Influence of acoustic, chemistry description and wall heat transfer in LES of the Volvo bluff-body stabilized flame dynamics

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Recent compressible turbulent reacting LES predictions of the Volvo configuration demonstrated the capacity of this approach to recover the three reported operating modes of the burner: ***i.e.*** **stable with no main oscillatory motion of the mean flow, buzz and screech with large thermo acoustic oscillations. Despite this success in recovering experimental observations, this advanced numerical approach is known to suffer from intrinsic limitations and difficulties which can explain the wide range of reported conclusions for the Volvo configuration. To better apprehend this working context, specific issues related to LES are detailed and gauged for this burner. Indeed, while numerics is clearly a key element of LES, boundary conditions are often approximative despite their importance, especially in the context of thermo acoustic instabilities. Connected to this inflow/outflow modeling, the actual computational domain extent should be chosen in agreement with the inflow/outflow boundary conditions while the cross stream dimensions need to cover the real geometry if associated acoustic eigen mode directions are to be properly captured by the simulations. In the same line, the thermal conditions of bluff-body are known to potentially infer different flame anchoring conditions more or less favorable to the triggering of oscillatory or non-oscillatory operating flows. Impacts and quantifications of such modeling difficulties are detailed in this work on the basis of the stable operating condition of the Volvo configuration.**

I. Introduction

Research on combustion instabilities (CIs) has been quite intense in the last hundred years but, as noted by Culick & Kuentzmann[1] in his classic 2006 monograph on CIs, High Performance Computing (HPC) applied to Computational Fluid Dynamics (CFD) has not entered the world of CI studies yet. This observation also arises despite the fact that combustion research has been one of the first HPC users over the last ten years: in the ASCI projects funded by DOE for example (www.llnl.gov/str/Seager.html), CFD of reacting flows has always been an essential element. Three-dimensional unsteady reacting flows can be computed today with high accuracy CFD codes using massively parallel computers.[2] These computers have revolutionized the field of numerical combustion: they have opened the door to the construction of virtual burners that can be fully simulated numerically instead of being built and operated experimentally. Interestingly, these HPC CFD codes have had a limited impact for the moment on CIs studies: most CI analysis tools[3,4,4] still rely on approaches that do not exploit the power of modern computers. The integration of exascale computing in CI methods is required now because it will bring unprecedented precision in this field and allow CI simulations to become truly predictive methods for practical applications.[5]

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All the physics required to predict combustion instabilities is contained in the full Navier-Stokes equations. Full equations indicate compressible, reacting, multi-species conservation equations including two-phase flows (for liquid fuels), radiation and heat transfer through combustor walls. Unfortunately, solving these equations in a turbulent flow is and will remain impossible for a long time. Simplifications are required but HPC allows to minimize them. The last ten years have shown that two methods can be used to study CIs using high-fidelity, large-scale simulation codes running on massively parallel systems. These methods can be split in two generic classes depending on the simplifications used to solve the compressible unsteady Navier-Stokes equations in a reacting flow: (1) Brute force computations where all the physics is to be simulated in a predefined computational domain along with associated boundary conditions and (2) Thermo-Acoustic (TA) solvers that intent to predict acoustic mode stability while relying on a flame/acoustic interaction models to be addressed *a priori*. Although both approaches appear today to be highly complementary and dependent on the target end usage: i.e. thermo acoustic limit-cycle analysis, flame/acoustic model generation or stability map generation for an entire range of operating conditions. For both working contexts, brute force computations seem unavoidable and today Large Eddy Simulations (LES) seem the most adequate CFD strategy to address the problem. A clear assessment of LES and associated modeling is however mandatory which may not be an easy task especially in the specific context of thermo acoustic problems or more broadly enclosed systems.

Naturally, experimental campaigns ranging from laminar[6,7] to highly turbulent flames[8,9] in academic and heavy-duty industrial configurations, have helped providing better understanding of fundamental mechanisms. However, most studies of combustion instabilities focus on longitudinal low-frequency modes[10,11] for which theory, experiments and simulations have been extensively developed. For transverse high-frequency instabilities (such as screech in afterburners, rocket engines or in certain gas-turbines), much less work is available[5,12] and even theory is still not complete today.[?,13–15] In this context, the Volvo configuration developed in the early 1990s is a good prototype to investigate combustion instability, both at low and high frequency: beside stable operation (for which velocity fields were measured), self-excited longitudinal and transverse combustion instabilities were observed during experimental testing.[?,16,17] The experimental data basis for the Volvo setup offers a large validation basis for numerical simulation.[18] While URANS (Unsteady Reynolds-Averaged Navier-Stokes) and LES have already been used to study combustion instabilities in the Volvo configuration,[19–24] most previous studies have concentrated on the low-frequency longitudinal mode appearing around 100 Hz in this configuration (buzz mode). Except for the work of Jourdain and Eriksson[22,23] who used URANS as well as linearized Navier Stokes equations to investigate both low-frequency and high-frequency modes, much less studies have addressed the other unstable mode, called screech,[25,26] at 1400 Hz which also appears in this setup.[24] For this burner, predictions are more or less satisfactory mainly because of the uncertainties present in the modeling and effective acoustic content of the burner at the various operating conditions. The description of chemistry itself in LES remains an open question. CERFACS has tested various formulations ranging from two-step scheme[24,27,28] to sophisticated reduced schemes.[29–31] In this specific context, an overview of recently obtained LES results at CERFACS[24] is provided here to clarify the potential acoustic content in this configuration. Based on such findings targeted towards the LES capability of reproducing acoustic instabilities and limit-cycles at given conditions, numerical setups and modeling required for LES in this burner.

This work is organized as follows. In §II a brief description of the Volvo experiment and the operating points considered in this study are presented followed by recent LES predictions obtained at CERFACS. In §III limits of the previously described predictions are detailed and overall modeling issues related to the proper computational domain definition, boundary condition treatments, chemistry and modeling issues are discussed to properly evaluate design rules for adequate assessment of LES modeling. To conclude, prospective remarks are provided in §IV.

II. Thermo acoustic stability predictions of the Volvo burner with LES

The Volvo configuration[?,16,17] consists of a rectangular chamber of constant cross section (0.12 m $\times$ 0.24 m) and a bluff-body for flame stabilization, Fig. 1. The total length of the configuration is 1.50 m. The flame holder is an equilateral triangle with an edge length of 0.04 m mounted $x = 0.82$ m downstream of the inlet. Three elements which were not clearly characterized in the experiments (fuel feeding line, honeycomb and exit section) are not considered in the computations but their modeling is addressed by their respective representation through the boundary condition specifications.[24]

Four cases are tested in the experiments: non-reacting, reacting stable, reacting low-frequency unstable (buzz) and reacting high-frequency unstable (screech). All simulation parameters discussed in this section are kept equal for the three different cases computed and which only address the reacting cases, Fig. 1(a). The operating condition is reported to be the primary parameter distinguishing the dynamics within the burner so they are at first to be adjusted: *i.e.* inflow mean equivalence ratio and bulk inflow velocity. Corresponding Schieleren photographs obtained from the experiment while operating at these three reacting points are pictured on Fig. 1(a). A fully compressible high-order code[32,33] is used for LES of these different conditions and which solves the reactive multi-species Navier-Stokes equations on unstructured grids. The two-step Taylor-Galerkin finite-element convection scheme[32] provides at least third-order accuracy in time and space. The Sigma model[34] is used to model the sub-grid stress tensor. The Dynamic Thickened Flame LES (DTFLES) model describes flame/turbulence interactions.[35–37]

Special attention is taken for inlet and outlet boundary conditions as they can control combustion instabilities: they are treated with Navier-Stokes Characteristic Boundary Conditions (NSCBC).[38] The outlet is modeled with the $3D$ NSCBC version derived by Granet et al.[39] and is assumed reflective: *i.e.* $p'\ approx 0$. The inlet is located at $x = 0$ in Fig. 1(b) and acts acoustically: *i.e.* $u' \approx 0$. Note that it is also used to inject turbulence using the method of Guezennec and Poinsot.[40] All walls are treated as no slip conditions and by default adiabatic unless specified otherwise. Note that bluff-body walls can be thermally adapted to evaluate their impact on the predictions. In this case, while side walls can be specified as convective loss conditions to reproduce the water cooling system, bluff-body walls can be specified as isothermal with a temperature value issued by the Conjugate Heat Transfert (CHT) solution of the LES/solid conduction problem.[41,42] Here, only convective loss conditions are used. Again for this first part where stability predictions of the burner are assessed by analyzing the limit-cycle reached by LES with fully adiabatic wall conditions.

