Can Combustion Models be Developed from DNS Data?

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Abstract

The development of accurate modeling strategies for Reynolds averaged Navier-Stokes (RANS) or large-eddy simulation (LES) models for turbulent combustion is often severely impeded by the lack of reliable data. Recent advances in direct numerical simulation (DNS) of turbulent combustion make the analysis of DNS data a powerful tool in the development process of combustion models. In this work, a systematic methodology of the development process will be discussed, which besides relying on experimental data makes use of the richness of DNS data. This methodology is then demonstrated using the example of model development for turbulent premixed flames on the border of the thin reaction zones and the broken reaction zones regime.

Introduction

Turbulent combustion is a topic of considerable interest with applications in internal combustion engines for transportation, stationary gas turbines for power generation, aircraft engines for propulsion, and large-scale furnaces, to name just a few. The physics of turbulent combustion and the involved interaction of turbulent and molecular transport with chemistry have a considerable complexity arising from the multi-physics nature, the wide scale-separation, and the highly non-linear character and interaction of the involved processes. Accordingly, the development of high-fidelity models for turbulent combustion is challenging and an area of ongoing research.

In the past decades, the use of computational fluid dynamics (CFD) has taken a pivotal role in the design and control of industrial combustion systems to reduce development costs and exploit the full potential of highly efficient ultra-low emission combustion devices. CFD of combustor flows initially started out with the classical Reynolds-averaged Navier-Stokes simulation (RANS) approach, where only ensemble mean quantities are considered for and the turbulence must be entirely modeled. Combustion models for RANS have been developed for different combustion regimes and applications [1], and models in the context of RANS are available in standard commercial CFD codes. The RANS approach is quite useful and has been applied in many fields of combustion applications, such as internal combustion engines, stationary gas turbines, and aircraft engines (e.g. [2, 3, 4]). However, this method has shortcomings in accuracy and flexibility, especially in the predictions of highly non-linear phenomena, such as the formation of pollutants.

More recently, large-eddy simulations (LES) have become more common in both research and the design of combustion devices [5, 6, 7, 8]. LES takes advantage of resolving the large-scale turbulent structures and only the effect of the small-scale structures on the large-scales needs to be modeled. In combustion simulations, this results in more accurate predictions of the mean flow and the scalar mixing process, which has been shown in numerous examples [6]. In LES, also the large-scale unsteadiness of flow and combustion are captured, so that unlikely yet dynamically important events and their effect on global quantities can be considered. This has been shown to be particularly important for the description of strongly non-linear combustion processes, such as for auto-ignition chemistry [9] or when there is complex interaction of processes with vastly different time scale, which is often the case for pollutant formation, such as the formation of soot, where typically a range of different chemical time scales interacts with large and small scale mixing [10].

Rapid advances in LES modeling accompanied by simultaneous progress in computer science and computer hardware have enabled LES of realistic combustion systems, such as gas turbine combustion chambers [8]. However, while combustion modeling is advancing, models often do not show acceptable predictability yet, especially for the more complex phenomena discussed above. Furthermore, modern combustion technology often explores new combustion regimes, which have not previously been considered in model development or validation. Examples for this from recent years are homogeneous charge compression ignition and low temperature combustion for internal combustion engines, oxy-combustion and MILD combustion for power generation, and lean direct injection for aircraft engines. Therefore, despite continuous progress of combustion LES, modeling of complex combustion phenomena, such as formation of NOx, CO, and soot, of thermoacoustic instabilities, and of transient operation conditions are still areas of active research. and improved and truly predictive models for these could have a tremendous impact for further improving combustion systems and for exploring more radical design changes. Accordingly, current research activities are directed towards developing combustion models which are regime independent, accurate for emissions, and computationally efficient.

Presently, the main impediment for the development and improvement of LES combustion models is the lack of data. While data sets from experiments and DNS both have their own limitations, the present paper discusses how these could be combined in a systematic way to provide more certainty in model development.

