Introduction

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Abstract The annual data published by IEA is analysed to get a projection for the combustion share in total primary energy supply for the world. This projection clearly identifies that more than 60% of world total primary energy supply will come from combustion based sources even in the year of 2110 despite an aggressive shift towards renewables. Hence, improving and searching for greener combustion technologies would be beneficial for addressing global warming. Computational approaches play an important role in this search. The large eddy simulation equations are presented and discussed. Potential terms which are amenable for using machine learning algorithms are identified as a prelude to later chapters of this volume.

Combustion is a socio-economically important topic for many tens of centuries and it still remains to be so because more than 90% of the world's total primary energy supply (TPES) is met through combustion in one form or another, see IEA (2021). Even the recently proposed changes towards low carbon or carbonless fuels, including E-fuels, will involve some sort of combustion employing concepts and technologies which could be substantially different from those used currently. Figure 1 shows the share of various sources for TPES which is about 606 EJ for the year 2019. This is nearly 139% of the energy used in 1973 which suggests about 3% increase per year over the past 46 years and this is inline with an estimate of about 40% increase in the global energy consumption for the next two decades by the National Academies of Science, Engineering and Medicine, see How we use energy (2022). This projected energy demand is likely to be larger because of the widespread use of energy-hungry

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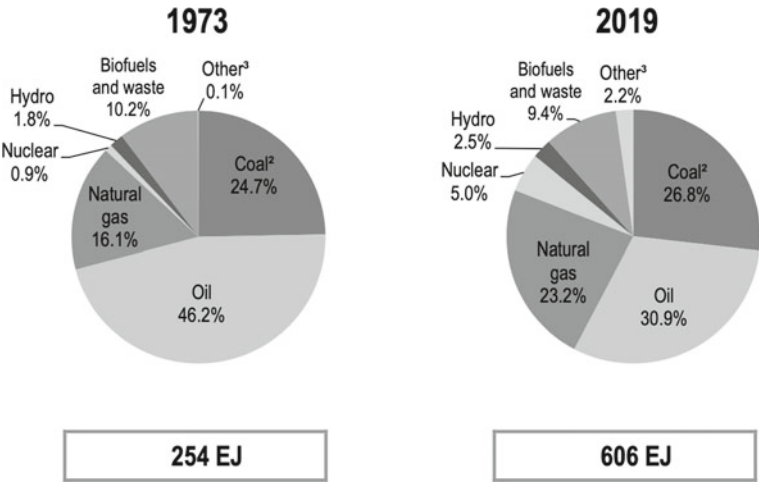

Fig. 1 World total primary energy supply, in exajoule, by source type. Adopted from IEA (2021), © IEA, 2021

consumer electronics and other technologies such as Internet of Things (IoTs), electric vehicles, etc. While these technologies bring their own advantages one cannot deny their impacts on the environment arising from their manufacturing, end-of-life treatments and more importantly higher demand for energy during their lifetime leading to global warming related issues. Indeed, the use of energy-hungry modern technologies and mitigation of global warming are at the opposite ends and bringing them together is a grand challenge requiring carefully constructed solutions.

The global temperature is expected to rise in the next 100 years according to the intergovernmental panel reports—Future climate changes, risks and impacts (2022), and as discussed by Hayhoe et al. (2017). If the emission of green house gases (GHG) follow a particular Representative Concentration Pathway (RCP 2.6) yielding Gigatons of carbon emission close to zero in the year of 2100 and the CO_2 concentration in the atmosphere is about 400 ppm then the temperature raise is expected to range from 0.3 to 1.7 °C. If the CHG emission is high following RCP 8.5 then the temperature rise may range from about 2.6 to 4.8 °C which may result in catastrophic effects.

The energy production using renewable and sustainable sources are gaining popularity and becoming wide spread in the past decade. The renewable sources include hydro, solar, wind and tidal. The nuclear energy may be considered as a renewable since the uranium deposits could provide energy for billion years (Cohen 1983) and there is no GHG emissions (Vasques 2014; Moore 2006). However, the safety issues and the concept of clean energy may exclude the nuclear energy from the renewables. Figure 1 shows that the share of this energy is 5% for the year 2019 whereas the renewables share, listed as Others, is only 2.2%. However, this substantial increase from 0.1% in 1973 is because of the advent of the renewable technologies in the

recent past. The photo voltaic, both rooftop and commercial, systems become popular but the capital cost projections in Winskel et al. (2009) (see their Fig. 4.1) does not seem to be realistic (the actual cost is nearly twice the projected cost of about £1000 per kW for 2019) because the price will increase as the demand grows unless the supply is in surplus.

