicit subgrid models be expressed as

\[ \mathbf{B} = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v} - \mathbf{b}_s = \tau_p (\nabla \cdot \mathbf{v}) - \mathbf{v} \times \mathbf{v}. \]
Another way of dealing with the complex flow physics in the near wall region and the conflicts in grid resolution and anisotropic flow physics is to use a DES, DDES or IDDES model, [33-36]. The most well-known example of such a model is the original DES model utilizing the Spalart-Allmaras, [63], turbulence model and modifying this so as to accommodate a seamless transition to an LES model, similar to the SMG model in the detached flow region outside of the near wall region. The compressible form of the DES model is

\[ \mathbf{B} = 2 \mu_{\ell} \tilde{D}_h, \quad \mathbf{b}_1 = \mu_{\ell}/\nu \nabla | \nabla \mathbf{b}_1, \quad \text{in which} \quad \mu_{\ell} = \tilde{f}_p \tilde{V} \] 

with \( \tilde{V} \) governed by the equation,

\[ \partial_t (\tilde{V} + \nabla (\nabla \tilde{V})) c = c_{\nu} (1 - f_2) \tilde{S} \tilde{V} c^{-1} \nabla (\nabla \tilde{V}) \tilde{V} c^{-1} \nabla \tilde{V} - (c_{\nu} f_2 - c_{\nu} f_2 \nu^2 \kappa^2) (\nabla \tilde{V})^2. \] (5)

Here, \( \tilde{a} = \min (0, \| D \tilde{h} \|_{\mathbf{B}} \), \( \tilde{S} = f_1 + f_2 \), \( \tilde{S} = \tilde{S} \nu \mathbf{B} \), whereas \( f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8 \) and \( \nu_1 \) are empirical constants and auxiliary functions, respectively, for the Spalart–Allmaras model. Other models, such as Menter’s k-ω model, [64], are also available.

2.2 Subgrid Combustion Models

To close the filtered reacting flow equations (3) a model is required for the filtered species reaction rates, \( \tilde{w}_s \), in addition to the subgrid models discussed in Section 2.1. The species reaction rates are highly non-linear functions of composition and temperature such that \( \tilde{w}_s (p, \tilde{Y}, \tilde{T}) \), and chemical reactions are usually confined to thin reacting layers at small scales that cannot be resolved on standard LES grids. Consequently, most of the turbulence-chemistry interaction needs to be modeled. A number of combustion models that have been proposed for LES follow concepts and modeling strategies developed for RANS, [14]. Different methods that have been formulated specifically for LES of combustion include flamelet models, [65-72], finite rate chemistry models, [73-95] and linear eddy models, [96-107]. In this paper only a few combustion models are mentioned, but those included have been used to compute real engineering combustion applications with good results.

2.2.1 Flamelet Models

In flamelet models the flame is considered thin compared to the length scales of the flow, and is thus an interface between fuel and oxidizer (for non-premixed combustion) or between reactants and products (for premixed combustion), [65]. It is then convenient to decouple the flow and interface from the combustion chemistry that can be represented by the laminar flame speed, \( s_f \), A mixture fraction, \( Z \), and its variance, \( \tilde{Z} \), is often used for non-premixed combustion and a progress variable, \( \tilde{c} \), or a kinematic G-field is usually used for premixed combustion, whereas both are needed for partially premixed or stratified combustion, [29, 66-68]. In a LES framework this typical flamelet model can be compactly expressed using the flamelet LES equations,

\[ \begin{aligned}
\partial_t (\tilde{V} + \nabla (\nabla \tilde{V})) &= 0, \\
\partial_t (\tilde{C}) + \nabla (\nabla \tilde{C}) &= \nabla D, \nabla \tilde{C} - \tilde{b}, \\
\partial_t (\tilde{P}) + \nabla (\nabla \tilde{P}) &= \nabla D, \nabla \tilde{P} - \tilde{b}, \\
\partial_t (\tilde{E}) + \nabla (\nabla \tilde{E}) &= \nabla D, \nabla \tilde{E} - \tilde{b}. \\
\end{aligned} \]

In addition to the previously defined quantities, \( D \) is the diffusion coefficient for \( \tilde{Z} \), \( \tilde{b} = \tilde{P} (\tilde{v}_e - \tilde{v}_c) \), \( \tilde{c} \) the scalar dissipation rate, \( D \), the diffusion coefficient for \( \tilde{c} \), \( \tilde{b} = \tilde{P} (\tilde{v}_e - \tilde{v}_c) \), \( \chi \) the chemical source term for \( \tilde{c} \). Most often are the thermodynamic properties computed using standard mixing rules thus accounting for changes in composition and temperature as described in conjunction to (3) and for this the species mass fractions, \( \tilde{T} \), are required. The species mass fractions as well as the chemical source term, \( \tilde{w}_s \), are typically obtained from a flamelet library \( \tilde{w}_s (\tilde{Y}, \tilde{T}) \), and \( \tilde{w}_e = \tilde{w}_e (\tilde{Y}, \tilde{T}) \) that is pre-computed using a detailed or quasi-detailed reaction mechanism. This pre-processing step typically consists in solving one-dimensional diffusion or premixed flamelets (depending on the nature of the flame considered) parameterized by the scalar dissipation rate or equivalence ratio. In a second step those solutions are convoluted with a β-PDF and tabulated along the three coordinate directions \( \tilde{Z} \), \( \tilde{Z} \) and \( \tilde{c} \). This tabulation is often non-trivial because of the large span of the table and also because of singular points that may arise in such a tabulation, [69]. An issue with the flamelet model not often discussed is the dependence of the chemical source term on other variables such as for example pressure, density and temperature that are very important for supersonic combustion. Terrapen et al, [70], developed a scaling procedure to take into account the effects of pressure such that \( \tilde{w}_e = \tilde{w}_e (\tilde{P} / \rho_0) \), where \( \tilde{w}_e \) is the tabulated chemical source term computed at the background pressure, \( \rho_0 \). The subgrid stress and flux terms (\( \tilde{b}_1, \tilde{b}_2, \tilde{b}_3, \tilde{b}_4 \) and \( b_b \) are computed with an adequate turbulence model such as one of those listed in Section 2.1. In addition we need also to model the scalar dissipation rate \( \chi = 2 D \nabla \tilde{Z} \). In most turbulent flows, \( \chi \) is viewed as a scalar energy dissipation and its role is to dissipate scalar variance (scalar energy) analogous to the dissipation of the turbulent energy, \( \epsilon \), and is often modeled as \( \chi = 2 D \nabla \tilde{Z} \) given the variance, \( \tilde{Z} \). The flamelet model constitutes a significant simplification compared to the reacting flow equations (3) in that the dimensions of the phase space is reduced from 5+N where N is the number of species, to eight. With careful selection of \( \tilde{c} = \tilde{c} (\tilde{Y}) \) this difference in phase-space can be minimized but never completely eliminated. Flamelet models of this type have been successfully used for engineering flames by many authors including Pierce & Moin, [67], Duwig & Fureby, [68], Di Mare et al., [71], and Larsson, [72].
For the LES-PaSR model (8) the residence time, $\tau^*$, and reacting volume fraction, $\gamma^*$, needs further specification. The modeling of $\tau^*$ is based on the fine structure area-to-volume ratio is given by the dissipative length scale, $\ell_D$, and that the velocity influencing these structures is the Kolmogorov velocity, $\nu_k$, so that $\tau^*=\ell_D/\nu_k$, which may be reformulated as $\tau^*=\sqrt{\varepsilon}/\nu_k$, in which $\tau^*$ is the shear time scale. 