The role of DNS

Numerous high quality experimental data sets have been obtained over the past years and are now available for many configurations. However, the provided details are often not sufficient for rigorous analysis of model deficiencies and unambiguous model development or improvement. Further, uncertainties in boundary conditions and systematic uncertainties in measurements and simulations constitute major challenges for rigorous validation. Although DNS are presently feasible only for a restricted range of the pertinent non-dimensional groups, the richness of DNS, the level of detail, the availability of all desired quantities at all locations, and the well-defined and well-known details of the boundary conditions motivate the use of DNS data for model development. Spatially and temporally resolved data for quantities like reaction rates including species and temperature distributions, high order moments, or correlation functions are challenging or impossible to obtain experimentally, yet these can enable very systematic analysis and

DNS of turbulent combustion was for a long time restricted to two-dimensional flows or one-step chemistry. Advances in supercomputing, in numerical methods, and in simulation codes for reacting flows have enabled a series of interesting DNS studies with more practical relevance for industrial combustion systems as reviewed by Chen [12]. In particular, besides a continuous rise of the Reynolds number, two main trends of recent DNS can be observed. First, the flow configurations have matured from isotropic turbulence and often feature a mean shear driving the turbulence or even resemble geometric features of realistic systems. Examples of advanced flow configurations comprise temporally evolving nonpremixed [13], premixed [14], and auto-igniting jet flames [15], a premixed swirl flame [16], a jet in cross flow flame [17], swirl-stabilized spray combustion [18], and a premixed flame interacting with wall [19]. Second, the chemistry of DNS flames becomes increasingly more detailed, which is for example demonstrated in a DNS of sooting n-heptane flames by Attilii et al. [20].

It is worth noting that despite the above mentioned progress of DNS of turbulent combustion, DNS remains a tool that, because of resolution requirements, is limited to certain ranges of the governing non-dimensional groups, such as to moderate Reynolds numbers, moderate Damköhler numbers, and high Karlovitz numbers Ka. Especially the fact that high Reynolds numbers are difficult to achieve in DNS with presently available supercomputing resources poses a challenge and calls for caution in drawing conclusions from DNS data for realistic combustion systems. As an example, although many models rely in one way or another on the high Reynolds number limit and Kolmogorov’s inertial range scaling, DNS typically cannot reach that limit. In that sense, models might be invalidated using low Reynolds number DNS data, while still yielding quite good results in actual applications to realistic engines and vice versa. In spite of this, DNS data have been found to be quite useful, especially when used in combination with experimental data.

Using DNS data for model development

For turbulent flow simulations, transport equations are typically derived for statistical expectations of the quantities of interest, such as ensemble averages (RANS) or spatially filtered quantities (LES). In applying averaging operators, unclosed correlations typically appear, for which in order to solve the equations, models need to be provided. This means, the unclosed terms have to be expressed as function of known quantities, which are those quantities, for which equations are being solved. Models typically do not use all known quantities. Hence, there is often a choice of which known quantities are best used as parameters in a model. To answer the question of what parameters should appear in a model, how a model should be formulated, and how a model then performs in simulations, DNS data could be helpful. DNS data can be used in different ways in model development or validation. Here, we will briefly discuss a priori testing, a posteriori testing, and data analysis.

A priori and a posteriori testing

Most often, DNS data are used for validation in a priori model testing, where a given model is evaluated by comparing the DNS values of the modeled quantity with the model prediction. Such tests are interesting, but typically suffer from the fact that the sensitivities of the real quantities of interest with respect to the modeled quantity are not known. Hence, it is difficult to judge how well a model has to perform in an a priori test in order to predict the quantities of interest within certain error margins. An example for this is shown in Fig. 1a. This figure demonstrates an interesting fact in modeling. The model shown in this figure [21] depends on two parameters, the subfilter velocity fluctuation $\Delta u_x$ and Fig. 1a shows data for a given value of $\Delta l / l = 2.1$, where $l$ is the nominal laminar flame thickness. For a given combination of the two parameters, the model apparently gives a unique result, while in the DNS there might be many realizations with the same values for both parameters, but each having a different value of the modeled quantity. In that sense, a model for an unclosed term with a given number of parameters can never be perfect and it cannot predict instantaneous data. However, one could judge the model prediction against the conditional mean, which is also shown in Fig. 1a, and which is very well predicted by the model. However, it is difficult to judge how much scatter should be allowed around the conditional mean. For the given example this implies that it is unclear whether the model shown in Fig. 1a is acceptable or not, despite the fact that it agrees quite well with the conditional mean.

