Chapter 5

LES of multi-burner chambers

This chapter addresses a question which is often ignored when studying gas turbine combustion: the interaction between the multiple burners installed in a chamber. These mechanisms are known to be important especially in annular combustion chambers where burners are very close to each other [96]. Acoustics experts also present results where burner/burner interaction can lead to instabilities. This has been clearly identified in rocket engines for example where installing plates between burners or injectors can reduce the level of oscillation. In an engine like Vulcain, the interaction between flames issued from the multiple injectors is a well identified source of instabilities [86, 87].

Even though all experts recognize the importance of burner/burner interaction, the cost of operating a chamber with all its burners in a laboratory is usually so high that single-burner experiments are chosen despite their obvious limitations. Here, the EU project DESIRE (Design and Demonstration of Highly Reliable Low NOx Combustion Systems for Gas Turbines n° NNE5/388/2001) brought the opportunity of studying a triple-burner set-up and comparing it to a single-burner set-up. This original work plan was proposed by SIEMENS PG who built the triple-burner devise with DLR (Deutsches Zentrum für Luft-und Raumfahrt).

In this chapter, LES of the single and triple-burner set-ups were performed and are described below. The chapter begins with a description of the DESIRE project (section 5.1) and of the work package WP3, dedicated to the triple-burner (section 5.2). Results are given in section 5.3 which compares mean and unsteady flows in both set-ups. For these test cases, the single-burner flow is systematically compared to the central burner of the triple set-up in terms of mean and RMS quantities. The objective is to check whether the LES performed on a single-burner differs or not from the LES performed on a burner surrounded by other burners. Section 5.6 presents an acoustic study of the single-burner and triple-burner geometries used for the LES and finally (section 5.7) the flame responses for the single and triple-burner are compared.
CHAPTER 5. LES OF MULTI-BURNER CHAMBERS

5.1 Context: the EU projet DESIRE

The following studies were conducted under the european projet DESIRE. The partners include the University of Twente (Netherlands), Siemens PG (Mülheim an der Rhur, Germany), CIMNE (Barcelona, Spain), E-on (United Kingdom), KEMA (Netherlands) and DLR (Germany). The objectives of the projet are:

- Reduction of $NO_x$ emissions from 25 ppm to levels below 15 ppm in premixed operation (No secondary emissions reduction means).
- Increase gas turbine reliability to values above 97%.
- Support efforts to increase efficiency from 55% to levels above 59%.
- Improve online monitoring to help power producers foresee and prevent any possible damaging behaviour for the turbine.

With this in mind, different studies were conducted or are ongoing. An important part of the project focused on fluid/structure interaction (Work Package 1), technical solutions for gas turbine application were developed in Work Packages 2 and 3 and applied to an industrial set-up in Work Package 4. CERFACS’s contribution to the project is part of Work Packages 1 (WP1) and 3 (WP3). This document will only deal with WP3, WP1 is the object of the Phd Thesis by Alois Sengissen [103].

5.2 Study of multi-burner combustors: WP3

In DESIRE, the objective of WP3 was to study a three burner test rig (built by DLR and Siemens PG) corresponding to $1/8^{th}$ of an annular combustor (see Fig. 5.1) and evaluate the correlation between its behavior and the real machine. Usually, experimental and numerical studies are performed on new designs to assess the potential issues that might arise during operation. However, because of the costs involved, it is unpractical to build a full engine for the tests. These tests are then often conducted on reduced geometries. Usually, a single-burner rig would be used for the tests and its behavior extrapolated to the turbine. This test-rig unfortunately does not have the same properties as the real set-up. Burner/burner interaction is totally neglected and the acoustic properties of the single-burner are different from the ones of the full set-up. Provided the data is available, it is possible to have the correct impedances at the inlet and outlet of the burner but the acoustic behaviour of the single-burner in the azimuthal direction is totally different.
This project presented the unique opportunity to evaluate the impact of the extrapolation from the behaviour of a single-burner to a multi-burner. Indeed, the same hypothesis inferred by the study of one burner to characterize a gas turbine can be applied to any multi-burner problem. Therefore it was decided to perform LES of a single periodic burner and of the triple-burner rig to compare the behaviour of both set-ups and check whether it is really worth performing tests on a three burner case or if the single-burner would yield the same results.

It is clear that a three burner rig behaviour might not (and probably does not) correspond to the full burner (which has an annular periodicity). However it is the smallest configuration that takes into account burner/burner interaction as well as the azimuthal component lacking in a single-burner test rig. Note that the procedure applied to experiments is also applied to numerical simulation. To reduce computational power, simulations are performed using reduced geometries taking advantage of periodicities of the design. Here the full three-burner case was simulated making it one of the largest full reacting LES performed on realistic industrial geometries.