The modeling of $\gamma^*$ is based on intermittency arguments and results in that $\gamma^*=\tau^*/(\tau^*+\tau)$, in which $\tau_m/\delta_s$ is the characteristic time scale of the chemical reactions with $\delta_s$ being the laminar flame thickness and flame speed, respectively. Combining (3) and (8) results in the LES-PaSR species transport equation model,

$$\partial_t(\rho \overline{Y})+\nabla \cdot (\overline{PV})+\rho \overline{F} \cdot \nabla \overline{Y}_i - \tau^* \overline{w}_i = \rho \overline{w}_i \overline{F} \cdot \nabla \overline{Y}_i,$$  

where the mixing, $\overline{w}_i$, and turbulent diffusivities should scale as $\overline{w}_i = \nu_t \overline{F} \cdot \nabla \overline{Y}_i$, whereas the species diffusivities should scale as $D_j = FD_j$. In order to take turbulence and turbulent wrinkling into account, $\nu_t$ is introduced so that $D_j = E_F D_j$. The LES-TFM species transport equation model then takes the form,

$$\partial_t(\rho \overline{Y})+\nabla \cdot (\overline{PV})+\rho \overline{F} \cdot \nabla \overline{Y}_i - \tau^* \overline{w}_i = \rho \overline{w}_i \overline{F} \cdot \nabla \overline{Y}_i,$$  

in which $E_F$ is often evaluated using the power-law flame wrinkling model, [94]. The LES-TFM model have been extensively used to study laboratory combustors, [95], and aeronautical gas turbine combustion in laboratory scale, [96], as well as in full scale, [97].

2.2.3. Linear Eddy Models

The linear eddy model, originally proposed and developed by Kerstein, [98-100], and further developed into a subgrid scale model by Menon et al., [101-103], is using a one-dimensional (1D) stochastic description of turbulent stirring and diffusion. The model explicitly distinguishes the effects of turbulent stirring, molecular diffusion and chemical reactions at all flow scales. Considering a species mass fraction, $Y_i$, and a decomposition of the velocity, $\nu = \nu_s + \nu_{\gamma} + \nu$, the resolved advect-
tion and subgrid processes are characterized by,
\[ Y^*_e = \frac{1}{\Delta t} \int_{t}^{t+\Delta t} \left( -\nabla v^* \cdot \nabla (\nabla Y) + M_p \delta \right) dt. \]  
(11)

In the above expressions, \( v^* \) is the subgrid velocity, which can be obtained using \( v^* = \frac{\sqrt{2k / \lambda}}{\lambda} \), \( v \) the unresolved subgrid velocity and \( t_{LES} \) is the LES time step. The superscripts \( n \) and \( n+1 \) indicate two consecutive discrete times, and \( Y^*_e \) is an intermediate state after the large-scale convection is completed. Equation (11) describes the LES model as interpreted on the LES space and time scales. The molecular diffusion and chemical reaction processes contribute to the small-scale transport are resolved on an embedded 1D domain for each LES cell and the 1D domain is aligned with the direction of the maximum scalar gradient. Equation (3) is reformulated in the 1D LES domain as \( \rho_0(x) \nabla \psi + \nabla \psi (\nabla \psi + \nabla (\nabla \psi) + M_p \delta \right) \), where \( \nabla \psi \) represents the effect of the subgrid turbulence on the scalar field and \( s \) is the spatial coordinate along the LES domain. The subgrid scalar field is discretized in each LES cell \( N_{LES}=N_{c} \) cells, where \( N_{c} \) is the subgrid number (typically based on \( v^* \) and \( \lambda \)). The LES scalar fields are ensemble-averaged to obtain LES-resolved scalar values.

Furthermore, subgrid stirring, \( F_{sub} \), is implemented using stochastic rearrangement events called triplets, [98]. Each triplet map represents the action of an isotropic ‘turbulent’ eddy on the subgrid field. The eddy size, \( \lambda \), is randomly selected from a distribution function, \( f(\lambda) = 5 \lambda^{-4/3} (\lambda^{1/3} - \Delta^{1/3}) \), [98], in the range from \( \Delta \) to \( \lambda \). Stirring events occur at a specified frequency, \( f \), [98], \( f = \frac{2}{\nu} N_{c} \Delta \), \( \Delta^{1/3} (\lambda^{1/3} - \Delta^{1/3}) \psi \) in which \( \Delta \psi = 15 \). The stirring intervals are controlled by the relation \( \Delta t_{stir} = \frac{f}{\Delta} \), [100]. The LES model has been successfully applied to mixing, [104-105], non-premixed combustion, [106-107], and premixed combustion, [108-109]. However, LES has some limitations: (i) the computational burden associated with LES is higher as compared to other models, (ii) molecular diffusion across LES cells is not fully incorporated, and (iii) in premixed combustion the flame-turbulence interaction is influenced by the flame front curvature, an effect missing in the 1D description. In addition, the triplet map assumes that eddies of all sizes affect the flame in the same way, which means that viscous dissipation is not considered properly.