The computational domain, Fig. 1(b), covers the entire axial and transverse extents of the experimental facility: *i.e.* from wall to wall in both transverse directions and from the reported honeycomb position to the exit section (sudden expansion of the chamber section into a tranquilization chamber that is not simulated here). As indicated, the mesh is fully unstructured with grid refinement in the bluff-body near wall region as well as in regions where combustion is expected to occur. It is composed of $3,685,066$ nodes and $20,919,678$ tetrahedral cells. For combustion, a reduced two-step scheme or an Analytically Reduced Chemistry (ARC) with 22 species for propane/air combustion designed for lean premixed combustion conditions[27] is used along with the DTFLES approach based on the Charlette efficiency function model[43] for turbulent combustion closure. As a result of the fixed grid resolution, the three reacting cases differing by their respective mean inflow equivalence ratios producing overall thickening factors of 15, for $\Phi = 0.65$ (stable case); 25, for $\Phi = 0.95$ (buzz mode) and 20, for $\Phi = 0.72$ (screech mode).

II.1. LES predictions of the thermo acoustic stable/unstable operation of the Volvo burner

Preliminary investigations of the LES capacity to reproduce large scale dynamics issued for the three different reacting operating conditions are first detailed.[24] Fixing the modeling and grid resolution, prior validation of the non-reacting flow predictions (not shown here) confirmed the adequacy of the strategy to retrieve most of the mean and dynamics features reported for this burner and in agreement with previous works.[24] With the same numerical setup, combustion is then activated using the DTFLES model and a two-step reduced model.[27] Note that activation of chemistry from the cold flow computation is obtained by replacing the cold flow behind the flame-holder with hot products of combustion at the adequate equivalence ratio. This generation of new initial conditions for each reacting case is obtained so as to preserve the local mass flux and pressure although composition, temperature and hence density are affected by this change. Naturally, adaptation of the flow to such changes is to be evacuated and only the resulting limit-cycle or statistically stationary reacting flows are studied in light of their thermo-acoustic content: *i.e.* are the three experimentally reported reacting modes of operation reproduced by the respective LES? For this exercise, boundary conditions correspond to: a fixed velocity at the inlet and a fixed pressure at the outlet.

Typical instantaneous views of the three resulting LES predictions are provided on Fig. 2. As expected

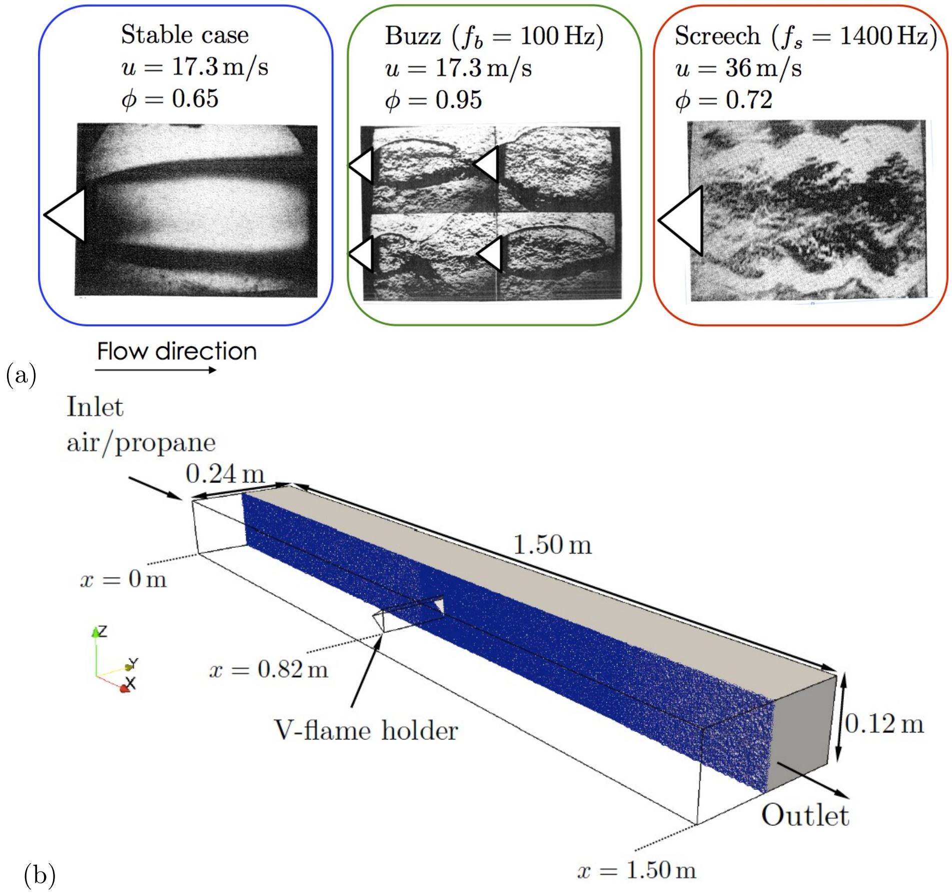

Figure 1: Volvo configuration: (a) experimental Schlieren photograph of the reacting cases and associated flow conditions complemented by (b) a view of the computational domain of the Volvo configuration retained for LES. Note that for visualization only half of the mesh is shown.

and in agreement with reported experimental observation, the dynamics of the bluff-body recirculation zone that is filled by hot products and resulting flames largely differ. The leaner case LES predictions, $\Phi = 0.65$ also referred here as the stable mode, Fig. 2(a), produces a rather quiet flame with weak perturbations of the velocity, pressure and flame front. The richer case, $\Phi = 0.95$ also referred as the buzz mode, on the other hand exhibits large levels of oscillations, Fig. 2(b), resulting in strong axial motions of the flame front that can even locate upstream of the flame holder. Finally, the intermediate case referred as the screech mode and obtained for $\Phi = 0.72$, Fig. 2(c), does exhibit strong pressure and flame oscillations. Spectral analyses of LES pressure signals recorded at the limit-cycles confirm the presence of acoustic oscillations at 95 Hz for the buzz mode and 1360 Hz for the screech mode respectively. These are to be compared to experimental findings reported at 100 and 1400 Hz respectively. Note finally that although the stable case is experimentally reported as having no thermo acoustic activity such a statement is to be pondered. Indeed, and contrarily to the other two reacting cases no clear or notable peak acoustic frequency arises for this operating point at least whenever faced with the natural turbulent background or flow activity of the simulation and at the locations probed. Such findings or comments do not disqualify totally the presence of acoustics which can readily imprint the flow either locally or globally. One can only infer that the sensitivity of the burner to many parameters including acoustics which can be amplified by combustion and thereby result in distinct limit-cycles as illustrated in this first and brief demonstration of LES capabilities.[24]