Figure 5.1 shows a global view of the full combustor (24 burners) while Fig. 5.1 shows a 3D view of the triple-burner installed on the experimental bench at DLR.
Burner characteristics

In the triple set-up like in the real machine all burners are identical. They are composed of co-axial co-rotating swirlers (see Fig. 5.3). The outer swirler is called *premix passage* and the inner swirler *pilot passage*. The premix passage swirler contains 24 vanes. Methane is injected through small holes on each vane, ensuring efficient mixing [93]. The pilot passage swirler contains 8 vanes. Upstream from the vanes, methane is injected through 4 tubes (see Fig. 5.3b). Note that some confidentiality concerns.

Since acoustics and flame response to perturbations are of great interest in a real turbine, an acoustic study (section 5.6) as well as forced LES cases (section 5.7) are considered.
5.3 Geometry, regimes and Boundary conditions

Figure 5.4 shows the computational domain for the single-burner configuration. The geometry of the single-burner is the same as the one used in chapter 4. Neither the axial nor the diagonal swirler are included in the computational domain. The computational domain starts right at the end of the swirler vanes for each passage. The tip of the burner inside the chamber is called Cylindrical Burner Outlet (CBO) (see Fig. 5.3b). To account for the vanes impact on the flow, proper velocity and mass fraction profiles were used as boundary conditions. The diagonal swirler is considered perfectly premixed \([100]\) whereas for the axial swirler has a non uniform species distribution (see Fig. 4.4b) already discussed in chapter 4.

<table>
<thead>
<tr>
<th>Table 5.1: LES runs designation: each run is characterized by the size of the domain, the regime and the type of BC applied in the azimuthal direction. For the single-burner, lateral boundaries can be either slip-walls (LES-SB-CI) or periodic boundaries (LES-SB-CII).</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cold flow LES</strong></td>
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<tr>
<td>Wall law BC</td>
</tr>
<tr>
<td>Single-burner</td>
</tr>
<tr>
<td>Triple-burner</td>
</tr>
</tbody>
</table>
These inlet boundary conditions are also used for the triple-burner set-up. To reduce the number of parameters in the simulations, the single-burner mesh was duplicated and concatenated to create the triple-burner mesh (Fig. 5.4). The final result is a 5,009,901 cells mesh (1,488,863 cells for the single-burner). Table 5.1 summarizes the studies that were conducted. Note that results for LES-SB-CI will not be discussed.
5.4 Cold flow results

Geometric simplifications (like using one isolated burner instead of the whole set-up) are often made without a posteriori analysis. Here, LES of a single versus triple-burner allows to check if a periodic burner suffices for this kind of study or on the contrary if a more detailed geometry is required. Figure 5.6 shows instantaneous views of the LES results for LES-SB-CII (a) and for LES-TB-CI (b). For the single-burner set-up a PVC at 300Hz is observed at the end of the burner. The Strouhal number for this PVC (based on the burner diameter $D$ and the bulk velocity at the outlet of the burner $U_b$) is $S_t = \frac{fD}{U_b} = 0.41$. This observation confirms many similar results obtained in similar combustors both numerically and experimentally [88, 101, 109]. In the triple-burner set-up, three PVCs at 300 Hz appear (one on each burner). In both cases the PVCs are visualized using a low pressure isosurface. In the triple-burner set-up, all PVC’s precess in the same direction: however since the CBO (Fig 5.3b) isolates each burner, the PVC’s are independent from one another.

![Figure 5.6: Precessing structure a) LES-SB-CII, b) LES-TB-CI (Cold flow).](image)

Figures 5.7a and 5.7b show profiles of averaged axial velocity and pressure fluctuations for LES-SB-CII (solid line) and the central burner of LES-TB-CI (circles) for the non-reacting case. Profiles are extracted at five locations on a horizontal plane along the axis of the burner (Fig. 5.5). All variables are normalized by reference parameters. The reference length $D$ is the burner diameter (Fig. 5.5). All velocities are normalized by the bulk velocity $U_b$ obtained with the following relation: $U_b = \frac{\dot{m}}{\rho S}$ where $\dot{m}$ is the total flow rate, $\rho$ is the fresh gases density and $S = \pi \cdot (\frac{D}{2})^2$. Pressure fluctuations are also normalized by a reference pressure $P_{ref}$ where $P_{ref} = \rho \cdot U_b^2$. Even though small differences are observed, it is clear that the mean flow but also the unsteady flow are the same in both burners (at least for the central burner of LES-TB-CI and the single
Figure 5.7: a) Mean axial velocity and b) pressure fluctuations. LES-SB-CII (solid line) vs central burner of LES-TB-CI (circles) (Cold flow).
burner of LES-SB-CII). A first simple conclusion is that, to study the non-reacting flow, using a single-burner set-up is sufficient. This information seems to confirm the validity of experiments and computations performed on single-burner set-ups. However, we have yet to account for the flame behaviour in such cases and especially the possibility of flame/flame interaction in the three burner case.