Models can also be tested in a posteriori model evaluation, where RANS or LES simulations of the actual DNS configuration are performed. The quantities of interest are being calculated and can be compared with the DNS data. The challenge though is that the modeled simulations depend not only on the tested model, but also on all other models used in the LES, such as subfilter models for the Reynolds stresses. Further, obtaining the proper resolution and adequately initializing the simulations is often difficult. An example for an a posteriori test using the model tested in Fig. 1a is shown in Fig. 1b in a comparison of the heat release. Apparently, the tested model yields very good results.

Systematic data analysis

Yet another use of DNS data is the analysis to understand the physical phenomena or to obtain more information that would constrain a model.

Two of the most important questions in the development of models are

- What parameters $\phi$ should appear in the model?
- Given a set of parameters $\phi$ that can appear in the model, what is the functional form between the model $g(\phi)$ and the known parameters $\phi$?

A powerful analysis tool to address the first question about the selection of the set of parameters is the concept of optimal estimators proposed by Moreau et al. [22], which we will review here briefly. Starting point is an unclosed term $g$, for which $\hat{g}_{\text{Model}}(\phi)$ is a model in terms of the set of parameters $\phi$. The concept of optimal estimators provides a method to determine the error caused by the choice the number and the actual set of parameters for the model.

The total error of a model can be assessed using DNS data and it can be defined as

$$\epsilon_{tot} = \left( \frac{\langle \Delta DNS - \hat{g}_{\text{Model}}(\phi) \rangle^2}{\epsilon_{DNS}} \right),$$

where $g_{DNS}$ is the unclosed term or quantity directly evaluated from the DNS and $\hat{g}_{\text{Model}}(\phi)$ is the model evaluated with a given set of parameters $\phi$ extracted from the DNS. The brackets denote an average over an appropriately defined ensemble. Note that, in principle, the parameters $\phi$ appearing in the model could already be modeled quantities and that Eq. 1 can be evaluated either with the modeled $\phi$ values or with these values evaluated from the DNS. The notation used in Eq. 1 suggests the latter, which is also what is used here in the examples.
Within the concept of optimal estimators, the total error for $\delta_{\text{Model}}(\phi)$ is split into two parts. One part of the modeling error results from the choice of the set of parameters, the remaining error originates from the functional form of the model given a certain set of parameters. The error due to the selection of the set of parameters is referred to as the irreducible error, and it is given as

$$e_{\text{irr}} = \left( \langle \delta_{\text{DNS}} \rangle - \langle \delta_{\text{DNS}}(\phi) \rangle \right)^2.$$  \hfill (2)

For a given parameter set $\phi$, the conditional average in Eq. 2 can be shown to lead to the smallest possible total error when used as a model in Eq. 1. This conditional average is therefore, for the given set of parameters, what the best possible model should predict and is therefore called the optimal estimator. A decrease of the irreducible error can only be accomplished by either changing the set of parameters or amending it.

The difference between $e_{\text{tot}}$ and $e_{\text{irr}}$ is the remaining error that stems from the functional form of the model for $g(\phi)$. The concept of optimal estimators is quite powerful and allows to determine the best set of parameters by repeatedly evaluating the optimal estimator with different sets of parameters. An example is the scalar dissipation rate model of Balarac et al. [23], where it was shown that using the kinetic energy as a parameter in a model is superior to using the strain rate. Another example will also be discussed in Fig. 6a below. Once the best parameter set has been determined, functional forms of the model can be assessed by comparing results with the total error with the irreducible error. However, since the optimal estimator concept is just a special form of a priori testing, it suffers from the same challenge, that the quality of a model in an a priori sense is difficult to correlate with predictions of the quantities of interest in an a posteriori sense, which was demonstrated in Fig. 1.

The application of the optimal estimator approach supports model development in two ways. It helps to understand errors of existing LES models and furthermore guides the choice of additional or alternative modeling parameters.