In addition to LES, acoustic studies using a TA solver with no flame coupling has been produced to understand the nature of the acoustic eigen modes (shape and frequency) of the system. To do so, the entire burner computational domain is retained along with the mean speed of sound given by LES and the

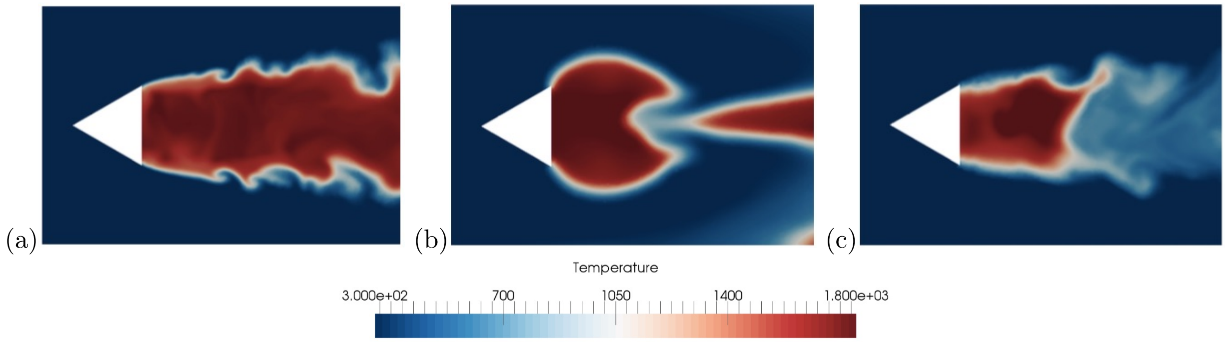

Figure 2: Instantaneous views of the temperature field produced by LES at the respective limit cycles of (a) the stable case ($\Phi = 0.65$), (b) the buzz mode ($\Phi = 0.95$) and (c) the screech mode ($\Phi = 0.72$).

Helmholtz equation[44–46] with $u' = 0$ at the inflow condition and $p' = 0$ as outlet condition is solved to look for potential acoustic modes of the burner. Modes of interest are provided on Fig. 3 in terms of acoustic pressure amplitude maps and structures as well as frequencies in Table. 1. Note that many other eigen modes are provided by the Hemholtz solver and only the modes with frequencies identified experimentally are discussed. Note also that mode structures are hereafter qualified by referring to the number of pressure nodes present and its directional composition in terms of dependency: *i.e.* $n\,L_x$ for the number of nodes in the longitudinal or axial direction, $p\,T_y$ for the spane-wise direction (main direction of the bluff-bod) and $q\,T_z$ for the cross-wise axis.

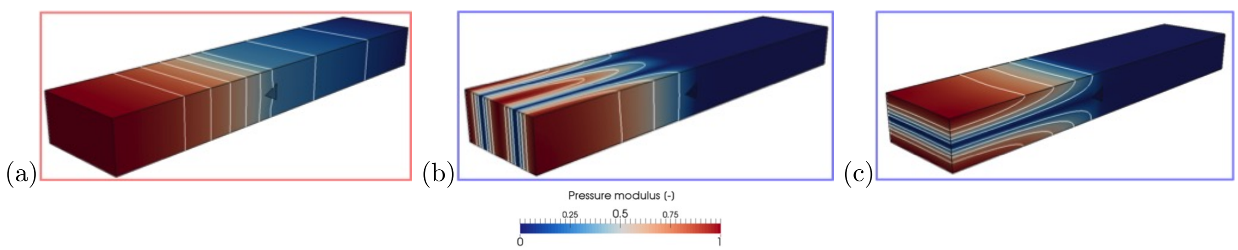

Figure 3: Spatial evolution of the pressure amplitude of the identified acoutic eigen modes of the burner: (a) purely longitudinal mode noted $(1\,L_x; 0\,T_y; 0\,T_z)$, (b) longitudinal and spane-wise mode noted $(1\,L_x; 2\,T_y; 0\,T_z)$ and (c) longitudinal and cross-wise mode noted $(1\,L_x; 0\,T_y; 1\,T_z)$. Details on the associated frequencies and denomination are provided in Table. 1.

Frequency [Hz]	$(n\,L_x; p\,T_y; q\,T_z)$	Figure
88	$(1\,L_x; 0\,T_y; 0\,T_z)$	Fig. 3(a)
1418	$(1\,L_x; 2\,T_y; 0\,T_z)$	Fig. 3(b)
1418	$(1\,L_x; 0\,T_y; 1\,T_z)$	Fig. 3(c)

Table 1: Acoustic eigen mode structures and frequencies provided by the TA solver and of potential interest to the understanding of the thermo acoustic stability of the Volvo burner. Note the coincidence of the second and third mode due to the fact that $L_y = 1/2\,L_z$ in the Volvo burner.

As indicated by these purely acoustic results, only three modes are potentially of interest at the experimentally reported frequencies of oscillation. These results show that most of the acoustic activity selected at the various limit-cycles focuses most of the pressure acoustic activity in the cold flow region of the burner: *i.e.* prior to the flame holder triangular body. The buzz mode involves a purely longitudinal acoustic activity, Fig. 3(a), mainly controlled by the burner inflow and outflow impedances. The screech mode on the other hand can result from a more complex pattern and may the consequence of the other two modes, Fig. 3(b)&(c), whose frequency is the same because of the geometrical symmetry and proportionality of the burner. In terms of effective content and mode selection, the screech mode at the limit-cycle, is found to resume to the $(1\,L_x; 2\,T_y; 0\,T_z)$ mode with at this stage a strong imprint on the mean flame shape and spatial dynamics[24] (at least based on the LES predictions).

II.2. LES mean predictions versus experimental data

Although the overall stability of the Volvo burner seems well captured by LES at least in terms of acoustic coupling and associated limit-cycles, more detailed investigations and qualifications are clearly needed. To evaluate these aspects and in light of the experimental data basis available, only the so called stable case is usually addressed in the literature. Note also that for this operating condition, although distinct sets of measurement campaigns exist, only the data from[?,17] are used here. Data from[47] could also be used since obtained at the same equivalence ratio but a lower Reynolds number and fresh gas temperature. In any case, it is important to underline that comparisons of the different data sets for this burner emphasize the fact that such configurations are experimentally sensitive. This is further confirmed by other group findings for similar flame holder configurations.[48] Variability is also clearly present in the accessible data and although such a configuration is qualified as stable, many complex processes are at play and compete in determining the statistically stationary state. For example, a small thermo acoustic mode will impact the level of RMS velocities in the mean flow results.

First, the LES axial evolution of the mean axial velocity component along the central burner axis starting at the backward facing step of the flame holder is presented on Fig. 4. Note that this axis is normalized with the bluff-body side length noted D. Overall, room for improvement is observed. Indeed, despite the fact that the backward bluff-body recirculation length is well predicted, its intensity (backward strength of the flow) is under-predicted. Likewise, the velocity constant acceleration as the exit is approached is under-estimated resulting in a mean axial velocity component that is slightly too slow. Such a finding is an indirect indication that along the axial distance the combustion is burning a little bit too slow resulting in a reduced expansion rate of the hot gases and thereby a slower velocity field.