5.5 Reacting flow results

Figure 5.8 shows the flame zone visualized by a 1000K temperature isosurface for LES-TB-HI (a) and LES-TB-H1 (b). All flames are anchored near the inner hub. Figure 5.9a displays profiles of averaged axial velocity on the same cuts as in Fig. 5.7. Here again, the average velocity profiles are very similar, showing that the jet opening and the central recirculation zones are the same in both geometries. However the unsteady pressure fields are very different (Fig. 5.9b): predicted pressure fluctuations are much larger in the three-burner case than in the single-burner case and exhibit a different structure. The geometry change alone, does not account for this kind of difference. Spectral analysis of the pressure signal at the center of each sector of the triple-burner set-up (Fig. 5.10a) reveals a 370 Hz component which is present only on the side sectors (spectral resolution for the reacting cases is 10Hz). The central sector seems unaffected. This 370 Hz component is also absent in the single-burner LES pressure signal (Fig. 5.10b). To understand why this mode appears only in the three burner set-up, an acoustic analysis of both configurations is performed in the next section.
Figure 5.8: Flame (1000K isosurface): a) LES-SB-HII b) LES-TB-HI.
Figure 5.9: a) Mean axial velocity b) Pressure fluctuations: LES-SB-HII (solid line) vs central burner of LES-TB-HI (circles).
Figure 5.10: a) Pressure spectra in the center of each sector of LES-TB-HI, b) Pressure spectra at the center of the domain of LES-SB-HII (both LES results)
5.6 Acoustic study of the set-ups

The LES highlights a difference of pressure fluctuations in both set-ups. The geometry of the triple-burner, which is a simple "triplication" of the single-burner, can not account for such a great difference: the explanation must lie somewhere else. This section shows that the discrepancies between LES-SB-HII and LES-TB-HI come from different acoustic characteristics of the two set-ups using a purely acoustic analysis of the set-ups.

Acoustic solvers are often used in combustion chambers to determine the frequencies and the mode shapes of acoustic modes [4]. The tool described in section 1.5 allows to learn more about the acoustics in the single and triple-burner configurations and to understand the meaning of the $370Hz$ component in the pressure signal.

Figure 5.11: Pressure fluctuations on a cylindrical plane intersecting each burner’s axis for LES-TB-HI, contour of pressure fluctuations (black line).

As a first element, Fig. 5.11 displays an LES result: the RMS pressure fluctuations in LES-TB-HI are plotted on a cylindrical plane that cuts through the axis of all three burners. These fluctuations show a clear structure with a pressure minimum at the central burner and two maxima at the lateral burners (consistently with Fig. 5.10a which shows a maximum pressure oscillation for the side burners). These results suggest that an acoustic mode with an azimuthal structure is excited in the LES. We try to track this mode in this section.
Boundary Conditions

Impedance is of great importance when dealing with acoustics, especially in a gas turbine. Unfortunately for industrial applications such data is not always available. No information was available on the acoustic properties of the inlets or the outlet of the test-rig. Therefore the current study the outlet was assumed to be totally non-reflecting. This condition matches the behavior observed in the LES (see Fig. 5.11) which shows that pressure fluctuations go to zero at the chamber outlet. An average field of mean sound velocity given by the LES is used for the Helmholtz solver. Table 5.2 shows the first three eigen-values for both configurations.

Table 5.2: Lowest eigen-frequencies (Hz) for one and three burner set-ups

<table>
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<th>Eigenvalue</th>
<th>One Burner</th>
<th>Three Burner</th>
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<tr>
<td>1</td>
<td>129</td>
<td>128</td>
</tr>
<tr>
<td>2</td>
<td>371</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>560</td>
<td>561</td>
</tr>
</tbody>
</table>

predicted by the Helmholtz solver described in section 1.5. Eigen-values 1 (128 Hz) and 3 (560 Hz) are longitudinal modes and they match in both configurations. Since the triple-burner corresponds to three single-burners assembled side by side this is no surprise. However, none of these frequencies is present in the LES suggesting that even though these modes are possible longitudinal modes of both set-ups, the unsteady combustion is not able to force them at this regime. On the other hand, the eigen value 2 (371 Hz) appears only for the three burner set-up and matches the LES data perfectly: Fig. 5.10a shows that the mode observed in LES-TB-HI has a frequency of 370 Hz (±10 Hz due to spectral precision) while the Helmholtz solver predicts 371 Hz. Obviously both LES and the acoustic solver capture the same mode. This can be confirmed by looking at the structure of the 371 Hz eigen mode (cf. Table 5.3), and comparing it with the prms/prref field from Fig. 5.11. The central sector sees little pressure disturbance and the side burners are subjected to intense fluctuations (cf. Fig. 5.12).

The excitation of the 370 Hz eigen mode explains the differences observed in the reacting LES in the two set-ups. The 370 Hz is not a mode of the single-burner set-up and does not appear in the acoustic analysis of Table 5.3. However, in the triple-burner, the 370 Hz mode is predicted by both the acoustic solver and the LES. The single-burner simulation is unable to reproduce this behaviour since 370 Hz is not a eigen-frequency for a one sector configuration. Performing a study of this set-up while considering only one burner would yield incomplete data on the behaviour of the set-up.