3. Numerical Methods for Engineering LES
Here we limit the discussion to unstructured Finite Volume Methods (FVM) since they are most appropriate for engineering LES. Unstructured grids typically allow greater flexibility in generating and adapting grids, but at the expense of increased storage needs. Central to FVMs is that the values of the dependent variables, \( u \), are represented by control volume averages, \( u_{i} = \frac{1}{V} \int_{V} u(x, t) dV \), representing implicit filtering. Discrete FVMs can be derived from Reynolds transport theorem so that,
\[ \frac{\partial}{\partial t} \int_{V} u_{i} dV + \int_{\partial V} \left( \nabla u_{i} \cdot \hat{n} \right) dS = \int_{V} \nabla \cdot (\nabla u_{i}) dV + \int_{\partial V} \left( \nabla \cdot (\nu \nabla u_{i}) \right) n_{i} dS. \]  
(12)

where \( F_{i} = \left( \rho v \right)_{i}, \left( \rho v e \right)_{i}, \left( \rho v Y_{i} \right)_{i} \), \( \nabla \cdot (\nabla u_{i}) \), \( \nabla \cdot (\nu \nabla u_{i}) \), \( \left( \nu \nabla v \right)_{i} \), \( \hat{n} \), \( dS \), \( dA \), and \( \partial V \) are the convective and diffusive fluxes, respectively, and \( B_{i} = 0, (b_{i})_{i} \), \( (b_{i})_{i} \), \( dA \), \( \partial V \) are the subgrid fluxes, and \( dA \), the area-element of integration. The semi-discretized LES equations (12) need to be integrated in time, and rules must be set for how to reconstruct the fluxes, \( F_{i}^{n} \) and \( B_{i} \), in order to be able to solve (12). For high-speed flows, explicit time integration, e.g. [110], is preferred, whereas for low-speed flows, requiring specific treatment of the pressure-velocity system, [111], semi-implicit multi-step methods, e.g. [112], are usually more appropriate. The choice of time-integration scheme is more important for the overall efficiency of the LES model than for the accuracy, provided that at least second order accurate time integration schemes are chosen. The choice of flux-reconstruction algorithms are however more important to the accuracy of the LES model than to the efficiency of the LES model. For the convective fluxes, \( F_{i}^{n} \), linear or cubic flux-reconstruction schemes (of second and fourth order accuracy, respectively) are recommended, but may not always work in complex engineering applications. The best choice is then to use flux-limiter based, [113], flux reconstruction schemes of the form \( F_{i}^{n} = \left( \phi F_{i}^{n} \right)^{+} + \left( 1-\phi \right) F_{i}^{n} \), in which the convective flux function is computed as a blend of a non-dissipative linear flux function, \( F_{i}^{n} \), and a dissipative upstream biased flux function, \( F_{i}^{n} \), with \( \psi \) \( 0 < \psi < 1 \) being a blending function that depends on the local state of the flow, [113-114]. For the other fluxes, \( F_{i} \) and \( B_{i} \), linear or cubic interpolation algorithms are usually applied. For LES, in which barely resolved vertical structures are to be transported across the domain, the time-step should be restricted so as to allow these structures to be transported across the grid. This puts some particular constraints on the time-step, and it is generally recommended that the Courant number should be less than about 0.5.

One way to estimate the accuracy of the numerical method is to estimate the leading order truncation error using the Modified Equations Approach (MAE), [115]. Briefly stated, given the differential equations of interest and the numerical method to be used, the MAE provides the differential equations solved numerically. These modified differential equations will thus include the original differential equations together with further terms related to the truncation error of the numerical method. One key aspect of the MEA compared with other approaches is that the truncation error will include whatever non-linearity is associated to either the differential equation or the numerical method. Expressions for the leading order truncation of the aforementioned FVM discretization can be found in [113] and [114], and for a 2nd order linear scheme, the leading order truncation error can be expressed as \( T_{n} = \frac{1}{2} \left[ \rho v \nabla \left( \nabla v \right) (d \delta) \right]_{n} + \ldots \), where \( d \) is the grid spac-
4. Verification and Validation

Information regarding general code verification and solution validation can be found in numerous references throughout the technical literature, e.g. [116-118]. Unfortunately, nearly all of this material has been directed toward RANS, which have different and more stringent requirements than those for LES. That notwithstanding, Oberkampf & Blottner, [116], provide a somewhat universal description of sources of error arising in nearly any fluid simulation. For validation of LES there exists a set of canonical and building block flows that are well suited for validation. Canonical flows are flows for which analytical, DNS and/or experimental data are available for validation. Canonical flows typically take place in simple geometries and have well-defined boundary conditions, and some examples are given in Table 1. Building block flows are typically more complicated flows for which experimental data and sometimes also DNS data are available for validation. Building block flows are typically associated with more complex geometries and more realistic boundary conditions, and some examples are provided in Table 1. There are a few joint efforts, e.g. by ERCOFTAC, [119], AGARD, [120], and the Sandia TNF workshop series, [121], to collect databases for validation of turbulent flow simulation techniques. As LES begins to be used for more complex flows it becomes harder to find data from well-controlled experiments that can offer well-defined boundary conditions and detailed, high-quality measurements in the flow regimes of interest. It is also essential that the LES model (or code) is compared with several canonical and building block flows in order to expand the regime for which the model (or code) has been validated. Besides canonical and building block flows, more complex flows, for which only experimental data and other LES predictions are available, should be used as validation cases in order to test the code or model as much as possible.