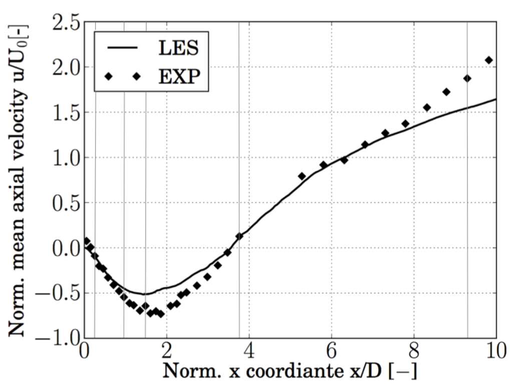

Figure 4: Mean axial velocity evolution along the central axis of the Volvo burner as measured experimentally and obtained by LES for the stable condition. The axis starts after the bluff-body vertical wall and oriented in the direction of the burner exit. Marked vertical lines indicate the location at which transverse profiles are taken in the experiment.

Cross stream profiles extracted in the experiment and LES at $x/D = 0.375, 0.95, 1.525, 3.75, 9.325$ are provided as complementary diagnostics on Fig. 5 not only for the mean axial and cross stream velocity components, Figs. 5(a)&(b), but also for their corresponding fluctuating contributions, Figs. 5(c)&(d), respectively. The data is taken along the cross stream direction at the axial locations indicated by the light grey lines on Fig. 4 and in the central vertical plane of the burner. Again, overall agreement is found between LES and experiment for these quantities at this operating condition. A deficit in the transverse activity as well as the axial activity is observed through the fluctuating component profiles. The deficit of mean axial velocity is also confirmed by Fig. 5(a) in agreement with the previous observation.

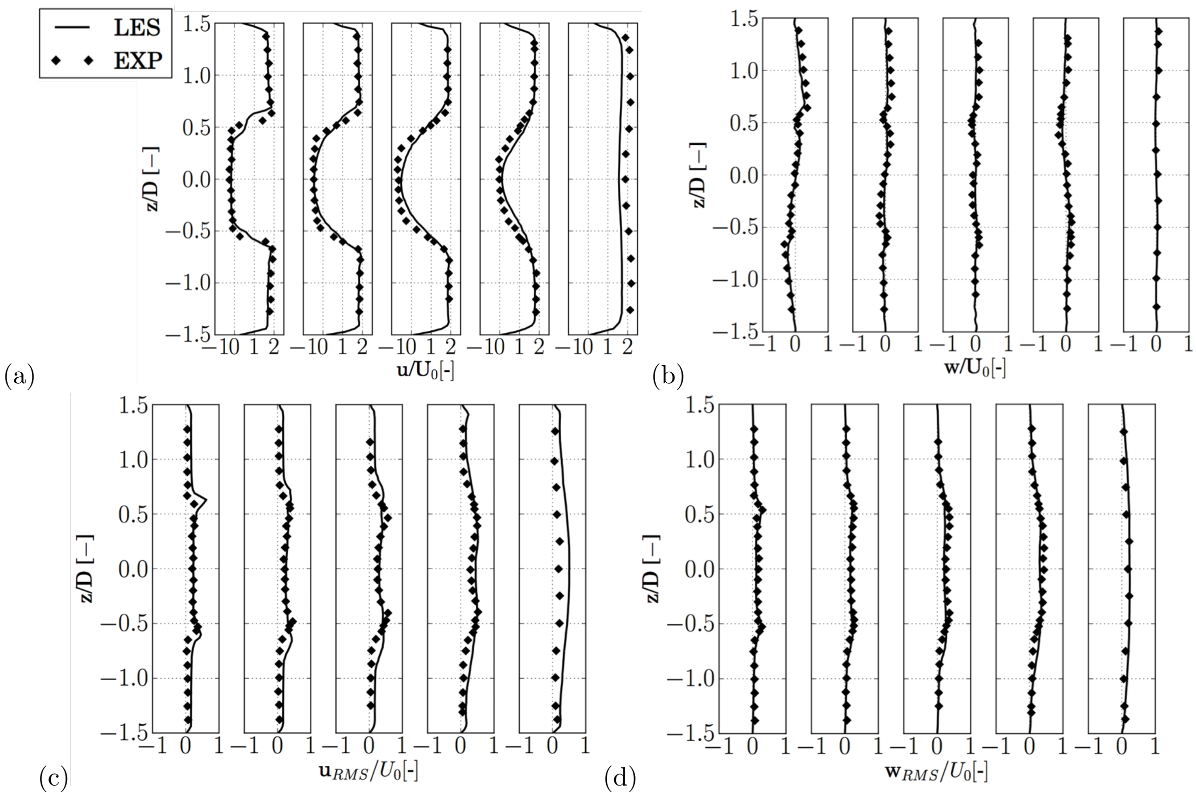

Figure 5: Transverse profiles of the mean velocity, (a) & (b), and fluctations, (c) & (d), at the axial positions indicated on Fig. 4 by the vertical lines.

To conclude on this preliminary discussion, although LES does not fully agree with available experimental data for the stable case, activity and stability of the Volvo burner seems to be satisfactorily captured by the methodology. Issues pertaining to the modeling and capabilities of the proposed modeling remain and it is of interest to assess the method in terms of sensitivity. This specific discussion is the topic of the coming sections (§III.1-§**??**) where different aspects of the observed physics described above are further investigated in the context of a broader modeling context. sec:

III. LES sensitivity analysis: Volvo modeling and associated difficulties

Analyses of the previous set of results highlight several fundamental observations which may be at the source of inaccuracies or uncertainties present in the LES problem definition. As detailed hereafter, some of these uncertainties may hinder from properly recovering the stable operating case of the Volvo burner.

- First, acoustics is ralways present in this simple burner: although the experimentally obtained data is qualified as being for a stable operating point, acoustics remains present and can imprint on the dynamics of the flame. The unknown is that for this operating point, no clear link is evidenced on the effective importance of the underlying acoustic mode strengthes and shapes compared to the flow large scale features. The only guaranty today is that identified acoustic modes (*cf.* §II.1, Fig. 3 & Table. 1) from the two thermo acoustic unstable conditions are likely to be selected and preferably amplified under these two conditions. Naturally it is reasonable to consider their presence in the stable case but with much weaker amplitudes.

- Second, preliminary assessment of the adopted LES modeling strategy points to under-estimations of the local heat release rate or burnt gas temperature. Many contributions of the modeling can be at the source of this observation and should therefore be addressed.

Different modeling features can address the above mentioned shortcomings. Among others, grid resolution or numerical scheme effects are usual LES work-horses that are known to control the expected flow dynamics. To go further and address the two points listed above, new LES have been initiated without changing the numerics or grid, keeping in mind the following observations. If acoustics is present, any incompressible CFD solver is naturally to be avoided. Likewise, domain size reduction on the basis of *a priori* hypotheses on the symmetries of the solution are dangerous as they can interfere with eigen mode selection as well as potential coupling with flame and hydrodynamics. Transverse dimensions of the Volvo burner are therefore retained. Inflow and outflow acoustic boundary conditions in that respect are under question and should be validated or at least gauged in terms of impact on the quantities and dynamics of the flow. As underlined above, under-predicted mean axial velocity components may be explained by the combustion modeling. Within the context of DTFLES, two sources or uncertainties are present: (1) the two-step chemistry model that has inherent limitations in terms of adiabatic flame temperature, laminar flame speed, near wall chemistry (although limited in the context of lean flames) and (2) the efficiency function that requires a model coefficient only valid in specific and ideal conditions.[43] Note that such combustion modeling difficulties can have indirect effects on the acoustic response of the system. At the exit of the burner for example where hot and unburnt gases are present and combustion proceeds, noise is generated and can participate in the system acoustic mode selection. Finally, if temperature levels are not adequate, issues pertaining to heat transfer to the solid bluff-body or side walls of the burner through conduction and radiation are also valid aspects of the problem definition. To evaluate both identified aspects, new simulations have been conducted for the stable operating condition.