Finally note that the experiment was not run on both a single and triple-burner for obvious cost reasons. However the 370 Hz mode had never been observed in previous experiments and it appeared very clearly in the triple-burner experiments, matching both LES and Helmholtz solver predictions within a few Hertz.
Table 5.3: Eigen-modes for both configurations (Helmholtz analysis). $|P_{RMS}|$ fields on the walls.
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5.7 Flame response

Another interesting question is whether the single-burner response to a given excitation matches the response of the triple-burner and of the full burner. The LES can be used in a “forced mode” to analyze the response for both set-ups [41, 48]. Based on previous experience from Siemens, a 90Hz axial excitation of the premix passage was considered with an amplitude equivalent to a \( p_1 = 20 \text{mBar} \) fluctuation at the middle of the chamber. Using the conservation of mass flow through the burner and the fact that \( p_1 = \rho_0 \cdot c_0 \cdot u_1 \), where 1 stands for perturbations and 0 for mean values, this pressure perturbation is equivalent in the case of an axial excitation to an inlet velocity perturbation with an amplitude of \( 12 \text{m.s}^{-1} \). Note that using the forcing method described in section 2.3.3, the swirl number remains constant. To simplify the discussion, these simulations have been labeled in table 5.4.

Table 5.4: Forced LES runs designation: each run is characterized by the size of the domain, the type of forcing, the forcing frequency \( f_p \) and the type of BC applied in the azimuthal direction.

<table>
<thead>
<tr>
<th>Single-burner (( f_p = 90\text{Hz} ))</th>
<th>Axial forcing</th>
<th>Wall law BC</th>
<th>Periodic-axi BC</th>
</tr>
</thead>
<tbody>
<tr>
<td>LES-SB-HI-AF90</td>
<td>Wall law BC</td>
<td>LES-SB-HII-AF90</td>
<td></td>
</tr>
<tr>
<td>LES-SB-HI-AP90</td>
<td>Periodic-axi BC</td>
<td>LES-SB-HII-AF90</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.5 shows the different transfer functions in the case of axial forcing at 90Hz. The change in boundary conditions (using wall-laws, LES-SB-HI-AF90, or periodic conditions for the side walls, LES-SB-HII-AF90) does not change the flame transfer function for the single-
5.7. FLAME RESPONSE

Table 5.5: $n - \tau$ values for the different simulations

<table>
<thead>
<tr>
<th></th>
<th>Single-burner</th>
<th>Triple-burner</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LES-SB-HI-AF90</td>
<td>LES-SB-HII-AF90</td>
</tr>
<tr>
<td>$n$ [ ]</td>
<td>3.7</td>
<td>3.6</td>
</tr>
<tr>
<td>$\tau$ [ms]</td>
<td>1.88</td>
<td>1.78</td>
</tr>
</tbody>
</table>

burner cases. However a slight difference is noticeable if we look at the $n - \tau$ values for the triple-burner case\(^1\). Actually, the $n - \tau$ formulation cannot be used for the triple-burner case because of the 370Hz mode as discussed below.

Table 5.6 shows snapshots at three different phases of the forcing frequency ($t=0$, $t=T_1/2$ and $t=T_1$ with $T_1 = 1/90$) for an horizontal plane for the central burner of LES-TB-HI-AF90 and for the single-burner LES-SB-HII-AF90. The flame position is visualized using a 1000K isoline. These figures show that only the flame length is affected by the acoustic forcing in both cases. Depending on the instant, the flame either extends or shrinks around a mean position corresponding to the non-forced flame. This confirms previous observations on the same kind of studies \([102, 9]\). The same visualization performed on the side burners of LES-TB-HI-AF90 (Table 5.7) reveals that the side burners behave quite differently. Flame anchoring is no longer guaranteed and the flame is more unstable. Periodic lift off and re-anchoring occurs out of phase for the side burners. This is a direct consequence of the 370Hz mode. The side burners in the triple-burner are located in pressure antinodes and the central burner is in a pressure node. Therefore, large acoustic perturbations occur at the sides, while the center of the domain is relatively calm. Looking at the pressure spectrum at the center of the single-burner domain (Fig. 5.13a) reveals only the 90Hz component induced by the axial forcing. This is also the case for the central burner of the triple set-up (Fig. 5.13b). However, the pressure spectra taken at the center of the side sectors of the triple-burner (Fig. 5.14) show that the 90Hz forcing amplifies the 370Hz component of the spectrum doubling its amplitude. This increase of amplitude gives enough strength to the perturbation to provoke periodic lift-off of the side burner flames making the set-up more unstable. Since the 90Hz forcing and the 370Hz mode are not exactly in phase, the lift-off and re-attachment of the flames is not perfect.