Other key issues for LES is to establish the quality of the computational grid and the accuracy of the numerical methods. These and other similar issues are treated in greater depth in [21] and [122], but the general guidelines are that (i) numerical schemes of at least second order accuracy should be used, although deviations may be needed close to shocks and discontinuities, and (ii) that at least 85% to 90% of the total kinetic energy should be resolved on the grid. In addition should grid refinement studies always be carried out, but since the solution changes with the grid only statistical moments of the flow solution can be compared and tested.

Next we will present two validation cases, a low Ma number building block flow and a reacting flow case for which experimental data is available for comparison.

The first example concerns the flow over a contoured ramp in a wind tunnel experimentally investigated by Song et al., [123], and computationally analyzed by several researchers, e.g. [124-127], using different LES models. The ramp experiments were carried out in a closed-loop wind tunnel equipped with an insert to mould the ramp. The computational set-up is designed to mimic the wind tunnel as closely as possible, including a 2 m long approach channel upstream of the ramp. Hexahedral grids with 1.0 and 8.0 million cells are used to discretize the computational domain. Open inflow-outflow boundary conditions are used together with no-slip wall boundary conditions and periodic spanwise boundary conditions. Based on the inflow velocity of $v_i=20.4$ m/s and the height of the ramp, the Re number is 28,560. Upstream of the ramp the flow is similar to a spatially developing channel flow, but as the ramp is approached the flow modifies due to the favorable pressure gradient developing close to the lower wall as a result of the curvature. In the vicinity of the ramp the expansion dominate, causing an adverse pressure gradient over the ramp section into the channel section after the ramp. From the velocity distribution, a small separation bubble can be observed over the trailing edge of the ramp. Comparison with experimental data for the static pressure coefficient, $C_p$, at the upper and lower walls shows that LES-LDKM and DES show the best agreement with experimental data whereas results from the LES-WALE and LES-MM show larger deviations at the bottom wall. Grid resolution studies (using the LES-LDKM model) show almost identical results. Comparison with experimental data for the axial velocity compo-

<table>
<thead>
<tr>
<th>Type</th>
<th>Case</th>
</tr>
</thead>
</table>


nent shows good agreement for the LES-LDKM and DES models, whereas the LES-WALE and LES-MM typically underpredict the recirculation region.

The second example concerns a lean propane air flame stabilizing behind a triangular shaped flame holder investigated experimentally by Sjunnesson et al. [128-137], and computationally by several researchers, e.g. [131-137], using different LES combustion models including flamelet, finite rate chemistry and linear eddy models. The set-up employ open inflow-out-flow boundary conditions together with no-slip wall boundary conditions and periodic spanwise boundary conditions. Grids with between 2.0 and 16.0 Mcells are typically used, and here results from a 6.7 Mcell grid will be presented. Results from two cases will be presented: Case I is characterized by $\text{Re}=47,000$ and $\varphi=0.61$ and Case II by $\text{Re}=28,000$ and $\varphi=0.58$. Figure 1b shows contours of the time-averaged instantaneous temperature distribution for the two cases. The unsteady separating vorticity shed off the wedge, rolls-up, generating a flow that wraps the flame around regions of intense vorticity and wrinkle the flame. This process is in both cases dominated by Kelvin–Helmholtz (KH) instabilities. As the shear layer mixing continues to support the flame with cold reactants Bénard von-Karman (BVK) instabilities starts to dominate over the KH instability, thus modifying the flame. Depending on the dilatation ($\rho_2/\rho_1$ or $T_2/T_1$) different ratios are reached between the KH and BVK instabilities resulting in either Case I, having suppressed BVK instabilities and a symmetric flame for $T_2/T_1 \approx 5.6$, or Case II, with a stronger relative influence of the BVK instabilities and a more asymmetric flapping flame for $T_2/T_1 \approx 3.2$. These observations are in line with the theoretical results of Erickson et al. [138], and the experimental data of Shanbhogue et al., [139]. Shown in figure 1b are also comparison between results from different flamelet and finite rate chemistry LES models using different reaction mechanisms.

![Figure 1](image_url)

**Figure 1.** Verification of LES models. (a) Flow past a contoured ramp, [123-127], and (b) combustion behind a triangular shaped flame holder, [128-137]. Legends for the ramp: (○) experimental data, (→) LES-MM, (←) LES-WALE, (↓) DES and (↑) LES-LDKM. Legends for the bluff-body combustor: (○) and (■) LDV and CARS experimental data, (→) flamelet LES, (←) LES-PaSR with 2 step chemistry, (↓) LES-TFM with 2 step chemistry and (↑) LES-PaSR with 15 step chemistry.

5. **Applications to Aerodynamics**

The determination of the stability and control characteristics of a new aircraft design is an iterative process involving computational, wind tunnel and flight test modeling techniques. Commonly used aerodynamic modeling tools are efficient but mostly linear and thus do not satisfactorily capture some non-linear aerodynamic effects such as vortex-boundary layer, shock-shock, and shock-vortex-boundary layer interactions. These non-linear effects may lead to instabilities such as wing stall, vortex ring state, tail buffet, and limit cycle oscillations, which can either limit the aircraft life span or
operational envelope. Correcting such issues after the initial flight tests is usually very expensive and can delay the project several years. Wind tunnel testing scale models is one approach to eliminate such issues at the design stage, but typically suffer from blockage, scaling, and Re-number effects together with support interference issues that prevent the proper modeling of the full-scale aircraft behavior. The use of high-fidelity computational tools capable of accurately predicting all important aspects of the flow over the aircraft at a range of operational conditions both at model and full scale is thus highly desirable.