III.1. Influence of acoustic boundary conditions

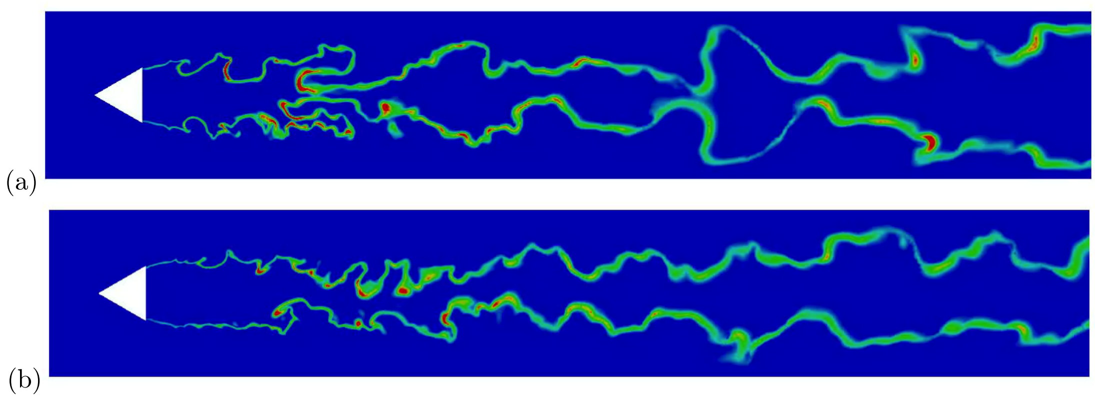

Figure 6: Instantaneous views of heat realease rate issued by the (a) *reflective* and (b) *anechoic* LES.

The issue of the inflow and outflow acoustic boundary conditions and their impact on the flow response is first addressed. To do so, the previous setup is retained to the exception of the boundary conditions which are switched to partially non-reflective conditions. Note that initially, the NSCBC boundary conditions are applied so that (1) at the exit, $p' = 0$, as equivalent to an axial pressure node considered as a good approximation of a sudden pipe expansion into a tranquilizing constant pressure chamber and (2) at the inlet, $u' = 0$, since the honeycomb essentially maintains a constant mean turbulent velocity flow. Through such changes, the burner goes from a acoustically closed system or *reflective* to an acoustically open system or *anechoic*. The main consequence of this change is illustrated on Fig. 6, where heat release rate contours in the axial mid plane of the rear part of the burner are provided for (a) the *reflective* simulation and (b) the *anechoic* prediction. Although in-depth diagnostics are missing, first direct comparaisons based on instantaneous snapshots indicate an overall different flame dynamics. In the case of a *reflective* system, Fig. 6(a), the flame shape in the mid axial plane takes on a quasi symmetric shape with a marked envelope whose axial size is of the oder of the axial length of the recirculation bubble positioned behind the bluff-body and evaluated at

$L_x/D \approx 3.5$ (Fig. 4) (to be compared to the experimental value of 3.55). Note that these structures seem to be born on the recirculation bubble outer edges and induce a transition zone in the flow recovery region at the end of the recirculation bubble that remains symmetric in mean and mark the flame shape throughout the remaining extent of the combustor. For the *anechoic* system, the pattern is much less pronounced and is partly antisymmetric near and prior to the recovery zone before recovering a more symmetric pattern.

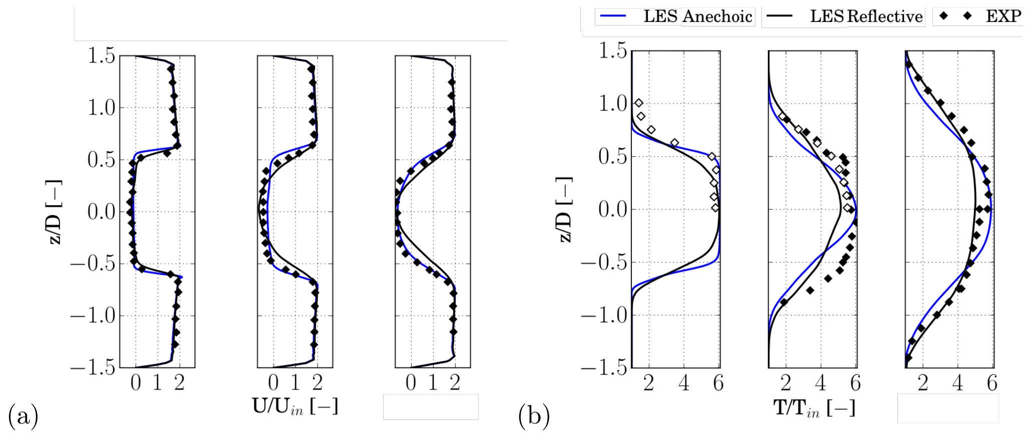

Figure 7: Mean (a) axial velocity and (b) temperature profiles across the recirculation bubble and issued by changes of acoustic boundary conditions of the Volvo burner. Profiles are here given for the first three axial locations in the mid plane of the combustor.

Figure 7 presents the comparison between the two LES transverse profiles of the axial mean velocity component and mean temperature for the first three axial positions reported on Fig. 4 that are crossing the bluff-body recirculation bubble. Both fields are affected by the change in dynamics observed previously. Conclusions are however uncertain because the acoustic characterization of the burner being difficult to obtain in the real experiment where impedances were not measured. The impact on the turbulent fields also indicate a potential degradation if non reflective conditions are used (not shown and to be confirmed at this stage). Note also that all computations have been reconducted and convergence issues may arise and partly explain differences observed between profiles of Fig. 5 &. 7.

III.2. Influence of the turbulent combustion model

The use of a reduced chemical scheme in conjunction with DTFLES is now investigated in more details. First and just like any turbulent combustion model, closure coefficients are present. In the preliminary set of results, the Charlette's efficiency function is used[43] and its unique closure coefficient is et equal to 0.55 from asymptotic developments. Changing this closure value will affect the turbulent flame speed issued by the model. To effectively quantify its effect on the predictions, the original value of 0.55 is artificially changed to 0.5 retaining the *reflective* boundary conditions. Overall behavior is again observed to affect the prediction as confirmed by Fig. 7 where mean transversal profiles of the mean axial velocity component and temperature as in Fig. 8 are shown. Although effects are present, they are at this stage not fully conclusive or at least less important than the observed boundary condition effects.