Tables 5.8 and 5.9 show a complete period of forcing (at 90Hz). The behavior of each flame is very unsteady. The side flames can be seen at different positions along the timeline. They try periodically to re-attach to the central hub, not always with success. Over a period of the 370Hz mode, the right flame detaches itself from the central hub and reattaches. The left flame is also subjected to strong perturbations, however it does not detach itself in the same way as the right burner. This is purely due to the choice of initial condition for the axial forcing. Had we proceeded to pulsate the case half a period of the 370Hz mode later, it would be the left burner that would have reacted more to the forcing. Also since 370Hz and 90Hz are not mul-

\(^1\)The reference point for the velocity fluctuations is in the central burner
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tiples one of the other, a low frequency modulation is observed going from a more unstable right burner to a more unstable left burner. The central flame sees none of these fluctuations and behaves similarly to a single-burner subjected to axial forcing. Since the 370Hz mode is not only present but very strong in the side burners, velocity but also pressure fluctuations occur at the side burners. The forcing frequency has less impact on the side burner than the self excited frequency does: using the $n - \tau$ for such a case where the forcing frequency is hidden by a self excited mode yields irrelevant results.

Figure 5.13: Pressure spectra at the center of domain for a) for the single-burner LES-SB-HII-AF90 and b) for the central burner of LES-TB-HI-AF90).

Figure 5.14: Pressure spectra for LES-TB-HI-AF90 at the center of domain: a) left burner and b) right burner.
Table 5.6: 1000K isoline on an horizontal plane for: (top) the single-burner LES-SB-HII-AF90 and (bottom) the central burner of LES-TB-HI-AF90 for \( t=0, t=T_1/2 \) and \( t=T_1 \) \( (T_1=1/90s) \). These two flows respond to forcing in similar ways.

This result in itself is not surprising: the forced response of any solution can be studied only if the eigen modes of this oscillation remain small. Here the 370 Hz mode of the triple-burner is much too strong to allow a proper measurement of the flame response at 90 Hz. What is interesting in addition to this result is that the triple-burner was built to match the real machine better than a single-burner configuration but it actually does not: the 370 Hz mode appearing in the triple set-up is not a mode of the full combustor, it has no practical applications for the full combustor but it prevents precise measurements in the triple set-up. This is another illustration of the facetious effects of acoustics in combustion chambers.
Table 5.7: 1000K isoline on an horizontal plane for: (top) the left burner of LES-TB-HI-AF90 and (bottom) the right burner of LES-TB-HI-AF90 for $t=0$, $t=T_1/2$ and $t=T_1$ ($T_1=1/90s$). The side burners respond very differently because a 370 Hz mode is present and leads to flames which are totally lifted from the central hub of the pilot passage.
Table 5.8: Temperature Isosurface for LES-TB-HI-AF90, unsteady behavior of the flame

<table>
<thead>
<tr>
<th>90Hz timeline</th>
<th>370Hz timeline</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>t=0</strong></td>
<td><strong>t=0</strong></td>
</tr>
<tr>
<td><strong>t=T₁/8</strong></td>
<td><strong>t ≈ T₂/2</strong></td>
</tr>
<tr>
<td><strong>t=T₁/4</strong></td>
<td><strong>t ≈ T₂</strong></td>
</tr>
<tr>
<td><strong>t=3T₁/8</strong></td>
<td><strong>t ≈ 3T₂/2</strong></td>
</tr>
<tr>
<td><strong>t=T₁/2</strong></td>
<td><strong>t ≈ 2T₂</strong></td>
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</tbody>
</table>
Table 5.9: Temperature Isosurface for LES-TB-HI-AF90, T=1/90, a) t=0, b) t=T/2, c) t=T.

<table>
<thead>
<tr>
<th>90Hz timeline</th>
<th>370Hz timeline</th>
</tr>
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<tbody>
<tr>
<td>$t=5T_1/8$</td>
<td>$t \approx 5T_2/2$</td>
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<tr>
<td>$t=3T_1/4$</td>
<td>$t \approx 3T_2$</td>
</tr>
<tr>
<td>$t=37T_1/8$</td>
<td>$t \approx 7T_1/2$</td>
</tr>
<tr>
<td>$t=T_1$</td>
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</table>
5.8 Towards full burner simulations

The previous sections demonstrate that the simplifications made in many numerical and experimental studies can provoke misinterpretations in the analysis of the stability of the set-up. The simplified set-up considered does not necessarily have the same acoustic properties of the full set-up and can therefore be subject to other or none of the acoustic perturbations that take place in the real turbine. We must strive to study cases as close as possible to real machines. Experimental cases are out of the question because of the costs involved. However, numerical studies are becoming possible. Computer power doubles every 18 months \[63\]. New technologies like the multi-threading system on Intel based chips or multi-core processors have increased immensely the possibilities for numerical simulations. Also, great effort is focused worldwide for the creation of ever more efficient and massively parallel computers with hundreds if not thousands of processors. Figure 5.15 shows a list of the 10 most powerful computers in the world taken form http://www.top500.org.