The first computational approach for complete aircraft configuration analysis is based on panel methods that are numerical schemes for solving (the Prandtl-Glauert equation) for linear, inviscid, irrotational, and steady flow, [140-141], using linear combinations of basic singular solutions. These methods are relatively general and have also been employed to compute the flow around ships, cars and other vehicles and configurations. As these methods cannot compute separation, skin-friction drag and transonic shocks more advanced models such as full potential flow models (also based on the Prandtl-Glauert equation) and Euler equation models were developed, [142-143], that still sees heavy use. However, as these methods cannot handle viscous effects the next step is to use the Navier-Stokes equations. During the 1990s the usage of RANS, [144-145], intensified significantly, and now RANS models are routinely used to analyze different aircraft configurations. Since only the mean (time-averaged) flow is explicitly computed in RANS, with statistical turbulence models accounting for turbulence effects, RANS is restrained to flows for which these have been carefully calibrated. For aerodynamics particular limitations of RANS includes issues with wake and separation predictions, particularly at large angles-of-attack. A wider range of flows can be computed with high accuracy using LES, DES and hybrid RANS-LES models, [146-147], though at a higher cost, since these methods are based on resolving the large energy containing flow scales whereas modeling is only restricted to small (hopefully more universal) flow scales, [20]. Recently, DES has been increasingly popular in aerodynamics as it gives improved accuracy and greater flexibility with affordable computational cost.

To illustrate the use of DES in aerodynamics figure 2 present some selected results from an analysis of Morton, McDaniel & Cummings, [148], in which several flight conditions were studied and compared with experimental data from the Cranked Arrow Wing Aerodynamics International (CAWAPI) flight test program, [149], of the F-16XL. For this study, the solver Cobalt, [150], was employed, and the baseline unstructured tetrahedral grids of a half-span F-16XL model contains about 15.0 million cells, with all control surfaces set to zero deflection. To allow simulation of engine effects at the inlet and nozzle exit, the engine inflow duct is meshed all the way to the compressor inlet plane and the nozzle is meshed from the engine mixing plane. More specifically, figure 2b shows the flow over the F-16XL at Flight Condition 7 (FC7), characterized by a Ma number of 0.30, an angle-of-attack of 11.89° and an altitude of 1600 m, in terms of an iso-surface of the vorticity magnitude colored by the instantaneous pressure. The primary flow features are the lead-

**Figure 2.** Vortical flow around a F-16XL-1 fighter aircraft model. (a) Symmetry plane of the F-16XL baseline unstructured grid, (b) iso-surfaces of vorticity magnitude colored by the pressure, (c) close up view of the iso-surfaces of vorticity magnitude over the wing colored by the pressure with labels for the key flow features and (d) cross-planes of time averaged (left) and instantaneous (right) vorticity.
ing edge vortex, the air dam vortex, the outer wing vortex, as well as a complicated set of vortices from the AIM-9 fins and forebody. Figure 2c clarifies that the leading-edge vortex develops from a coherent structure to a complex structure with helical windings, similar to vortex breakdown in the region of the actuator pod. Note also that the helical vortex structure is located above the vortex emanating from the air dam creating a very complex structure. Figure 2c shows a cross-plane of time-averaged and axial vorticity far aft across the fuselage-wing. Here, the air dam vortex has lifted off the skin and begun to pair with the leading-edge vortex. The crank outer-wing vortex is also evident in red as well as the AIM-9 fin vortices (colored blue and red).

6. Applications to Hydrodynamics

Much of the understanding of ships hydrodynamics has been obtained through systematic tests in model and full scale. Because of the cost of such tests, current design and analysis practices involve only selected parameter variations of the hull and/or the propulsor. This is merely possible due to the presence of historic series data and experience gathered over decades at the model basins. Systematic and continuous analysis of the experimental data has significantly contributed to the understanding of ship hydrodynamics, and hence also to the improved hull and propulsor designs currently entering into production. The classical topics of ship hydrodynamics are resistance, propulsion, seakeeping and manoeuvring, [151], whereas for naval vehicles signatures are also of significant importance. These topics include many disciplines of classical physics such as fluid mechanics, turbulence, free-surface flows, cavitation, six degree-of-freedom hydromechanics, acoustics and fluid structure interactions. For both ship hydrodynamics the turbulent flow results in a wide range of scales, from the smallest scales of turbulence, the Kolmogorov scales, to the scales of the hull, and with Re numbers on the order of 10^3 to 10^7 there are six to eight orders of magnitudes of flow scales that interact. In addition to the critical complexities associated with high Re number wall bounded turbulent flows, ship hydrodynamics also includes other challenges such as propellers, turning rudders, free surface flows, bubbles, manoeuvring, etc. making this a challenging and computationally demanding field, [151-152].

Classical potential flow models, [152], are frequently used in industry to estimate resistance and Taylor wake fields but with the prompt advancement and easier access to high performance computers RANS models, [153-155], are fast becoming more and more used. Since only the mean (time-averaged) flow is explicitly computed in RANS, with statistical turbulence models providing information about how turbulence affects the mean flow, RANS is limited to flows for which the statistical turbulence models have been prudently calibrated. For ship hydrodynamics particular limitations of RANS includes underestimation of the size of separation and recirculation regions and underestimation of turbulent kinetic energy in wakes. These shortcomings limit the use of RANS for innovative and unconventional hull, as well as propulsor designs. By using more advanced methods such as LES, DES and hybrid RANS-LES, [156-158], a wider range of flow problems can be computed with high accuracy but at an increased computational cost since these methods are based on resolving the large energy containing flow scales whereas modeling is only restricted to small (more universal) flow scales, [20]. The use of LES/DES in ship hydrodynamics was reviewed by Fureby, [159], and since then the number of LES/DES ship flow studies has increased notably due to the rapid increase in computational hardware.