A systematic approach to model development

Model development and validation are inherently coupled. A very common challenge for both is that models are typically developed for certain applications, for instance, combustion in premixed stationary gas turbines or non-premixed gas turbines for applications in aviation. Validation for the actual application, however, is difficult, because data are typically sparse. Often, only averaged engine-out data for some pollutants are available. In-combustor data are usually restricted to quantities that are easy to measure, such as the pressure. Simpler lab-scale experiments or DNS allow for more detailed data, but they are less relevant for the application. This has led to the picture of a tier-based validation strategy that includes a broad base of unit problems and performs validation through a hierarchy of benchmark cases and sub-system cases all the way to the full system [24, 25]. This concept has been borrowed here to develop the model development strategy shown in Fig. 2. Here, however, the base of the pyramid is not the number of unit experiments, but spans a new direction. Its width represents the data completeness for one unit experiment or DNS of a unit configuration. The pyramid shows the connection between one unit experiment and the system scale as a hierarchy of DNS in simple configuration with lots of data, which then leads through DNS in more relevant configurations and lab-scale experiments all the way to the system scale. It should be pointed out here that the sub-system scale is omitted in the following, but it could be added without changing the character of the subsequent discussion.

![Validation pyramid](image_url)

Figure 2: Validation pyramid

Here, a systematic guide for developing a combustion LES model from DNS data is suggested. This methodology is based on both DNS and experiments. It takes advantage of the richness of DNS data on the one hand, and uses the proximity of experiments to practical combustion systems on the other hand. One could argue that the procedure is self-evident, but it is
Starting point here is an interesting and relevant modeling question. Considering the full validation hierarchy, this should be obtained from system-scale simulations with comparisons to experiments that identify model deficiencies. Sensitivity studies should then identify important parts of the model, which will be the focus for further improvements. Then, well-documented lab-scale experiments should be identified that on the one hand represent the combustion characteristics of the considered system, and on the other hand have a similar sensitivity to the same model parts. This step is listed below, but is not discussed here any further.

The sequence in the model development then follows the depiction shown in Fig. 3 and includes the following steps:

0. LES of system scale configuration demonstrating modeling need; identification of important parts of the model; identification of relevant lab-scale experiment.
1. LES of well-documented experimental validation case and demonstration of modeling need.
2. Identification of DNS representing the same combustion regime and demonstrating the same model deficiency.
3. A posteriori test of the model using the DNS results.
4. Error analysis and model development including good modeling idea based on understanding of the underlying processes.
5. Potentially, identification of additional unit problem DNS configuration for further analysis.
6. A priori and/or a posteriori test using unit problem DNS results.
7. A posteriori test of model using DNS with newly developed model.
8. LES of experimental validation case with newly developed model.

Assuming that a modeling question important for a full scale simulation is known and that a lab-scale experiment has been identified that represents some important features of the full system with respect to the modeling problem, in the first step, LES of this experiment is performed. It is essential that the experiment satisfies certain conditions, such as well-defined boundary conditions and the availability of reliable and extensive sets of measurements. Further, cold flow data should be available for the case and in the ideal scenario, the experimental data set has a number of cases with a systematic variation of the important non-dimensional group, such that models typically work under some condition, but not under other conditions. A potential target flame could be an experiment of a validation workshop in some condition, but not under other conditions. A potential target flame could be an experiment of a validation workshop in some condition, but not under other conditions.

Next, the model failure should be reproduced in an a posteriori test of a DNS configuration. For this, in step 2, a DNS database has to be identified or produced that mimics the experiment as closely as possible, so that the model assumptions leading to the model failure can be analyzed and identified. This DNS should resemble the flow features and complexities of the lab-scale experiment, so it is typically a DNS of a jet or a swirling flow, a wall bounded flow, or other shear-driven turbulence case. Most importantly, the model has to fail in predicting this DNS case for the same reason as for the lab-scale experiment, which implies that the combustion regime should be the same. This step is a crucial part of the process, which is particularly difficult, since a DNS has to make compromises: It is not the same as the lab-scale experiment, but should resemble the experiment at the same time. Furthermore, this step typically involves very expensive DNS simulations that do not leave much room for an unsuccessful trial.

Following this, in step 3, an a posteriori test using the DNS data set is performed, which should again demonstrate the modeling need. This simulation should also provide data for the subsequent model uncertainty analysis, and serve as a reference for subsequent simulations with an improved model. As in step 1, if the model does not fail, the test case has been chosen well or it hints at other issues in the comparison in step 1.