III.3. Influence of flame holder temperature

The next step relates to the thermal equilibrium of the system. In this context, it is now recognized that bluff-body flame stabilization is a fundamental problem still not fully mastered which involves strong coupling between various physics around the flame foot position. Indeed, flame stabilization is the result of the heat conducted to the solid, the heat stored in the recirculation zone and the capacity of the mixture to sustain combustion in the associated aerodynamic field. For the Volvo burner, flame stabilisation can hence be critical

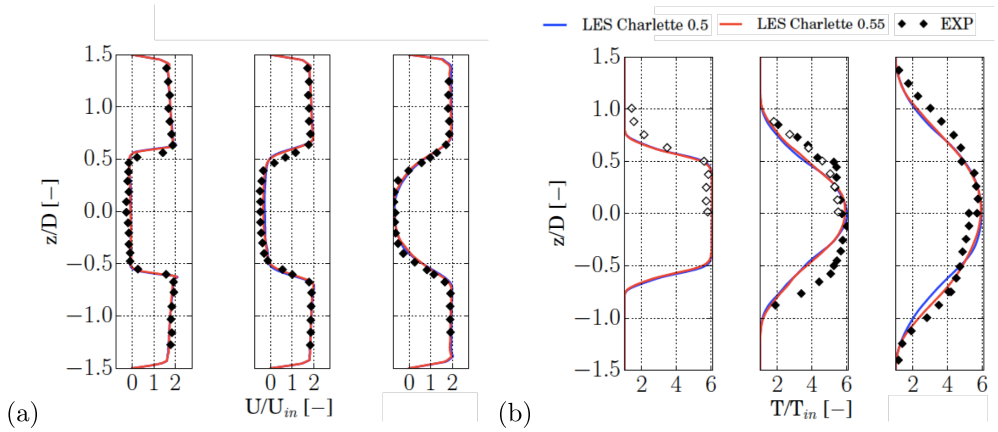

Figure 8: Effect of the efficiency function model value on: (a) the mean axial velocity transversal profile in the mid plane of the burner and at the first three axial locations in the recirculation zone with (b) the corresponding mean temperature profiles.

as it can dictate the dynamics of the resulting flame and its response to perturbations (either acoustics or aerodynamics). To evaluate the sensitivity to the solid thermal state, a new LES is produced switching the initially adiabatic wall condition of the bluff-body to a loss condition using the thermal resistivity of the solid body and the fresh gas temperature as reference. As illustrated on Fig. 9(a)&(b) for the adiabatic and loss wall conditions respectively, the recirculation bubble shape and mean temperature is affected, a clear indication that this region and the flame position is a sensitive matter that can help improving the quality of the predictions.

III.4. Influence of the chemical scheme

Whenever faced with a turbulent reacting flame and the thermal state of such a system, flame chemistry can rapidly become an issue as demonstrated in the problem of a bluff-body stabilized flame by.[49,50] Although the modeling strategy proposed has been tailored for lean premixed combustion and has shown multiple successes, more advanced chemistry schemes are still needed to alleviate inherent limitations of reduced schemes. Today such options are readily maturing and Algebraically Reduced Chemistry (ARC) tools can produce tractable chemical schemes that LES can fully resolve.[29–31] An example of such an approach is given on Fig. 10(a) and compared to the reference two-step reduced scheme on Fig. 4(b). For information, the used propane/air ARC scheme treats 22 species and associated reactions among which 12 are obtained from a Quasi-Steady State (QSS) method. Note that both schemes ensure the same laminar flame speed at $\Phi = 0.65$: *i.e.* 0.16 m/s. Aside from the feasibility of such LES, again this specific part of the modeling for the Volvo burner is seen to affect the prediction. Similarly to previous findings, the bluff-body mean recirculation zone is the primary marker of the changes, Fig. 10. With the ARC scheme, Fig. 10(b)&(d), it gets shorter and is filled with hotter gases when compared to results obtained with the reduced two-step scheme, Fig. 10(a)&(c). The main consequence of such differences is a stronger recirculating flow within the bubble and a stronger acceleration of the flow in the recovery region, Fig. 11.

Note that at this stage, although these tests are encouraging in terms of impact and understanding of the required modeling capacities a LES approach should provide, care is still required. Indirect consequences issued by the change of models or boundary conditions are present. For example, thickening issued by DTFLES will differ simply due to the fact that the flames do not fully locate at the same positions and because the mesh is unstructured and with variable cell edge length depending on where it stands in the fluid. Mesh resolution is hence again to be considered. Indication for improvements are however evidenced here at least for the stable conditions of the Volvo burner.

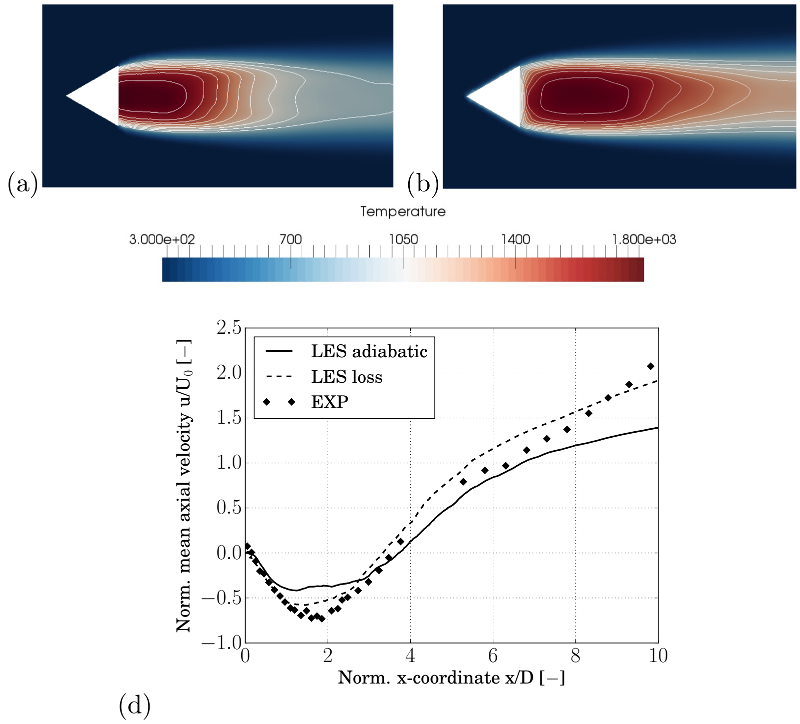

Figure 9: bluff-body thermal effect on the mean recirculation zone temperature: (a) for an adiabatic solid wall and (b) for a heat conductive solid (same views as in Fig. 7). The evolution of the two mean axial velocity profiles along the centerline of the burner starting at the backward face of the bluff-body are provided in (c).

IV. Conclusion

Large Eddy Simulations have at multiple occasions demonstrated their capacity in addressing the problem of thermo acoustic instabilities. In the case of the Volvo burner, where the geometry is simple but not necessarily easier, LES can distinguish between different operating modes of the burner:[24] *i.e.* no thermo acoustic oscillation for lean conditions, longitudinal thermo acoustic activity (buzz) for richer conditions and transverse thermo acoustic activity (screech) for intermediate conditions. Such a rich range of operation is typical of this bluff-body stabilized straight duct burner and although LES captures limit-cycles with the correct acoustic activity in terms of frequency, it is found not to fully recover experimental data at the nominal condition (where no thermo acoustic instability is reported) and room for improvement appears just as found by other researchers. Although many studies have indicated and confirmed that LES is grid and scheme dependent, the adopted analysis focuses here on the actual definition of the problem and its potential impact on the prediction. In that respect, it is clearly demonstrated that acoustic boundary conditions to be prescribed to a fully compressible LES will impact the dynamics of the system even in the so-called thermo acoustically stable case. Turbulent combustion models, which are usually the main difference between the research groups involved in such studies along with the numerics used, is found here to play a minor role at least in the context of the DTFLES approach. Contrarily, bluff-body thermal conditions seem to be of importance at least as much as the chemical scheme to be used in this application. Note that at this occasion, the capability of resolving ARC schemes is demonstrated for the Volvo burner. The various sensitivities identified resume in a problem definition which differs from the more conventional arguments present in the LES community which tend to first incriminate turbulent combustion issues or code capacities. Although these sensitivities do not rule out these facts, they are observed to impact the Volvo burner near bluff-body flow organisation and flame dynamics. Chemistry and solid thermal state indeed are seen to affect results in the same proportions, similarly to the acoustic boundary conditions. As such, perspectives are therefore to keep pursuing the analysis minimizing as much as possible the effect inherent to the problem definition: *i.e.*

