A systematic approach for combustion models development

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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 close to the broken reaction zones regime.

1. 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.

The process of model development and validation crucially depends on reliable high-quality data, which could be obtained either from experiments or from direct numerical simulations (DNS). In fact, the main impediment for the development and improvement of LES combustion models today is the lack of such data. Numerous high quality experimental data sets have been obtained over the past years. However, not all data sets are suitable for validation and most data sets have never been taken for this purpose. Ideal data sets are based on accurate and verified diagnostics, sufficiently well-characterized boundary conditions including information about heat transfer, mean velocity profiles, and turbulence at the inlets, they include cold flow data, provide a comprehensive set of measured quantities, and very importantly, they include a series of cases from cases that are easy to predict to cases featuring more complex combustion physics. Several data sets satisfying most of these criteria if not all are now available for different configurations including piloted nonpremixed [1, 2] and premixed [3, 4] jet flames, bluff body stabilized flames [5, 6], or swirling flames [7]. Still, even the most complete and accurate validation-type experiments typically cannot provide sufficient details for rigorous analysis of model deficiencies and unambiguous model development or improvement. Further, uncertainties in boundary conditions, systematic uncertainties in measurements and simulations, and uncertainties in chemical kinetics are difficult to completely rule out. These issues constitute major challenges for rigorous validation of models for turbulent combustion.

Although DNS are presently feasible only for a restricted range of the relevant non-dimensional groups, the richness of DNS, the level of detail, the availability of all desired quantities at all locations, the well-defined and well-known details of the boundary conditions, and the fact that uncertainties in chemical kinetics are not a prime concern motivate the use of DNS data for model develop-

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ment. 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 analyses and model development [8].

In light of this, the objective of the present paper is to discuss a systematic strategy for the development and validation of combustion models. 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.

2. 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 [9, 10]. This concept has been borrowed here to develop the model development strategy shown in Fig. 1. 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.

Here, a systematic guide for developing a combustion LES model from DNS data is suggested.

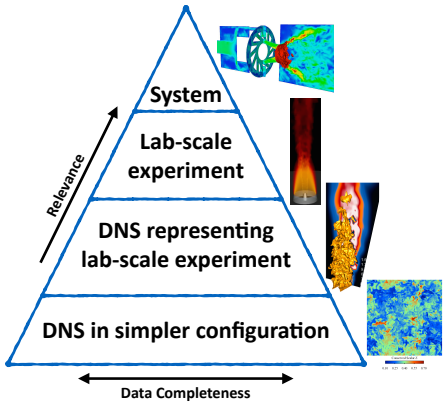


Figure 1: Validation pyramid

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 nonetheless useful to formalize and discuss such an approach and it is instructive to follow the method in model development. Unfortunately, the approach does not automatically lead to a model and still relies on good ideas of the model developer. In the following, the approach is first introduced. Subsequently, one example of the application of this procedure will be shown.

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 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 initial step is listed below, but is not discussed here any further.

The sequence in the model development then follows the depiction shown in Fig. 2 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.

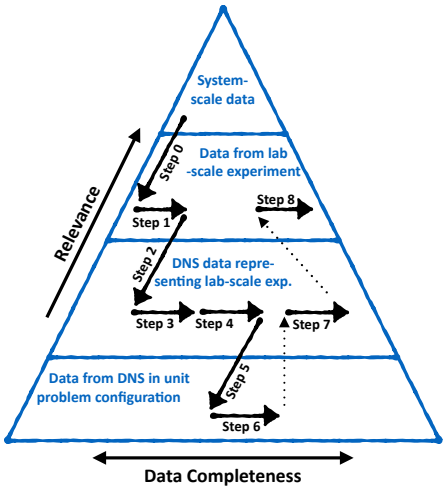


Figure 2: Model development strategy.

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, then, 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. A potential target flame could be an experiment of a validation workshop in combustion, such as the Turbulent Nonpremixed Flames (TNF) or the International Sooting Flame (ISF) workshop, which ensures well-documented experimental conditions and measurements. In case good agreement between experimental data and simulation results is found, no further modeling is required, and the model can be used with more confidence for similar flow and combustion configurations. This would also hint at issues in the prior validation process and comparison of simulation and experimental data at the system scale (step 0). In case the model fails to predict the experiment, the modeling need is identified and demonstrated in the lab-scale experiment.

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 it failed 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 a unsuccessful trials.

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 not 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 might be very useful and should precede model formulation. In this step, 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.

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 [11] 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 Ka at gas-turbine conditions. An adequate lab-scale experiment is the piloted premixed jet burner (PPJB) by Dunn et al. [4], 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. [4], 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. 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.

Results from LES show, as expected, good agreement between simulation and experiment for flame PM1-100, while the axial velocity is overpredicted further downstream for flame PM1-200.