The levelised cost of electricity for renewable technologies at utility-scale is becoming lower than that for the traditional fossil fuels—0.038 to 0.076 USD/kWh depending on the renewables compared to 0.05 to 0.18 USD/kWh for fossil fuels (IRENA 2020)—which is an excellent progress. However, the consumer energy prices do not reflect this lower cost for the renewables yet. Perhaps, this may take some more time. Although the renewable power generation has increased by nearly 50% (a total of about 780 GW) for the year 2020 compared to 2019 (IRENA 2021), this is substantially lower than the 2019 projection of 1.5 TW for 2020 (IRENA 2019). This clearly suggests that the renewables share is growing slowly and one may have to accelerate it but the accelerated growth may have its own consequence on the environment for the reasons argued in Lørstad et al. (2022a), which are based on the data for GHG emissions and cradle-to-grave life cycle analysis (LCA) published in past studies. For example, the electric vehicles projected to have zero emission is not so in reality according to cave-to-case analysis showing that one has to drive a 110 kW size EV for about 35,000 km *without recharging* to offset the CO_2 emitted by the battery pack production alone (Alvarez 2019). This is not practical. It is likely that combustion will remain as one of the components in the energy technology mix and will play an important part for specific applications, such as transport and energy-intensive industries, requiring high energy densities but its form and type are likely to be different.

1 Combustion Technology Role

The mitigation of global warming requires solutions, targeted towards reducing GHG emissions, which arise from efforts concerted across various continents and countrywide solutions are inadequate. While a complete shift towards renewables seems attractive and achievable over longer timescales but the accelerated shift set by various governments independently does not sound pragmatic. Perhaps, this may worsen the situation because the additional energy required to achieve the accelerated shift towards renewables has to come from non-renewables. Thus, a balanced approach to meet the ever increasing energy without aggravating the global warming is needed.

Combustion technologies play important role in this respect as suggested by the results in Fig. 2 showing future projections for the combustion share of world TPES under three different scenarios (Swaminathan 2019). The inset is the actual data from the International Energy Agency (IEA 2021) showing a gradual decrease in the combustion share while a small rise in 2012 is because of the increase in coal combustion in some countries in that year. If one makes a naive projection by assuming that the progress in renewable technologies is steady and organic following the current trends

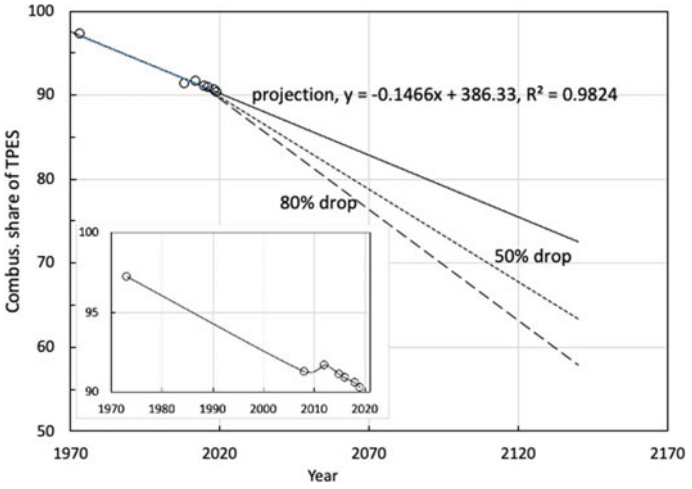

Fig. 2 Combustion share of world TPES and its future projections. Adapted from Swaminathan (2019)

then the combustion share will be more than 75% even by the year 2110 (the solid line). The slope of this curve is related to the progress and advancement of alternative energy technologies. If one keeps an optimistic view for these technologies and presumes that they are progressing at about 50% faster pace compared to the current trend then the combustion share falls to about 70% in 2110. This share decreases further to 66% for the year 2110 if one assumes that the alternative technologies progress at 80% faster pace. To achieve this, a radical paradigm shift is needed and whether this is practical or not from the economical consideration is an open question. Even the heavily accelerated shift (80% scenario) reduces the combustion share only by 40% and thus a pragmatic approach is to seek for alternative combustion concepts and technologies which can significantly reduce GHG emissions and can act as retrofits to the existing combustion systems which can also aid a quicker shift towards renewables in the longer run.