The modeling work is in step 4. Here, the existing model is either extended or reformulated, or an alternative new model is eventually formulated. For this, systematic analysis methods, such as the concept of optimal estimators described above might be very useful and should precede model formulation. For this, the richness of the DNS data is important and after identifying the shortcomings of the model through the analysis, additional unit problem DNS addressing that issue in a more targeted way might be added, which involves identifying such a DNS case in step 5 and performing a priori or a posteriori testing of that case in step 6. Such DNS cases could be, for instance, isotropic turbulence or non-reactive cases.
Afterwards, the newly developed model is validated in two ways. It has to predict both the DNS resembling the lab-scale experiment in step 7 and the original experimental target in step 8 with improved accuracy compared to the simulations in steps 1 and 3.

**Application: Modeling premixed turbulent flame with strong finite-rate chemistry effects**

Increasing thermal power and power density of combustion devices is often desirable. This is typically accompanied by increasing the flow Reynolds number and, accordingly, the turbulence intensity. If operated in a premixed fashion, such combustion systems are likely to be operated on the border of the thin reaction zones regime and the broken reaction zones regime. In the broken reaction zones regime, the time scales of the chemistry inside the reaction zone and small scale turbulence are of the same order, and hence, strong finite rate chemistry effects can be expected. Since conventional unstretched premixed flamelet models [26] do not account for these effects, further modeling is needed in the framework of these models as outlined in the following example. It is worth noting that while the following example is chosen to discuss the individual steps of the model development procedure given above, the final very important step is missing.

**Step 0: Choosing a lab-scale experiment**

A full-scale simulation should be the starting point, which is omitted here, since the modeling need is clear. It is the adequate modeling of the combustion process at high Karlovitz number $\text{Ka}$ at gas-turbine conditions. An adequate lab-scale experiment is the piloted premixed jet burner (PPJB) by Dunn et al. [27], which consists of a series of turbulent premixed jet flames from low to high Re and Ka numbers with an extraordinarily large pilot flame that can sustain the flame even when strong local extinction occurs. In that sense, the PPJ burner is similar to a high Ka number gas turbine combustion case, where the large pilot represents the recirculated hot combustion products in a typical swirl-stabilized gas turbine combustor.

**Step 1: LES of the PPJ burner**

From the PPJB experiments by Dunn et al. [27], two different flame configurations were chosen, one with a smaller Ka number, where experimentally very little extinction was observed and one with a higher Ka number with substantial extinction. For the two cases, velocities of 100 m/s (PM1-100) and 200 m/s (PM1-200) were used, which results in Reynolds numbers of 25,000 and 50,000, respectively. The corresponding Karlovitz number $\text{Ka} = \frac{\text{U}^2}{\text{g}^2}$ that characterizes the small scale turbulence-chemistry interaction, varies from 1,600 to 3,500. Because no significant extinction and reignition regions are detected for the case with lower inflow velocity PM1-100, the present level set based combustion model is expected to capture this flame accurately. For the PM1-200 flame, however, substantial regions with extinction are observed. Therefore, modeling of this flame is quite challenging.

A comparison of the radial profiles of the mean axial velocity at two different measurement positions for cases PM1-100 and PM1-200 is shown in Fig. 4 [28]. As expected, good agreement between simulation and experiment is noted for flame PM1-100 at both measurement positions, while the axial velocity is overpredicted further downstream for flame PM1-200. This discrepancy originates from the inability of the premixed flamelet model formulation used in the simulations to account for extinction and reignition occurring primarily in the downstream section of the burner for flame PM1-200.

**Figure 4: LES of the PPJ burner. Radial velocity profiles of axial mean velocity for flame cases PM1-100 and PM1-200 at $x/D = 5$ and $x/D = 25$.**

**Step 2: Identification of relevant DNS**

The DNS database chosen for the analysis should be at high Ka number and have shear driven turbulence to resemble the experimental case. Here, the DNS target is a premixed methane/air planar jet flame by Sankaran et al. [29], where the Reynolds number is Re$_j = 2100$ and the associated Karlovitz number is Ka = 225, which implies that the flame is located just inside the broken reaction zones regime of the turbulent premixed flame regime diagram. Hence, turbulence is expected to influence premixed flame structures to a leading order degree. Although both the Karlovitz and Reynolds number are an order of magnitude lower than in the PPJ burner and no extinction and reignition events are observed in the DNS in contrast to flame PM1-200, this DNS is suggested to mimic the experiment well due to strong finite-rate chemistry effects. However, implications and modeling attempts on the basis of this DNS analysis have to be rigorously validated in the PPJ burner as well.