![26th List: The TOP10](image)

<table>
<thead>
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<th>Manufacturer</th>
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<th>Year</th>
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</tr>
<tr>
<td>10 Cray</td>
<td>Jaguar Cray XT3</td>
<td>20.53</td>
<td>Oak Ridge National Lab</td>
<td>USA</td>
<td>2005</td>
<td>5200</td>
</tr>
</tbody>
</table>

**Figure 5.15:** 26th List: The TOP10 computers (November 2005: http://www.top500.org).
This list shows that many of these computers contain of thousands of processors. In the case of single-burner studies like the one presented in the chapter 4, the LES uses 32 processors over 200 hours\(^2\). If 5000 processors were available during the same period a much larger study could be undertaken. However, having a lot of computer power is not sufficient. We need to be able to use it properly. The numerical code must be parallel to take advantage of these new computers of course, but it must also be efficient with a high number of processors. With the help of IBM, a feasibility test was performed with a full burner LES on a Bluegene/L machine in the USA. Performance tests were made for two cases, the three burner case (LES-TB-HI) and a full chamber case\(^3\) (see Fig. 5.16). Performance measurements up to 5000 processors are shown on Fig 5.17. The LES code used (AVBP) is able to take advantage of all the processors that are allocated to the task. However, the triple burner case shows an interesting phenomenon that must be kept in mind when dealing with such super-computing tasks. If the simulation is too small (meaning the memory usage per processor is very low), performance will drop too. Computer power needs must be scaled correctly for each task.

![Figure 5.16: Full chamber case: a 40.10^6 tetrahedra mesh](image)

With the increase in power and the availability of new computational resources, ever more complex cases will be studied. We are confident that a full burner LES is within our grasp.

\(^2\)This value is strongly dependent on the flow condition and in the mesh quality which can affect greatly the time step.

\(^3\)The full burner case represents a 40 million cells mesh, the largest reactive LES performed on a industrial configuration so far.
Other studies, focusing on purely unsteady phenomena like ignition in full turbines are already under study (http://www.cerfacs.fr/cfd/movies/Ignition_high.mov).

**Figure 5.17:** Speedup for AVBP performed on Bluegene/L: (dotted line) ideal set-up, (squares) three burner cases, (circles) full burner case.
Conclusion

This thesis has presented studies on the influence of large and small scales in LES of realistic industrial burner geometries:

Pilot flames:
The present document demonstrates the importance which pilot fuel can have on flame stabilization. A high quantity of pilot fuel ensures a robust and stable flame. However, the mixture burns at high equivalence ratio creating a high temperature zone that increases pollutant emissions so a compromise between stability and emissions must be reached. If the quantity of pilot fuel is too low, although the pilot fuel is injected pure, it rapidly mixes with the other gases. The mixing process impedes the formation of a rich zone that ignites easily and the flame behaves almost as if the pilot fuel was turned off.

Azimuthal interaction:
Due to costs, interactions in multi-burner combustion chambers in the azimuthal direction are almost always neglected both in experimental and numerical studies. The study of the influence of azimuthal interaction on a multi-burner set-up was possible using a test-rig especially built for project DESIRE. It was demonstrated that although the influence in cold flow is negligible, the flame presence changes the burner behavior dramatically. A natural mode of the set-up is excited in the reacting flow case. This mode is purely azimuthal and can not be evidenced in a single-burner study. It is demonstrated than this mode can influence greatly flame stabilization. A numerical method to simulate the effects of an azimuthal mode on the burners of an annular combustor while using only a single-burner domain is presented and used in an industrial configuration. Results demonstrate that although the impact of the transverse component is less important than the impact of the axial component, burner/burner interaction is modified which might lead to wrong estimation on burner stability if neglected.

Although not directly linked to mechanics of fluids, one aspect also studied during PhD is the feasibility of a full chamber LES using massively parallel computers. Today's high end computers are more than capable of performing this task. A single burner LES could be performed in a couple of minutes using this computers but also a much larger domain could be used for
the study, even the full chamber. However, optimization of the LES code is required since not all codes are able to take full advantage of a very large number of processors. Even though access to this computers is still restricted to a small portion of the scientific community, with time availability will increase as this computers become more widespread.

In summary, this work demonstrates the importance of the azimuthal interactions on flame behavior. Current computer performance allows to consider a larger part of the turbine. The work shows that even considering only three of the twenty four burners of an annular gas turbine yields important results on flame stabilization that are not evidenced in the equivalent single-burner simulation. Therefore, the thesis highlights the importance of considering as much as possible the real geometry of the turbine in order to correctly predict the flame stabilization process, including low frequency phenomena possible only in the full chamber. Moreover, the feasability of full chamber LES is demonstrated although computer power requirements are still too high for today’s standards, they will soon be available on a large scale.
Appendix A

Présentation étendue de la thèse

La combustion et la production d’énergie.