Many alternative combustion concepts such as fuel-lean and MILD (moderate, intense or low dilution) combustion emerge as potential solutions since they could deliver both low emissions and high efficiency. However, using them for practical applications bring their own challenges as discussed by Swaminathan and Bray (2011) and Lørstad et al. (2022a). Also, carbon-free and E-fuels are emerging as potential alternative solutions to mitigate CO_2 emission while catering to the ever-increasing energy demand. Specifically, hydrogen combustion seems to be gaining momentum with a view to use hydrogen as a main energy carrier. Although this solution addresses the CO_2 emission directly it brings additional challenges for its safe usage, controlled combustion for practical applications and potential increase in NO_x emissions. One of the current NO_x reduction technologies can be utilised to control this emission from hydrogen or E-fuel combustion. Nevertheless, the distri-

bution of hydrogen from production sites to consumers is challenging which requires a complete infrastructure overhaul and the scale of economy for this cannot be underestimated adding further challenges.

Modern computational methods and approaches play significant parts in developing these alternative technologies and taking them to fruition. The use of machine learning algorithm (MLA) and techniques in computational fluid dynamics (CFD), specifically for turbulent flows and turbulent combustion are gaining renewed momentum in recent times for two reasons, *viz.,* (i) these algorithms and techniques have evolved and developed for a wide-spread use across various disciplines and (ii) to take advantage of their robustness, accuracy and computational efficiencies so that the CFD codes with MLA can be employed for quick evaluations of design changes. Before discussing the role of MLA in computational simulations of turbulent flows with chemical reactions, let us briefly review the governing principles and equations, and various computational methods used for turbulent combustion. The topic of turbulent reacting flow simulations has been discussed elaborately in many books, see for example Swaminathan and Bray (2011), Libby and Williams (1980), Poinsot and Veynante (2005), Echekki and Mastorakos (2011), Swaminathan et al. (2022b), only a brief review with detail required to fulfil the aim of this volume is discussed in the next section.

2 Governing Equations

The computational simulations of turbulent reacting flows use three numerical approaches, namely direct numerical simulation (DNS), large eddy simulation (LES) and Reynolds-Averaged Navier Stokes calculation (RANS). These approaches involve different levels of detail, approximations and modelling. The complete set of conservations equations are solved with no models using high order numerical schemes in the DNS approach and further detail can be found in many books, for example Poinsot and Veynante (2005). This approach resolves and captures the range of, from dissipative to energy containing, scales in the flow without using any modeling approximations and this range increases with turbulence Reynolds number, Re_t. The ranges of spatial and temporal scales vary as $Re_t^{3/4}$ and $Re_t^{1/2}$ respectively and thus the computational cost for using DNS at Re_t relevant for practical application in appropriate geometry is prohibitive. Hence, this approach is typically used to gain fundamental understanding of turbulence and its interaction with chemical reactions, and these knowledge are important for devising engineering models for practical use. There are many examples for this which are discussed and summarised in Swaminathan and Bray (2011), Poinsot and Veynante (2005), Echekki and Mastorakos (2011), Swaminathan et al. (2022b). Appropriately averaged conservation equations are solved in the RANS approach along with closure models and approximations, which are discussed elaborately in many past works, for example see the books edited by Libby and Williams (1980, 1994) and the works in Swaminathan and Bray (2011). The RANS equations are deterministic and do not have the stochastic

aspects required for statistical inference and hence one must be cautious in using MLA for RANS calculations. However, it is possible to use some of the machine learning algorithms to address the uncertainties of RANS model parameters. LES approach is well suited to make use of MLA since there is inherent stochasticity. Before identifying the potential avenues to use MLA for LES, let us briefly review the required governing equations.