**Step 3: A posteriori test: LES of the Sandia Bunsen flame DNS**

LES of the DNS configuration was performed and as shown in Fig. 5, it was found that the LES vastly underpredicts the correct flame height [30]. Furthermore, it was shown by Knudsen et al. [30] that a distinct difference between temperature and velocity profiles of LES and DNS is observed, such that the LES overestimates the temperature, which results in an underprediction of the axial velocity. Similar to the LES of the PPJ burner, this discrepancy stems from strong finite-rate chemistry effects that are not accounted for in the LES combustion model.

**Step 4: Strained flamelet model development**
This step is the core of model development. DNS data are used in the analysis and to test models and suggest modeling strategies. The starting point of the modeling work is an analysis by Sankaran et al. [29], who reported that in the upstream region of the Bunsen flame, an unstretched premixed flamelet model cannot reproduce the flame structure, while further downstream the flame structure is predicted well by the unstretched flamelet model. Furthermore, they found that the flame structure smoothly transitions into that of an unstretched flamelet with increasing downstream position. A single strained flamelet solution was compared to the DNS Bunsen flame and was shown to be close to the flame structure in the upstream section. Here, an interesting analogy to the PPF burner exists, where unstretched flamelet modeling leads to good results in some regions, whereas in other regions, unstretched flamelets cannot predict the flame with good accuracy.

This motivates modeling flame stretch by means of strained flamelets in a transient manner meaning that an entire set of strained flamelets is incorporated into the combustion model. In this approach varying flame structures are considered by choosing the closest flamelet depending on the local strain effect on the flame structure. Knudsen et al. [30] observed that the H radical reasonably correlates with the strain showing a monotonic decrease when increasing the strain. The newly formulated strained flamelet model takes advantage of this characteristic and captures strain in form of the local hydrogen concentration. This is accomplished by solving an additional transport equation for the filtered H radical mass fraction and tabulating strained flamelet solutions, which are then parameterized as function of a reaction progress variable and the H radical.

Another aspect of the model development is the subfilter modeling and closure for the joint subfilter probability density function (PDF) of progress variable and hydrogen radical mass fraction. In an a priori analysis, this subfilter distribution was investigated and subfilter PDFs were presumed accordingly.

Step 5: Choice of additional unit problem DNS

The model proposed in the previous step assumes from empirical evidence that incorporating stretch effects in the model should lead to an improvement of the model and that the H radical mass fraction can be used to parametrize stretch effects on the chemical source term of progress variable. It was shown by Knudsen et al. [30] that both quantities correlate in the laminar flame simulations, but there could be better parameters. The choice of parameters, the quality of this particular parameter, and the general improvement of the model with the additional stretch parameter can now be assessed using the same DNS or, as done in the present example, with DNS data from an even simpler configuration, in this case a planar periodic time-developing premixed turbulent jet flame. The DNS of Hawkes et al. [14], already discussed above in the context of Fig. 1, is in general a good case for this. It features a relatively high Karlovitz number of Ka = 92, which is very close to the broken reaction zones regime and it has shear-driven turbulence. However, it uses hydrogen as a fuel, which could lead to differences in what the best strain parameter is. This could therefore be seen as a disadvantage of this database for the present question. On the other hand, it also allows to test the model for a different fuel, which could be seen as an advantage.

Step 6: A priori analysis of periodic jet DNS

In this step, several model variants can be tested using, for instance, the concept of optimal estimators to identify the best set of parameters in the model. Here, several parameter sets for a strained flamelet model are tested, which use a reaction progress variable, here the H2O mass fraction, and in addition different choices for a strain parameter, here the strain, the progress variable dissipation rate, the H2 mass fraction, the H mass fraction. These models are compared with a base model only using the progress variable that was already tested in steps 1 and 3. The results are shown in Fig. 6. The irreducible error, the error only caused by the choice of the parameter set, for all models is given in Fig. 6a. Obviously, the irreducible error of the strained flamelet model using the H2 mass fraction is at least one order of magnitude lower than that of the base model, which shows that the consideration of flame stretch in the model has a strong effect and that the parameter used for this is reasonable. The other parameters are less good and most interestingly, using the strain rate as a parameter, which has often been proposed in the literature, and similarly the progress variable dissipation rate, do not improve the irreducible error over the unstretched model. Also the use of the H radical as a strain parameter improves the results. However, here the improvement is mostly for low progress variable values, where the source term is small. Large values of the source term occur at high progress variable, where the molecular hydrogen is preferable as a parameter. It should be mentioned that it was found that for methane flames, which are considered in the LES test case, the H radical was found to be an appropriate strain parameter and it is used in the subsequent LES modeling.