Le développement industriel est directement proportionnel à la production énergétique. La forme d’énergie la plus répandue est l’électricité. Elle a l’avantage de pouvoir facilement être transformée dans toutes les autres (énergie mécanique, thermique, etc.). Les ressources pour créer de l’électricité sont variées (barrages, panneaux solaires, etc.). Malgré un consensus général sur leur épuisement à plus ou moins long terme, les sources fossiles tel que le pétrole ou le charbon restent dominantes. Elles fournissent près de 80% de l’énergie mondiale. Cette dominance est expliquée par le manque d’alternative aussi efficace et rentable:

- Le déploiement de centrales hydroélectriques a atteint sont maximum.
- L’énergie solaire reste chère et peu efficace pour le moment
- L’énergie nucléaire, malgré son fort rendement, pose des problèmes à long terme (traitement des déchets). De plus, l’opinion publique est grandement opposée à ce type d’installation.
- De nos jours, la fusion nucléaire est purement théorique à l’échelle humaine.
- L’énergie éolienne est trop peu efficace et pose des problèmes de par son cote intermittent.
- Les sources géothermiques nécessitent des conditions géologiques particulières. De plus, les scientifiques craignent à long terme des problèmes de refroidissement de la couche terrestre (avec pour conséquences potentielles l’augmentation des tremblements de terre et des éruptions volcaniques).
Ainsi les sources fossiles ne peuvent être remplaçées pour le moment. La question est alors de brûler ces éléments de façon efficace et sans produire trop de pollution. Dans ce but, les producteurs d’électricité se tournent de plus en plus vers la technologie des turbines à gaz. Leur efficacité (57% pour le moment) les rend très attractives, ainsi que leur facilité d’installation. Des normes de pollution de plus en plus rigoureuses poussent les manufacturiers de turbines (Siemens, Alstom, General Electric mais aussi Rolls Royce, Snecma, etc.) à accélérer le cycle de recherche et développement. Par le passé, les formules empiriques et les études expérimentales étaient les outils dominants. De nos jours, les études numériques se sont rajoutées à l’arsenal des chercheurs et sont utilisées de plus en plus dans l’industrie.

La simulation numérique: Les outils classiques et leurs limita-
tions

L’utilisation de la simulation numérique dans l’industrie est grandement répandue. Les manufacturiers de turbines à gaz utilisent des codes commerciaux (CFX, Fluent, etc..) et des codes ”maison” pour évaluer l’écoulement moyen à froid comme à chaud. Ces codes sont devenus essentiels dans la phase de recherche et de développement. La majorité de ces codes résolvent les équations RANS (Reynolds averaged Navier Stokes) [46, 77, 69] ou seules les moyennes dans le temps des variables (pression, température, vitesse, etc.) sont résolues. Malgré un développement de plusieurs décennies, cette approche atteint ses limites:

- Les modèles RANS pour la combustion turbulente sont difficiles à dériver et manquent souvent de précision. Malgré une forte contribution de la communauté scientifique [8, 13, 39, 50, 69]), il est envisageable d’annoncer que les méthodes RANS ont atteint leur limite.

- De par leur principe de base, les codes RANS ne peuvent être utilisés pour étudier des phénomènes purement instationnaires comme l’allumage, l’extinction et les instabilités et les solveurs RANS sont en général peu adaptés aux calculs instationnaires.

Le besoin d’augmenter l’efficacité des turbines et de respecter les normes internationales a poussé les manufacturiers de turbines à utiliser des régimes d’opération ou ces deux problèmes deviennent trop importants pour être ignorés. L’allumage et l’extinction sont des thématiques de grand intérêt pour les industriels. Il suffit aussi de regarder les publications issues de laboratoires industriels pour voir l’importance qu’ils accordent aux instabilités de combustion.
La Simulation aux Grandes Echelles

Les récents développements informatiques ainsi que les progrès dans la modélisation de la turbulence ont propulsé la Simulation aux Grandes Echelles (SGE) sur le devant de la scène. La communauté scientifique reconnaît les progrès apportés par la SGE dans les simulations des écoulements à froid [90, 53, 54]. La SGE capture non seulement l’écoulement moyen mais aussi toutes les fluctuations instationnaires, ce qui ouvre de nombreuses voies pour les études aéroacoustiques, la prédiction et le contrôle d’instabilités. Il est important de souligner que l’évolution rapide de la SGE provient des avancées effectuées en simulation numérique directe (DNS)[62, 61, 81, 80].

La validation incontestable de la SGE dans les écoulements réactifs reste à faire même si de nombreuses études passées [14, 25, 28, 38, 43, 70, 71, 73, 88, 91, 102, 106] et en cours ont démontré son potentiel. Des problèmes persistent, notamment la modélisation de tous les régimes de combustion. De nombreux projets expérimentaux sont en cours pour valider la SGE. Des besoins de plus en plus pressants poussent l’adoption de plus en plus urgente de la SGE dans l’industrie.

Les limites de la SGE

La validation ponctuelle de la SGE dans quelques cas ne suffit pas à démontrer qu’il s’agit de la méthode la plus intéressante pour l’avenir. Il reste de nombreux challenges à surmonter:

Tout d’abord, tous les cas académiques doivent être résolus. L’interaction flammes/flammes ainsi que la résolution de la turbulence restent des thèmes ouverts. Le nombre de papiers traitant de la combustion turbulente en est la preuve.