3 Equations for LES

In large eddy simulations, the low-pass filtered governing equations for mass, momentum, energy and species mass fractions are solved. The filtering, or separation of the scales, is done with a spatial filter, which is applied to the governing equations for the above quantities. The various filters and their attributes are discussed in many text books, for example see Pope (2000) and Favre-filtering, also known as density-weighted filtering, is commonly used for flows such as turbulent combustion involving strong density variations. The filtering implies that the dynamic large scales, which are larger than the filter cut-off scale, are resolved and the scales smaller than the cut-off scale, known as subgrid scales (SGS), are modelled. Hence, the computational cost for LES is much lower than that for DNS because coarser grids and larger time steps can be used for similar level of numerical fidelity.

The Favre-filtered governing equations are written as

$$\text{Mass:} \qquad \frac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\,\widetilde{\mathbf{u}}) = 0 \tag{1}$$

$$\text{Momentum:} \qquad \frac{\partial \overline{\rho}\,\widetilde{\mathbf{u}}}{\partial t} + \nabla \cdot (\overline{\rho}\,\widetilde{\mathbf{u}}\,\widetilde{\mathbf{u}}) = -\nabla \overline{p} + \nabla \cdot \overline{\tau} - \nabla \cdot \overline{\tau}^{S} \tag{2}$$

$$\text{Energy:} \quad \frac{\partial \overline{\rho}\,\widetilde{h}}{\partial t} + \nabla \cdot \left(\overline{\rho}\,\widetilde{\mathbf{u}}\,\widetilde{h}\right) = \frac{\mathrm{D}\overline{p}}{\mathrm{D}t} - \nabla \cdot \overline{\mathbf{q}} - \nabla \cdot \left(\overline{\rho \sum_{i=1}^{N_s} Y_i \mathbf{U}_i h_i}\right) + \overline{\tau : \nabla \mathbf{u}} + \overline{Q_r} + \Pi_{\text{dil}} - \nabla \cdot \overline{\theta}^{S} \tag{3}$$

$$\text{Species:} \qquad \frac{\partial \overline{\rho}\,\widetilde{Y_i}}{\partial t} + \nabla \cdot \left(\overline{\rho}\,\widetilde{\mathbf{u}}\,\widetilde{Y_i}\right) = \nabla \cdot \left(-\overline{\rho\, Y_i \mathbf{U}_i}\right) + \overline{\dot{\omega}_i} - \nabla \cdot \overline{\psi}_i^{S} \tag{4}$$

using standard notations and $\mathbf{U}_i$ is the diffusion velocity of species i.

The filtering procedure yields extra terms, SGS stress tensor $\overline{\tau}^{S}$, SGS enthalpy flux $\overline{\theta}^{S}$, SGS pressure-dilation Π_{dil}, and SGS species flux $\overline{\psi}_i^{S}$, given by

$$\overline{\tau}^S = \overline{\rho}\left(\widetilde{\mathbf{u}\mathbf{u}} - \widetilde{\mathbf{u}}\,\widetilde{\mathbf{u}}\right) \tag{5}$$

$$\overline{\theta}^S = \overline{\rho}\left(\widetilde{\mathbf{u}\mathbf{h}} - \widetilde{\mathbf{u}}\,\widetilde{h}\right) \tag{6}$$

$$\Pi_{\text{dil}} = \overline{\mathbf{u}\cdot\nabla p} - \widetilde{\mathbf{u}}\cdot\nabla\overline{p} \tag{7}$$

$$\overline{\psi}_i^S = \overline{\rho}\left(\widetilde{\mathbf{u}\,Y_i} - \widetilde{\mathbf{u}}\,\widetilde{Y}_i\right) \tag{8}$$

These unknown quantities represent the influence of unresolved scales on the resolved scales and need closure models. The pressure-dilation in Eq. (7) is sometimes less important in compressible flows and therefore commonly neglected (Piomelli 1999; Martin et al. 2000). A plausible modelling for it and its limitation are explored in Langella et al. (2017). Closure models are required for all the SGS quantities in Eqs. (6) to (8), molecular diffusion related quantities in Eqs. (2) to (4) and the species reaction rate $\overline{\dot{\omega}}_i$. The molecular diffusion of momentum (viscous shear, $\overline{\tau}$), energy (heat flux, $\overline{\mathbf{q}}$), and species (diffusive flux, $-\overline{\rho\, Y_i \mathbf{U}_i}$) are modeled following classical ideas of gradient diffusion after neglecting the fluctuations in viscosity, diffusivity and heat conductivity (Piomelli 1999; Gicquel 2012). Further detail on these models and the LES governing equations are discussed in Pope (2000), Poinsot and Veynante (2005) and Garnier et al. (2009).