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. [12], where the Reynolds number is $\mathrm{Re}_j = 2100$ and the associated Karlovitz number is $\mathrm{Ka} = 225$, 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.

Step 3: A posteriori test: LES of the Sandia Bunsen flame DNS. LES of the DNS configuration was performed and as shown in Fig. 3, it was found that the LES vastly underpredicts the correct flame height [13]. Furthermore, it was shown by Knudsen et al. [13] 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, to test models, and to suggest modeling strategies. The starting point of the modeling work is an analysis by Sankaran et al. [12], 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.

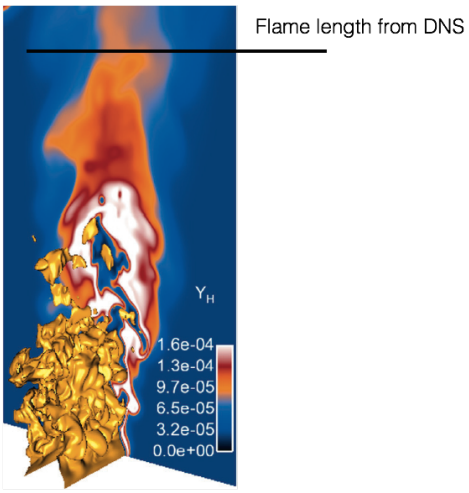


Figure 3: Instantaneous realization of the LES using an unstretched flamelet model. Compared to the DNS, the flame height is underpredicted.

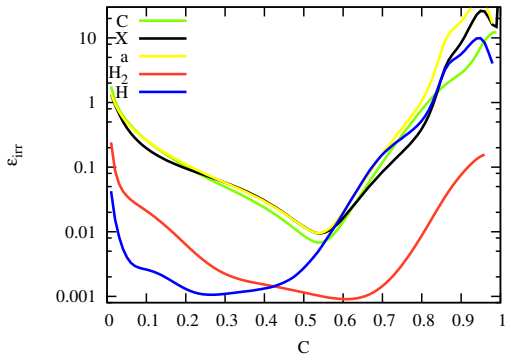
Here, an interesting analogy to the PPJ burner exists, where unstretched flamelet modeling leads to good results in some regions, whereas in other regions, unstretched flamelets cannot predict the flame with good accuracy.

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. [13] 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.

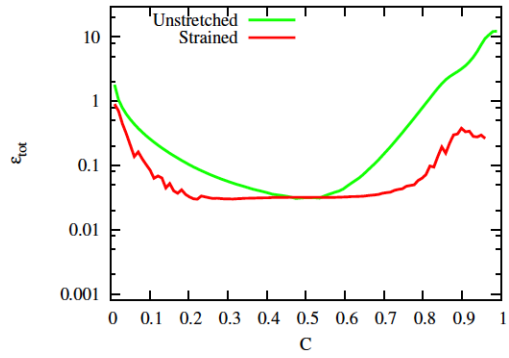
Step 5: Choice of additional unit problem DNS. The model proposed in the previous step assumes from empirical evidence that incorporating stretch effects in the model should lead to an improvement of the model and that the H-radical mass fraction can be used to parametrize stretch effects on the chemical source term of progress variable. It was shown by Knudsen et al. [13] 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] 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.

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 H_2O mass fraction, and in addition different choices for a strain parameter, here the strain, the progress variable dissipation rate, the H_2 mass fraction, and 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. 4. The irreducible error, the error only caused by the choice of the parameter set, for all models is given in Fig. 4a. Obviously, the irreducible error of the strained flamelet model using the H_2 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 unstrained 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 this is hence used in the subsequent LES modeling.

The total error, shown in Fig. 4b only for the model using H_2 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.



(a) Irreducible error for the progress variable chemical source term as function of reaction progress variable C from the models using unstretched (green line) and strained (other lines) flamelet solutions for different strain parameters.



(b) Total error for the progress variable chemical source term as function of reaction progress variable C from the models using unstretched (green line) and strained (red line) flamelet solutions using H_2 mass fraction as strain parameter.

Figure 4: Optimal estimator analysis using results from the hydrogen/air premixed combustion planar jet DNS of of Hawkes et al. [14].

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. 3 for the base model, is now predicted quite well. The comparison with the data has been omitted here for brevity.

4. Conclusions

Thinking beyond the present example, despite certain limits, DNS is anticipated to play an important role in forthcoming modeling studies. In particular, modeling pollutant formation in turbulent flames is an ideal candidate for DNS assisted model development, since DNS provides invaluable data of important quantities, such as reaction rates of pollutant chemistry, which are difficult to obtain experimentally. However, it is important that validation and model development using DNS data is embedded in a coordinated validation strategy based on both DNS and experiments at different levels of complexity.

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