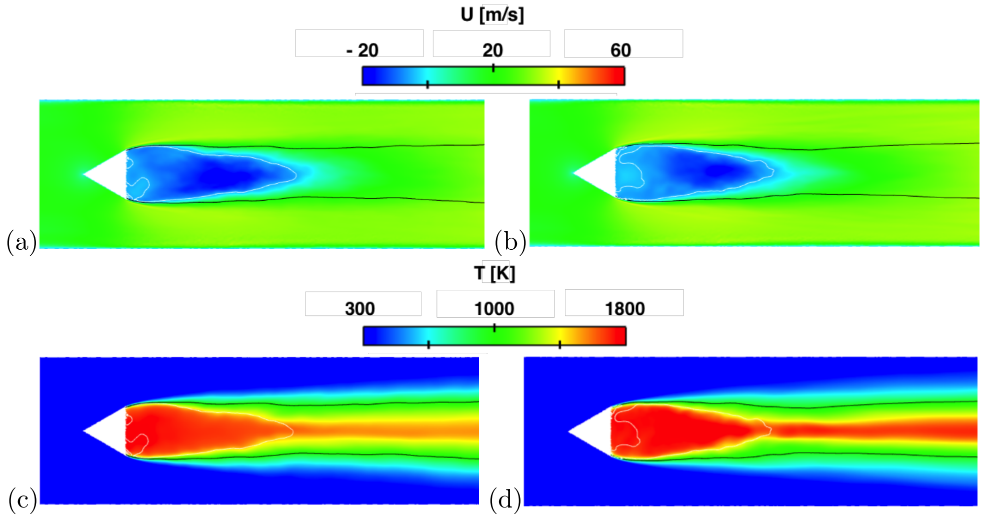

Figure 10: Mean flow comparisons in the mid transerval plane of the burner and restricted to the bluff-body recirculation zone: (a) & (b) are the mean axial velocity distributions obtained by use of a 2 step chemistry or a ARC model respectively, while (c) & (d) are the associated mean temperature distributions.

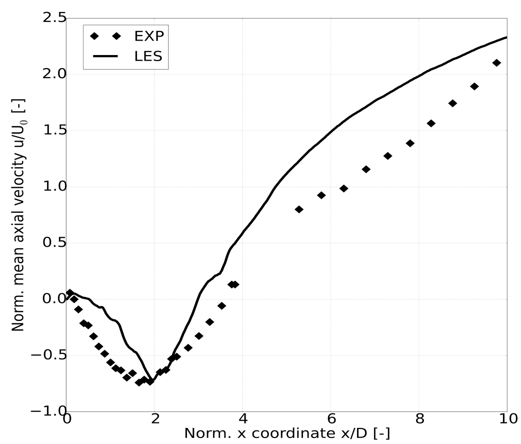

Figure 11: Mean axial velocity profile issued by LES using an ARC propoane/air chemical scheme and along the centerline of the burner starting behind the bluff-body backward facing face.

chemistry and thermal condition of the system. A difficulty will however remain: *i.e.* the inflow/outflow acoustic boundary conditions which are not known. However, it seems that only in such conditions can turbulent modeling or numerics be adequately assessed in the context of the stable operating point of the Volvo application.

References

[1]Culick, F. and Kuentzmann, P., *Unsteady Motions in Combustion Chambers for Propulsion Systems*, NATO Research and Technology Organization, 2006.

[2]Gicquel, L. Y. M., Staffelbach, G., and Poinsot, T., "Large Eddy Simulations of gaseous flames in gas turbine combustion chambers," *Prog. Energy Comb. Sci.* , Vol. 38, No. 6, 2012, pp. 782 – 817.

[3]Crighton, D. G., Dowling, A. P., Williams, J. E. F., Heckl, M., and Leppington, F., *Modern methods in analytical acoustics*, Lecture Notes, Springer Verlag, New-York, 1992.

[4]Lieuwen, T. and Yang, V., *Combustion Instabilities in Gas Turbine Engines. Operational Experience, Fundamental Mechanisms and Modeling*, Prog. in Astronautics and Aeronautics AIAA Vol 210, 2005.

[5]Poinsot, T., "Prediction and control of combustion instabilities in real engines," *Proceedings of the Combustion Institute*, Vol. 36, 2016.

[6]Fleifil, M., Annaswamy, A. M., Ghoneim, Z. A., and Ghoniem, A. F., "Response of a laminar premixed flame to flow oscillations: A kinematic model and thermoacoustic instability results," *Combust. Flame* , Vol. 106, No. 4, 1996, pp. 487–510.

[7]Ducruix, S., Durox, D., and Candel, S., "Theoretical and experimental determinations of the transfer function of a laminar premixed flame," *Proceedings of the Combustion Institute*, Vol. 28, No. 1, 2000, pp. 765–773.

[8]Krebs, W., Flohr, P., Prade, B., and Hoffmann, S., "Thermoacoustic stability chart for high intense gas turbine combustion systems," *Combust. Sci. Tech.* , Vol. 174, 2002, pp. 99–128.

[9]Schildmacher, K.-U., Hoffman, A., Selle, L., Koch, R., Schulz, C., Bauer, H.-J., and Poinsot, T., "Unsteady Flame and Flow Field Interaction of a Premixed Model Gas Turbine Burner," *Proc. Combust. Inst.* , Vol. 31, 2007, pp. 3197–3205.

[10]Schuller, T., Durox, D., Palies, P., and Candel, S., "Acoustic decoupling of longitudinal modes in generic combustion systems," *Combustion and Flame*, Vol. 159, 2012, pp. 1921–1931.

[11]Poinsot, T. and Candel, S., "Nonlinear studies of low-frequency combustion instabilities," *Mathematic modeling in combustion and related topics*, edited by Nijhoff, Vol. 140, NATO ASI Series, Dordrecht, 1987, pp. 185–215.

[12]Bauerheim, M., Nicoud, F., and Poinsot, T., "Progress in analytical methods to predict and control azimuthal combustion instability modes in annular chambers," *Physics of Fluids*, Vol. 28, No. 2, 2016, pp. 21303.

[13]Mery, Y., Ducruix, S., Scouflaire, P., and Candel, S., "Injection coupling with high amplitude transverse modes: Experimentation and simulation," *Comptes Rendus Mécanique*, Vol. 337, No. 6, 2009, pp. 426–437.

[14]Méry, Y., Hakim, L., Scouflaire, P., Vingert, L., Ducruix, S., and Candel, S., "Experimental investigation of cryogenic flame dynamics under transverse acoustic modulations," *Comptes Rendus Mécanique*, Vol. 341, No. 1, 2013, pp. 100–109.

[15]Baillot, F. and Lespinasse, F., "Response of a laminar premixed V-flame to a high-frequency transverse acoustic field," *Combust. Flame* , Vol. 161, No. 5, May 2014, pp. 1247–1267.

[16]Sjunnesson, A., Nelsson, C., and Max, E., "LDA measurements of velocitites and turbulence in a bluff body stabilized flame," *Fourth International Conference on Laser Anemometry - Adavnces and Application*, edited by ASME, Vol. 3, Cleveland, 1991, pp. pp. 83–90.

[17]Sjunnesson, A., Henrikson, P., and Lofstrom, C., "CARS measurements and visualization of reacting flows in a bluff body stabilized flame," *28th Joint Propulsion Conference and Exhibit*, No. AIAA 92-3650, Nashville, TN, 1992.