3.1 SGS Closures

A few common closures for the SGS terms given in Eqs. (6) to (8) are discussed briefly here. The eddy viscosity models are the most simple ones for the SGS stress in Eq. (5) and the popular of these is the classical Smagorinsky model (Smagorinsky 1963), which has been extended to the SGS kinetic energy by Yoshizawa (1986). The Smagorinsky model, in tensor notation, is

$$\begin{aligned}\tau_{ij}^S - \frac{\delta_{ij}}{3}\tau_{kk}^S &= -2\,C_s^2\,\Delta^2\overline{\rho}\,|\widetilde{\mathbf{S}}|\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right)\\ &= -2\,\overline{\rho}\,\nu_{\text{SGS}}\left(\widetilde{S}_{ij} - \frac{\delta_{ij}}{3}\widetilde{S}_{kk}\right), \quad \text{and} \end{aligned} \tag{9}$$

$$\tau_{kk}^S = 2\,C_I\,\overline{\rho}\,\Delta^2|\widetilde{\mathbf{S}}|^2 \tag{10}$$

where $\widetilde{S}_{ij} = 0.5\left(\partial\widetilde{u}_i/\partial x_j + \partial\widetilde{u}_j/\partial x_i\right)$ is the resolved symmetric strain-rate tensor and $|\widetilde{\mathbf{S}}| = \sqrt{2\,\widetilde{S}_{ij}\widetilde{S}_{ij}}$. The filter width estimated typically using the local numerical cell volume is denoted as Δ. Equation (9) defines the SGS eddy viscosity, ν_{SGS}, and the symbols C_s and C_I are model constants. The τ_{kk}^S, which is twice the SGS kinetic energy, is likely to be small or negligible in low Mach number flows as noted by Martin et al. (2000) but may not be so for flows with strong heat release.

The Smagorinsky models is relatively simple and robust, but it has its limitation for near-wall and transition flows since it can give a non-vanishing eddy viscosity, which is unphysical and this can be remedied by invoking damping functions, but an alternative approach is to use a dynamical procedure to determine C_s and C_I as proposed in Moin et al. (1991). This approach is used widely by applying a second filter of typical width $\hat{\Delta} = 2\Delta$ to the resolved fields to compute the resolved stress near the filter cut-off. Assuming similarity of the stresses near the cut-off scale, Δ, this resolved stress can be used to find an expression for C_s and C_I in terms of the resolved velocity gradients, see Pope (2000), Martin et al. (2000) and Garnier et al. (2009).

The dynamic procedure allows the model to adapt itself to the local flow changes and hence ν_{SGS} naturally approaches zero near solid walls and in laminar regions which retains physical behaviour. The dynamic procedure can produce $\nu_{\text{SGS}} < 0$ implying an instantaneous reverse cascade of kinetic energy locally which may occur in turbulent flows. However, this can lead to numerical instabilities and therefore, it is common to clip C_s to avoid negative ν_{SGS} or by averaging it in either space or time.

Other algebraic approaches have also been developed in past studies to over this specific issue of ν_{SGS} not approaching zero near a wall in wall bounded flows. Details can be found in Vreman (2004), Nicoud and Ducros (1999), Nicoud et al. (2011). An alternative approach to estimate ν_{SGS} uses the SGS turbulent kinetic energy, $\widetilde{k}_{\text{SGS}}$, obtained directly by using its transport equation, see Yoshizawa and Horiuti (1985) and Ghosal et al. (1995). Various approaches have also been proposed, developed and tested for the SGS stresses in many past studies and detail can be found in Zang et al. (1993), Lesieur and Métais (1996), Layton (1996), Kosovic (1997), Misra and Pullin (1997), Meneveau and Katz (1997), Armenio and Piomelli (2000), Domaradzki and Adams (2002), Chaouat and Schiestel (2005), Lucor et al. (2007).