Figure 3 presents selected results from a recent joint computational and experimental study of submarine hydrodynamics, [160], using RANS and LES in conjunction with measurements of the wake total pressure, surface pressure, skin friction, and sail and hull wakes using Particle Imaging Velocimetry (PIV) and hot-wire anemometry. This is a very exhaustive study giving as the unique opportunity to elucidate many aspects of the high Re number flow past the fully appended hull as well as providing information about the computational capabilities of both RANS and LES. For the fully appended Joubert hull configuration two grids of 8.5 and 68 million cells were used. For RANS the SST k-ω model, [28], was employed whereas for the LES the MM was used together with a wall model, [41]. Figures 6a and 6b present side views of the instantaneous velocity at the meridian plane from the fine grid LES and from the PIV measurements. Good qualitative agreement is found with the flow dominated by the wake and the sail-tip vortex pair. In addition to these key flow features the horseshoe vortex system around the fin is very important for the flow over the tapered stern with the x-shaped rudder configuration. The legs of the horseshoe vortex system pass between the upper rudders resulting in a non-uniform and unsteady approach flow into the propeller. This type of detailed information is not available from RANS and assists in optimizing the design of the propeller both with respect to performance and reduced vibrations and flow noise. Figure 3c and 3d compares predictions of the skin friction coefficient, C_f, on the meridian plane of the hull and the normalized axial velocity profiles, v/v_{in}, downstream of the fin between the experimental data and the LES-MM and RANS SST k-ω simulations.

Figure 4 show selected results from DES and LES investigations of the flow past the DTMB 5415 and 5512 model hulls, [161-162], respectively, from [153, 156, 163-165]. Both models were intended to represent a preliminary design for a US Navy surface combatant of around 1980, with and without bilge keels, but due to the extensive experimental data, [161-162], this case have become an important validation test case for CFD as well as a valuable case for understanding the flow physics around a surface ship. The hull geometry in-
include a sonar dome below the bow and a transom stern, making geometry and grid generation quite challenging in particular as the free water surface, being part of the DES/LES solution, also requires high resolution in order to capture the developing bow- and Kelvin wave patterns. Typical grid resolutions range from 7 to 58 million cells, [165, 168-169], but very high grid resolutions (about 300 million cells) have been employed by Stern, [7], to investigate high performance computing scalability issues as well as grid resolution requirements of computational free surface ship hydrodynamics. As for submarine hydrodynamics the incompressible LES equations (1) are solved but now together with a separate equation describing the evolution of the sea-air interface. Different numerical techniques can be used to describe this and the most common approaches are the Volume of Fluids (VoF) method, [166-167], and the Level Set method, [168-169], which includes a transport step and a re-initialization step. Figures 4a and 4b shows the vorticity distribution in the air and water, respect-

Figure 3. LES predictions of the Joubert submarine hull configuration. (a) Predicted instantaneous axial velocity in the meridian plane and at a cross-section halfway between the trailing edge of the fin and the stern from LES-MM, (b) experimentally measured axial velocity in the meridian plane, (c) skin-friction coefficients, $C_f$, along the meridian plane and (d) normalized axial velocity, $v/v_0$, profiles along lines across the wake of the fin. Legend: (—) RANS SST k-ω on the coarse grid, (—) LES-MM on the fine grid, (—) LES-MM on the coarse grid, (○) experimental data from a bare hull configuration and (+) experimental data from a fully appended hull configuration.

Figure 4. Surface ship hydrodynamics (a) Instantaneous vortical structures colored by streamwise vorticity for DTMB 5512 at Fr=0.41 in the air phase, [164]. (b) Instantaneous vortical structures colored by streamwise velocity for DTMB 5415 at Fr=0.28 in the water phase, [165]. Figures (c) to (g) shows velocity contours for DTMB 5415 at x/L=0.2, 0.4, 0.6, 0.8 and 0.935 from experiments, [161], (left) and LES, [165], (right), whereas figures 4h and 4i present the water surface elevation from experiments, [161], and from DES, [169].
tively. Underneath the hull the main vortex structures are the sonar dome vortex and the forebody keel vortex, both being unsteady as evident from figure 4b. Figures 4c to 4g present velocity contours at x/L=0.2, 0.4, 0.6, 0.8 and 0.936 from experiments, [161], (left) and LES, [165], (right), whereas figures 4h to 4i show the water surface elevation from experiments, [161], and DES, [169]. As can be found, good agreement is obtained between the experimental results and the DES and LES computations, also providing more information than contemporary RANS, [153].

7. Applications to Chemically Reacting Flows

Even though combustion has always been related to human evolution, understanding the details of combustion has been predominantly empirical. Only in the last few decades has there been some systematic efforts to understand combustion using theoretical and experimental tools. This effort is extremely challenging since many disciplines within classical physics and chemistry – fluid mechanics, thermodynamics, heat and mass transfer as well as chemical kinetics – interact at the continuum level. In addition to the variety of physical and chemical processes included, combustion covers a wide range of scales from the molecular scale of the chemical process, via the scales of droplets, mixing and turbulence, to the scale of the device. This means that there is over eight orders of magnitudes of scales that interact in the combustion process within a typical combustor. An additional complication can arise in combustors in practical devices due to confinement. Interaction among vortical motion, combustion heat release and the system acoustics (i.e. pressure waves) may give rise to complex interactions that can lead to issues of fundamental concern, such as combustion instabilities which is an important design concern for aero and power generation gas turbines, [170]. Emissions and combustion efficiency are also fundamental issues that are important to the global economy and world climate, [171].

During the last two decades, computational investigations of combustion have emerged to become feasible with the rapid increase in computer speeds and architectures, especially with the advent of massively parallel computers. DNS of combustion, [31, 172-173], help to understand the fundamental processes involved whereas combustion RANS, [174-175], previously has been the preferred engineering approach assisting in designing combustors, [176]. LES of combustion has evolved significantly during the last two decades, [8-9, 11, 29, 65], and is now both contributing to the design of advanced combustion systems, and to understanding fundamental physical and chemical processes in complex combustors (e.g. annular multi-burner combustors). Combustion LES suffers, as the same was as combustion RANS, from that the flame is typically thinner than what can be resolved on the grid, rendering subgrid combustion modeling unavoidable, e.g. [8-9, 29, 65]. In flamelet LES, [29, 65-72], the flame is infinite-ly thin and the transport equations for the species concentrations are replaced with an equation for the progress variable, $c$, measuring the advance of the flame, and a mixture fraction, $z$, measuring the degree of mixing, thus reducing the complexity of the LES model considerably. The flamelet approach is, however, only valid in the flamelet regime, [29], and is thus not usually applicable to real combustion systems. Alternatively, some kind of finite rate chemistry model, [73-95], must be used for these cases. In these models the pacing item is (i) how to find a compact, but yet accurate, reaction mechanism and (ii) how to close the filtered reaction rate source term in the species concentration equations. Many alternatives are available for the latter, e.g. [8, 26, 73-74, 93], often resulting in small differences, e.g. [86-87], whereas for the former large differences can take place subject to which reaction mechanism is used. For LES, the use of detailed reaction mechanisms, including hundreds of species and thousands of reaction steps, e.g. Westbrook et al., [177], is currently prohibitively expensive and in its place global or reduced mechanisms are often used, [178-179]. The pacing item in LES of combustion is now the selection of an appropriate global or reduced reaction mechanism that allows accurate but still not to expensive computations of real applications.