[18]Cocks, P., Sankaran, V., and Soteriou, M., *51st AIAA Aerospace Sciences Meeting*, edited by AIAA, No. 2013-0170, 2013, pp. 1–29.

[19]Fureby, C., *Proceedings of the Combustion Institute*, Vol. 28(1), 2000, pp. 783–791.

[20]Giacomazzi, E. and Battaglia, V. abd Bruno, C., *Combustion and Flame*, Vol. 138, No. 4, 2004, pp. 320–335.

[21]Erickson, E. and Soteriou, M., *Combustion and Flame*, Vol. 158, No. 12, 2011, pp. 2441–2457.

[22]Jourdain, J. and Eriksson, L.-E., *18th AIAA/CEAS Aeroacoustics Conference (33rd AIAA Aeroacoustics Conference)*, edited by AIAA, No. 2012-2147, 2012, pp. 1–11.

[23]Jourdain, J. and Eriksson, L.-E., *ASME Turbo Expo 2010* , AMSE, 2010, pp. 269–278.

[24]Ghani, A., Poinsot, T., Gicquel, L., and Staffelbach, G., "LES of longitudinal and transverse self-excited combustion instabilities in a bluff-body stabilized turbulent premixed flame," *Combust. Flame* , Vol. 162, No. 11, November 2015, pp. 4075–4083.

[25]Rogers, D. E. and Marble, F. E., "A mechanism for high frequency oscillations in ramjet combustors and afterburners," *Jet Propulsion*, Vol. 26, 1956, pp. 456–462.

[26]Culick, F., "Combustion instabilities in liquid-fueled propulsion systems- An overview," *AGARD 72B PEP meeting*, 1988.

[27]Franzelli, B., Riber, E., Sanjosé, M., and Poinsot, T., "A two-step chemical scheme for Large-Eddy Simulation of kerosene-air flames," *Combust. Flame* , Vol. 157, No. 7, 2010, pp. 1364–1373.

[28]Roux, A., Reichstadt, S., Bertier, N., Gicquel, L. Y. M., Vuillot, F., and Poinsot, T., "Comparison of numerical methods and combustion models for LES of a ramjet," *C. R. Acad. Sci. Mécanique*, Vol. 337, No. 6-7, 2009, pp. 352–361.

[29]Jaravel, T., Riber, E., Cuenot, B., and Bulat, G., "Large Eddy Simulation of a model gas turbine burner using reduced chemistry with accurate pollutant prediction," *Proceedings of the Combustion Institute*, Vol. 36, 2016.

[30]Schulz, O., Jaravel, T., Poinsot, T., Cuenot, B., and Noiray, N., "A criterion to distinguish autoignition and propagation applied to a lifted methane-air jet flame," *Proceedings of the Combustion Institute*, Vol. 36, 2016.

[31]Felden, A., Riber, E., and Cuenot, B., "Effect of the chemistry description on LES of a realistic swirled non-premixed combustor," *Proceedings of the Combustion Institute*, Vol. 36, 2016.

[32]Colin, O. and Rudgyard, M., "Development of high-order Taylor-Galerkin schemes for unsteady calculations," *J. Comput. Phys.* , Vol. 162, No. 2, 2000, pp. 338–371.

[33]Schønfeld, T. and Poinsot, T., "Influence of boundary conditions in LES of premixed combustion instabilities," *Annual Research Briefs* , Center for Turbulence Research, NASA Ames/Stanford Univ., 1999, pp. 73–84.

[34]Nicoud, F., Baya Toda, H., Cabrit, O., Bose, S., and Lee, J., "Using singular values to build a subgrid-scale model for large eddy simulations," *Phys. Fluids* , Vol. 23, No. 8, 2011, pp. 085106.

[35]Schmitt, P., Poinsot, T., Schuermans, B., and Geigle, K. P., "Large-eddy simulation and experimental study of heat transfer, nitric oxide emissions and combustion instability in a swirled turbulent high-pressure burner," *J. Fluid Mech.* , Vol. 570, 2007, pp. 17–46.

[36]Colin, O., *Simulations aux grandes échelles de la combustion turbulente prémélangée dans les statoréacteurs*, Phd thesis, INP Toulouse, 2000.

[37]Sengissen, A., Giauque, A., Staffelbach, G., Porta, M., Krebs, W., Kaufmann, P., and Poinsot, T., "Large Eddy Simulation of piloting effects on turbulent swirling flames," *Proc. Combust. Inst.* , Vol. 31, 2007, pp. 1729–1736.

[38]Poinsot, T. and Lele, S., "Boundary conditions for direct simulations of compressible viscous flows," *J. Comput. Phys.* , Vol. 101, No. 1, 1992, pp. 104–129.

[39]Granet, V., Vermorel, O., Leonard, T., Gicquel, L., , and Poinsot, T., "Comparison of Nonreflecting Outlet Boundary Conditions for Compressible Solvers on Unstructured Grids," *AIAA Journal* , Vol. 48, No. 10, 2010, pp. 2348–2364.

[40]Guezennec, N. and Poinsot, T., "Acoustically nonreflecting and reflecting boundary conditions for vorticity injection in compressible solvers," *AIAA Journal* , Vol. 47, 2009, pp. 1709–1722.

[41]Duchaine, F., Mendez, S., Nicoud, F., Corpron, A., Moureau, V., and Poinsot, T., "Conjugate heat transfer with Large Eddy Simulation application to gas turbine components," *C. R. Acad. Sci. Mécanique*, Vol. 337, No. 6-7, 2009, pp. 550–561.

[42]Jauré, S., Duchaine, F., and Gicquel, L., "Comparisons of Coupling Strategies for Massively Parallel Conjugate Heat Transfer with Large Eddy Simulation," *In IV International Conference on Computational Methods for Coupled Problems in Science and Engineering*, Kos Island, Greece, 2011.

[43]Charlette, F., Veynante, D., and Meneveau, C., "A power-law wrinkling model for LES of premixed turbulent combustion: Part I - non-dynamic formulation and initial tests," *Combust. Flame* , Vol. 131, 2002, pp. 159–180.

[44]Benoit, L. and Nicoud, F., "Numerical assessment of thermo-acoustic instabilities in gas turbines," *Int. J. Numer. Meth. Fluids* , Vol. 47, No. 8-9, 2005, pp. 849–855.

[45]Martin, C., Benoit, L., Sommerer, Y., Nicoud, F., and Poinsot, T., "LES and acoustic analysis of combustion instability in a staged turbulent swirled combustor," *AIAA Journal* , Vol. 44, No. 4, 2006, pp. 741–750.

[46]Sensiau, C., Nicoud, F., and Poinsot, T., "A tool to study azimuthal and spinning modes in annular combustors," *Int. Journal Aeroacoustics*, Vol. 8, No. 1, 2009, pp. 57–68.

[47]Sanquer, S., Bruel, P., and Deshaies, B., "Some specific characteristics of turbulence in the reactive wakes of bluff bodies," *AIAA journal*, Vol. 36, No. 6, 1998.

[48]Veynante, D. and Knikker, R., "Comparison between LES results and experimental data in reacting flows," *J. Turb.* , Vol. 7, No. 35, 2006, pp. 1–20.

[49]Kedia, K., Altay, H., and Ghoniem, A., "Impact of flame-wall interaction on premixed flame dynamics and transfer function characteristics," *Proc. Combust. Inst.* , Vol. 33, 2011, pp. 1113–1120.

[50]Kedia, K. S. and Ghoniem, A. F., "The blow-off mechanism of a bluff-body stabilized laminar premixed flame," *Combust. Flame* , Vol. 162, No. 4, April 2015, pp. 1304–1315.