The total error, shown in Fig. 6b only for the model using H2 as additional parameter does not show much improvement for the strained model at around C = 0.5, but at higher values of progress variable, which are most important for the heat release, the model improvement leads to a decrease in the error of almost an order of magnitude.

Step 7: LES of the Sandia Bunsen flame DNS with new model

In this step the newly developed model is validated by performing LES of the more complex DNS case already considered in step 3. The flame length, which was shown in Fig. 5 for the base model, is now predicted quite well. The model improvement is also quite evident from radial temperature profiles shown in Fig. 7. Coarse and fine LES simulations are shown for both the base and the improved models. The mesh resolution has only a minor influence indicating that even the coarse grid simulations are mesh converged. Further, the modified model leads to...
In addition to providing data for model validation, Fig. 9(a) highlights an interesting combustion process that occurs in the DNS (see Fig. 12). This value of $\varepsilon_{\text{irr}}$ is the dominant effect.

The rapid advances of DNS of turbulent combustion have not yet been completed. However, DNS provides invaluable data of important quantities, such as reaction rates of pollutant chemistry, which is illustrated by a modeling study of premixed flames on the configuration and the initial experimental target. This procedure is further assisted by an a posteriori test of this DNS configuration is performed in order to reproduce the model failure. In the fourth step, the richness of the DNS data is being used to directly assess model assumptions and identifying model deficiencies. This step can be supported by systematic analysis tools, such as the optimal estimator approach. Based on the analysis, a new model including subfilter closure may be formulated. Note, however, that while the systematic analysis can suggest certain aspects of a model, the full model formulation is not suggested by the analysis. Analysis and model formulation can be further assisted by other DNS more targeted to the specific modeling question in steps 5 and 6. Steps 7 and 8 finally are the a posteriori validation of the newly developed model against the DNS configuration and the initial experimental target. This procedure is illustrated by a modeling study of premixed flames on the border of the thin reaction and broken reaction zones regime with strong finite rate chemistry effects. Results of steps 1–7 are presented and it is demonstrated that the developed strained flamelet model is a significant improvement over the conventional unstretched flamelet model for the investigated flames.

**Conclusions**

The development of high-fidelity LES models for turbulent combustion is challenging due to its multi-physics nature and the fact that turbulence-chemistry interactions occur primarily on subfilter levels, which means that they require modeling. While continuous progress is being made in combustion modeling, one of the main impediments today is the sparsity of validation data. In that regard, data from DNS might be quite useful. The rapid advances of DNS of turbulent combustion in recent years has significantly improved data quality in terms of fuel chemistry, flow configuration, and flow and combustion regimes. This makes DNS a powerful tool in the development of RANS and LES models. This paper discusses a systematic approach for model development from DNS and describes how DNS data and experimental data can be combined for systematically developing high-fidelity LES models.

The methodology discussed here has eight individual steps. Given an interesting modeling question, first LES of an experimental validation case is performed with an existing LES model. If the model fails to predict the experiment, in the second step, an appropriate DNS database is selected, which is characterized by the same combustion regime, and in the third step, an a posteriori test of this DNS configuration is performed in order to reproduce the model failure. In the fourth step, the richness of the DNS data is being used to directly assess model assumptions and identifying model deficiencies. This step can be supported by systematic analysis tools, such as the optimal estimator approach. Based on the analysis, a new model including subfilter closure may be formulated. Note, however, that while the systematic analysis can suggest certain aspects of a model, the full model formulation is not suggested by the analysis. Analysis and model formulation can be further assisted by other DNS more targeted to the specific modeling question in steps 5 and 6. Steps 7 and 8 finally are the a posteriori validation of the newly developed model against the DNS configuration and the initial experimental target. This procedure is illustrated by a modeling study of premixed flames on the border of the thin reaction and broken reaction zones regime with strong finite rate chemistry effects. Results of steps 1–7 are presented and it is demonstrated that the developed strained flamelet model is a significant improvement over the conventional unstretched flamelet model for the investigated flames.

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References