Figure 5 show results from LES of flow, fuel injection, mixing, ignition and combustion in a generic small-aircraft gas-turbine combustor with 12 fuel injectors, [180]. The aim if this study was to elucidate the understanding of gas turbine combustion in a realistic engine and to examine the influence of grid resolution and chemical kinetics. Three computational grids with 27, 54 and 108 million cells were employed together with a global two-step reaction mechanism, [181], and a more advanced global eight-step reaction mechanism, [182-183], that includes a simplified fuel breakdown sub-mechanism that models the low-temperature combustion modeling of kerosene fuel blends. In these LES the LES-PaSR finite rate chemistry model, [26], was used following [88], whereas in other similar annular multi-burner gas turbine studies, e.g. [96-97], a LES-TFM finite rate chemistry model, [93], was used. Figure 5a shows an exploded view of the flames and temperature contours across the combustor and at the turbine outlet. Figure 5b shows cross-sectional views of pressure, temperature, velocity magnitude, fuel mass fraction, CO mass fraction and the Takeno flame index, respectively. From these figures it is clear that the pressure affects the flames, and if azimuthal or longitudinal pressure variations takes place, notable flame modulations can occur, [184]. From figure 5c we find that the mixing holes allows cold air to enter the combustor and to divide the combustion zone into a rich burn zone, followed by a mixing zone and a lean burn zone, in which any remaining fuel is oxidized. The staging also help lower the temperature of the combustion products and thus also the NOx emissions. Figure 5d shows a histogram of the equivalence ratio, $\phi$, revealing rich combus-
tion at $\phi=2.0$ and lean combustion at $\phi=0.5$. Figure 5e summarizes the effects of the grid refinement and reaction mechanism study, showing that the predictions with successively finer grids and the predictions with more detailed combustion chemistry converge to the same results.

![Figure 5](image)

**Figure 5.** LES predictions of Jet-A combustion in a generic aero-gas turbine combustor. (a) explosive views of temperature and flames, (b) cross-sectional views of the pressure, temperature, velocity magnitude, fuel mass fraction, carbon-monoxide mass fraction and Takeno flame index (with red regions representing premixed flame elements and blue regions representing non-premixed flame elements), (c) enlargement of one of the combustor sections showing the flame together with the velocity magnitude and the temperature distribution, (d) histogram of the equivalence ratio and (e) volume-averaged variances of pressure, temperature and carbon monoxide mass fractions for three grids (27, 54 and 108 million cells) for (■) two step chemistry and (●) eight step chemistry.

Figures 6a and 6b present LES results, [90-91], of the shock-tunnel experiments, [185-187], at combustor pressures and temperatures of $p_f=57$ kPa, $T_f=1500$ K, and $p_f=130$ kPa, $T_f=1300$ K, respectively, emulating the HyShot II scramjet flight tests at flight altitudes of 33 and 28 km, respectively, [188-189]. These figures illustrate the flow in the combustor in terms of iso-surfaces of the second invariant of the velocity gradient, $\lambda_2$, colored by temperature (center), pressure contours on the lower combustor wall and through the combustor (upper left), as well as an enlargement of the injection and mixing region in terms of $\lambda_2$ colored by the heat-release (lower right). The computational grids typically use between 25 and 100 million cells, [90-91], with the finer grids resulting in richer vortical flow structures. The combustor pressure primarily influences the jet penetration, characterized by the jet-to-freestream momentum flux ratio, $J$, whereas the combustor temperature mainly influences the chemical kinetics ignition delay time, $\tau_{ign}$. For the two cases portrayed in figures 6a and 6b the different jet penetrations result in dissimilar vortical flow patterns and therefore also distinctive mixing patterns. The different mixing patterns in turn result in different flame characteristics: For the low pressure case the relatively high value of $J$ results in a very steep bow shock and comparatively wide jet wakes. Fuel-air mixing takes place in the shear-layers of the jet-wake and around the entwining legs of the horseshoe vortices of neighboring jets. Self-ignition occurs far downstream when fuel and air are mixed properly. For the high-pressure case the lower value of $J$ results in a shallow bow shock and more narrow jet wakes. Fuel-air mixing takes place in the shear-layers of the wake, and self-ignition occurs as a result of interacting shock waves. Figures 6c and 6d illustrate pressure and heat-flux comparisons along the lower combustor wall. Here, results from Chapuis et al., [91], using the LES-PaSR model, Larsson, [72], using the LES flamelet model, Cesare et al., [190], using a different LES model, and Karl, [191], using a RANS-PDF model are included. From these comparisons we find that LES capture the trends in heat flux and pressure due to the differences in operating conditions between the cases. This is by no means obvious as the turbulent flow, mixing, self-ignition and exothermicity are all affected and contributes to the different pressure and heat flux profiles obtained experimentally.
8. Other Applications

Besides the engineering applications of aerodynamics, hydrodynamics and combustion, LES been extensively and successfully employed to study other fluid mechanical related subjects such as contaminant transport, e.g. [192-194], illustrated in figure 7, and different astrophysics applications, e.g. [18-19, 195-197], illustrated in figure 8.