Further to the SGS stress discussed above, the SGS fluxes needing modelling and a straightforward approach is to use an eddy diffusivity model written as

$$\overline{\psi}_i^S = \frac{-\overline{\rho}\,\nu_{\text{SGS}}}{\text{Sc}_{\text{SGS}}}\nabla\widetilde{Y}_i, \qquad \text{and} \qquad \overline{\theta}^S = \frac{-\overline{\rho}\,\nu_{\text{SGS}}}{\text{Pr}_{\text{SGS}}}\nabla\widetilde{h} \tag{11}$$

for species and enthalpy respectively. The symbols Sc_{SGS} and Pr_{SGS} are the SGS Schmidt and Prandtl numbers respectively. These quantities may be estimated using a static or dynamic procedure, see Martin et al. (2000), Garnier et al. (2009) and Moin et al. (1991). Many other models for the SGS stresses and fluxes have been developed and tested in past studies (Martin et al. 2000; Garnier et al. 2009; Silvis et al. 2017) and these models are introduced and discussed in later chapters, specifically in chapter "Machine-Learning for Stress Tensor Modelling in Large Eddy Simulation". The statistics obtained using these models could show some sensitivities to errors introduced by the numerical scheme, especially for second order statistics and thus some care is needed. Perhaps, one way to address these issues is to use MLA to estimate the model parameters, which is discussed in chapter "Machine-Learning for Stress Tensor Modelling in Large Eddy Simulation".

The chemical reaction rate in the species equation, Eq. (4), is important for turbulent combustion. The physical processes represented by this term typically occur at SGS level. Also, the reaction rate is a highly nonlinear function of temperature, T, and species mass fractions, Y_i, and, hence it cannot be expressed in a meaningful way using only the resolved temperature and species mass fractions. Formulating a robust yet accurate SGS closure for the reaction rate is challenging and important and this has been studied in past studies which are reviewed and summarised in many references, see for example Swaminathan and Bray (2011), Poinsot and Veynante (2005), Swaminathan et al. (2022b), Gicquel et al. (2012), Peters (2000), Pitsch (2006), Rutland (2011). Each of these approaches has their advantages and limitations in terms their predictive abilities, simplicity, ease of use, computational expenses, physical basis and these aspects are discussed in past works, for example see Swaminathan et al. (2022b). In the following, we give an brief overview on the challenges involved in LES and the role of MLA to tackle them which also helps us to articulate the objectives for this volume.

3.2 LES Challenges and Role of MLA

The SGS closures are predominantly based on the gradient flux hypothesis as discussed in the previous subsection and it is well known that in reacting flows there are processes which defy this hypothesis. Hence, modelling counter-gradient subgrid scalar fluxes are still an outstanding issue, specifically for low Reynolds number reacting flows. Despite this, LES calculations with the gradient flux models have shown good agrements between the computed and measured statistics suggesting that these models are sufficient for flows of interest to practical systems. Another challenge for LES is on the near-wall flow characteristics. It is quite well known that practical LES cannot recover the law of the wall and some special numerical treatments are required as noted by Nikitin et al. (2000) and Brasseur and Wei (2010). Recovering the law of the wall becomes important when the heat and momentum fluxes through the walls (of the combustor, for example) need to be evaluated as design variables.

It is observed generally that the numerical grids used for LES of reacting flows resolve instantaneous flame structure to some extend, which is acceptable for atmospheric pressure. High pressure flows in complex geometries are common in practical applications and thus resolving the instantaneous flame structure will likely to yield impractical grid cell counts because the flame thickness approximately scales as $\delta_{th} \sim p^{-1/2}$ (Turns 2006) and some of the important geometry detail need to be captured in the grid. Thus, the common practice of using grids having cell sizes of the order of δ_{th} is unattractive for practical LES. Consequently, SGS combustion models have to be robust and accurate in representing the relevant physical processes and machine learning algorithms can play important role here. Probably, it is useful to design or select a grid resolving most of the kinetic energy in the flow and let the SGS closures, specifically for combustion, to handle the turbulence-chemistry interactions

and their intricacies for LES of reacting flows in practical systems. The guidance suggested by Pope (2000), which is $\mathcal{K} = k_{\text{sgs}}/\left(k_{\text{res}} + k_{\text{sgs}}\right) \leq 0.2$, where k_{sgs} and k_{res} are subgrid scale and resolved kinetic energies respectively, may be used. It is to be noted that this condition can only be evaluated after completing a preliminary LES of non-reacting flow in a given geometry. Alternative measures to evaluate LES grid requirement have also been suggested in past studies. However, the parameter $\mathcal{K}$ is quite practical and useful, and thus it is recommended. This requirement is to be applied for flows before igniting the flame and thus checking and satisfying this grid requirement are quite straightforward since the LES of non-reacting flow is the first step in conducting LES of turbulent combustion.