Reducing health risks from accidental or deliberate release of chemical, biological or radiological agents and pollutants from industrial leaks, spills, and fires motivate simulating the air-flow and species flow of contaminants through large terrain or urban canopy models. Configurations with complicated geometries and unsteady buoyant flow physics are usually involved. The widely varying temporal and spatial scales exhaust current modeling capacities. Crucial technical issues include turbulent fluid transport and boundary condition modeling, and post-processing of the simulation results for practical use by responders to actual emergencies. Appropriate physical processes to be simulated include vortex shedding from multiple buildings, flows in recirculation zones, and approximating the subgrid turbulent and stochastic backscatter. The model must also incorporate a consistent stratified urban boundary layer incorporating realistic effects from wind fluctuations, solar heating, aerodynamic drag and heat losses due to the presence of trees, surface heat variations and turbulent heat flux. The model must thus take mixing into account from first principles at the widest possible range of scales. Additional physics includes deposition and

Figure 6. LES predictions of the HyShot II combustor for (a) the high altitude case with $p_c=57$ kPa, $T_c=1500$ K and (b) the low altitude case with $p_c=130$ kPa, $T_c=1300$ K in terms of vorticity, pressure, temperature and heat release. (c) Comparison of wall pressure and (d) heat flux at the lower combustor wall. Legend: ($\circ$) and ($\bigtriangledown$) experimental data, [187-189], (---) and (----) RANS of Karl, [191], (---) and (----) LES of Chapuis et al., [90-91], (----) LES of Larsson, [72], and (----) LES of Cesare, [190].

Figure 7. Other applications. (a) Contaminant transport: Contaminant dispersion from an instantaneous release in Times Square, New York City predicted by the FAST3D-CT model, [198]. (b) Results from a validation study in the USEPA metrological wind tunnel at LANL.
evaporation of contaminants. The most appropriate contaminant transport models currently available are based on LES, e.g., [198–199], validated primarily on experimental data in model scale, e.g. [192], but also on simplified field measurements such as [200]. Figure 7a shows a snapshot from contaminant dispersion from an instantaneous release in Times Square, New York City as predicted by the FAST3D-CT model, [198]. This model is based on ILES, but contain sub-models for additional physical phenomenon. Figure 7b shows results from a validation study involving data from the USEPA metrological wind tunnel at LANL.

Many problems of astrophysical fluid dynamics share two important features: the ubiquitous presence of spatially localized features such as shocks, clumps, or composition discontinuities that need to be numerically resolved or at least adequately modeled and the high Re numbers of the baryonic component indicating that fully developed turbulence is responsible for the mixing and dissipation properties of the fluid almost everywhere. Despite great advances in CFD, an accurate handling of both aspects has so far proven to be very challenging, as specialized numerical techniques have seemed to be almost mutually incompatible. Figure 8 presents results from two different astrophysical subject areas in which LES have and will continue to make a difference. Figure 8a shows a projection along the axis of rotation of a stellar disk evolving in time in terms of the density distribution after 100 Myears from Hupp, [201]. These simulations clearly show the evolution of early fragmentation and the build up of irregular web of filamentary density enhancements as well as the subsequent fragmentation into small clumps of cold dense gas. At later times during the simulation, the disk settles into a less dynamical state where it only marginally changes in size and structural appearance. These LES were carried out using the adaptive mesh refinement LES code FEARLESS, using a OEEVM-type subgrid model with additional terms dealing with compressibility. These LES were performed in a box with side length of 1 Mpc (=3.0985·10^23 m) that is resolved by a baseline grid with 128^3, and 8 levels of refinement. Figure 8b shows the initial and final stages of a simulated thermonuclear deflagration in a carbon-oxygen white dwarf star, from [18]. This is now believed to be the consensus model by which a Supernovae of type Ia is formed. The burning process proceeds as subsonic deflagration driven by turbulence. The production of turbulence is primarily a consequence of Rayleigh-Taylor instabilities due to the lower mass density of nuclear ash as compared to the density of unprocessed material. These LES were performed using ILES, and also employ adaptive mesh refinement to resolve shock waves, steep density, pressure and composition gradients as well as wrinkled flame fronts. Typical grid sizes range between 384^3 and 770^3 cells.

Figure 8. Other applications. Astrophysics: (a) Turbulence regulated star formation in an isolated disk galaxy from [201]. (b) Early and late times in the development of a thermonuclear deflagration appearing in a carbon-oxygen white dwarf star characteristic of a Supernovae of type Ia, from [18].

9. Concluding Remarks and Perspectives

Predictive modeling of turbulent flows is becoming increasingly important for the development of cars, aircrafts, ships, medical equipment, process devices, power plants etc. The increase in computational power in the past decade has made many of these flow configurations numerically accessible. Nevertheless, the interaction of turbulence with physical processes, such as chemical kinetics and phase change processes is a great challenge. Significant advances in modeling turbulent flow are now possible with the development of LES and similar methods. The philosophy of LES is to explicitly solve for the large scales of the flow, directly affected by boundary conditions, whilst modeling the small (less energetic) scales of the flow. For historical and practical reasons, the development of LES models is based on concepts from corresponding RANS models, resulting in improved predictions, due mainly to that in LES the large turbulence scales are resolved. However, to meet the future demands in more accu-
rate predictions, more detailed predictions and predictions at conditions out of range with present LES models and computational resources, a paradigm shift is needed. Emerging LES models that are developed with these demands in mind, make use of multi-scale techniques, and are believed to be in practical use within the next five to ten years. In this review we have also illustrated typical engineering problems that can be handled with present day models and hardware systems, and we have summarized some of the very important practical aspects that has to be taken into account in order to successfully carry out LES on an engineering scale.

Acknowledgement
The presented work was supported by the Swedish Armed Forces and the Swedish Defense Material Agency and Drs F. Stern, J. Larsson, A. Inginito, S. Karl, G. Patnaik, E. Oran, S. Menon, D. Jones, D. Clarke, D. Norrisson, K. Pettersson, M. Liefvendahl, O. Parmhed, F. Grinstein and V. Sabelnikov are greatly acknowledged for providing simulation results and for valuable support and many fruitful discussions.

References