Machine learning algorithms can play a vital role in turbulent combustion calculations. These algorithms can be leveraged to build SGS models which can reduce computational requirements substantially. However, using MLA for these purposes are not common yet and there is a surge of research activities in this direction. The subgrid fluid dynamic and combustion processes and their interactions are highly non-linear stochastic events and thus MLA is well suited to infere the SGS statistics required for LES. Typically, machine learning methods are used for pattern recognition in various fields (Hinton et al. 2012; Sathiesh et al. 2016; Gogul and Sathiesh Kumar 2017) and are finding their ways into other fields such as climate modelling (Watson-Parris 2021), drug discovery (Bhati et al. 2021) and fluid mechanics (Brunton et al. 2020). Their application to reacting flows is gaining momentum although it is still at an early development and validation stage. Hence, the objective for compiling this volume is to bring together the latest developments in MLA and its application to chemically reacting flows and make it readily accessible for researchers and graduate students interested in this multi- and cross-disciplinary topic.

4 Objectives

The broad aim here is to bring together the recent developments in the field of MLA applied to reacting flow calculations. These flows in practical systems are invariably turbulent and hence there are three important aspects, *viz.,* turbulence, chemical reactions and their interactions, requiring close attention. The chemical reactions are because of molecular collisions but, at continuum level of description used commonly for turbulent reacting flow simulations, they are modelled using Arrhenius rate expressions involving kinetic parameters. These parameters, related to the atomic potential energies, are obtained typically using shock tube experiments but recent advances in ML techniques is helping to estimate these parameters using atomistic molecular dynamic simulations as described in chapter "Machine Learning Techniques in Reactive Atomistic Simulations". This chapter also gives an overview of various ML algorithms. One needs large data sets to train and validate these algorithm before using them for inferring quantities of interest and thus their robustness depends on the conditions covered in the data sets and hence these data sets can be huge. Hence one needs a clever and intelligent algorithm to

detect events/patterns of interest in the data. Machine learning algorithms can come handy for this purpose as discussed in chapter "A Novel In Situ Machine Learning Framework for Intelligent Data Capture and Event Detection" suggesting an interesting idea—in situ training—to train MLA. The application of MLA to infer SGS stresses and fluxes are described in chapter "Machine-Learning for Stress Tensor Modelling in Large Eddy Simulation". The combustion chemistry is quite complex even for a simple fuel like methane or hydrogen and involves a large number of elementary reactions with disparate time and length scales. Hence integrating these reaction into numerical simulations of turbulent combustion can make the simulations to be prohibitively expensive. Machine learning can be leveraged to accelerate chemistry integration by helping us to understand combustion chemistry closely as described in chapter "Machine Learning for Combustion Chemistry". The third aspect, turbulence-chemistry interaction, of turbulent combustion noted above can be addressed using different modelling approaches which helps us to estimate the filtered reaction rate of a chemical species or a reaction progress variable depending on the modelling approach used. The application of machine learning algorithms to these approaches are discussed in chapters "Deep Convolutional Neural Networks for Subgrid-Scale Flame Wrinkling Modeling" to "AI Super-Resolution: Application to Turbulence and Combustion". Obeying constraints coming from physical conservation laws and requirements (for example species mass fractions have to positive or zero) can become an issue for machine learning methods and some extra care is required while defining the *cost function* needed in the training step for machine learning algorithms, see chapters "Machine Learning Techniques in Reactive Atomistic Simulations" and "AI Super-Resolution: Application to Turbulence and Combustion". The interaction between fluctuating heat release rate and pressure in turbulent combustion established inside a tube as in many practical combustion systems, for example gas turbines and rocket engines, will have thermoacoustic oscillations which can become an issue for safe operation of these systems if these oscillations are not controlled. Predicting these oscillations and their on-set are challenging machine learning algorithms can be applied to these problems as described in chapter "Machine Learning for Thermoacoustics". The concluding remarks are drawn in the final chapter.

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