L’extrapolation des résultats obtenus sur des expériences réduites en laboratoire vers les vraies machines pose beaucoup de problèmes. Le même problème peut se présenter quand on parle de simulation dans des cas très simples ou le phénomène est très bien connu et que l’on effectue une extrapolation vers les vraies turbines. Cette thèse propose d’étudier ces deux questions.

Pour répondre à ces deux questions, il ne suffit pas d’avoir beaucoup de puissance de calcul, la modélisation de certains aspects spécifiques est également nécessaire. Le saut d’une configuration réduite et simple vers une configuration beaucoup plus grande et vers les brûleurs réels implique de nouveaux phénomènes:

- Premièrement, le nombre de Reynolds dans les vraies turbines est beaucoup plus grand que celui des configurations de laboratoire. Par exemple, dans l’étude effectuée par S.
APPENDIX A. PRÉSENTATION ÉTENDUE DE LA THÈSE

Roux [88] sur un brûleur (P= 1atm) installé dans un laboratoire, le nombre de Reynolds basé sur la vitesse débitante et le diamètre du swirler est de 170 000. Dans le brûleur V94.3 de Siemens, le nombre de Reynolds basé sur le diamètre du swirler extérieur et la vitesse débitante est de 5100 000. Les modèles éprouvés dans le premier cas ne seront pas nécessairement adaptés pour le second. Ce problème est bien connu des aérodynamiciens qui utilisent la SGE. La SGE est capable de prédire correctement une couche limite ou le comportement d’un canal mais elle a des problèmes pour recréer le comportement d’un avion à cause du changement de nombre de Reynolds.

• Deuxièmement, la turbine à gaz utilise des artefacts qui rendent le régime de combustion hétérogène, ce qui complique la tâche des modèles. La plupart des études en laboratoire traitent de flammes parfaitement pré-mélangées [9, 41, 42] ou totalement non pré-mélangées (aussi appelées flammes de diffusion)[18, 73]. Les turbines à gaz industrielles utilisent une combustion partiellement pré-mélangée avec une flamme pilote. De très petits jets de méthane pur sont utilisés pour créer cette flamme pilote. Ainsi tous les régimes depuis la diffusion pure jusqu’au régime partiellement pré-mélangé sont présents dans la turbine.

• Troisièmement, la géométrie utilisée dans les laboratoires est souvent une géométrie réduite. En laboratoire, on étudie généralement un seul brûleur. Celui-ci peut correspondre exactement à un brûleur de la vraie turbine, mais il est possible d’avoir plusieurs dizaines de ces brûleurs dans la vraie machine. Généralement, ils sont distribués de façon homogène le long de la circonférence de la turbine et soufflent dans une chambre de combustion commune. Il est donc possible d’observer des interactions entre les brûleurs qui peuvent provoquer des effets violents d’après le peu de cas accessibles dans la littérature [76, 86, 87, 116]. Ces phénomènes sont impossibles à observer en étudiant un brûleur seul. Il est à noter que en plus la taille des injecteurs est de quelques millimètres alors que la taille de la turbine est de l’ordre de quelques mètres.

• Pour finir, l’acoustique est un point crucial qui est grandement affecté par la taille et la géométrie. Les interactions entre les flammes et l’acoustique sont reconnues comme étant la source de beaucoup de problèmes dans les chambres à combustion, notamment des instabilités de combustion [77]. La géométrie et les conditions aux limites impactent grandement sur l’acoustique. L’objet de notre étude est focalisé sur les turbines à gaz annulaires. Dans ce type de configuration, beaucoup de modes acoustiques sont possibles. Certains ne dépendent que d’un brûleur mais d’autres sont le résultat de l’interaction brûleur/brûleur. Les modes azimutaux, jamais observés sur des configurations monobrûleur, sont un exemple de ces modes. Leur fréquence est de l’ordre de la centaine de Hertz. Ils interagissent et influencent de manière significative la combustion. Une validation de la SGE pour ce type de thématique reste à faire.
Objectifs

Le but de cette étude est d’appliquer la SGE à des géométries réelles correspondant aux plus grandes turbines existantes. Les thèmes spécifiques abordés sont :

- Comment se comporte la SGE lorsque que l’on passe d’un bas nombre de Reynolds (configurations de laboratoire) vers un très haut nombre de Reynolds (vraie turbine) ?

- Par quel mécanisme les flammes pilotes aident à avoir une meilleure stabilité de flamme dans des brûleurs vrillés turbulents ?

- Est-ce que l’interaction entre brûleurs est un facteur déterminant lors de l’étude de l’écoulement moyen dans une turbine à gaz ? Son influence est-elle plutôt perceptible sur les phénomènes instationnaires ? Ces questions sont déterminantes pour savoir si, pour étudier une turbine annulaire qui comporte 24 brûleurs, il suffit d’en étudier un seul ou la totalité.

- Est-ce que le calcul massivement parallèle est prêt pour des tâches aussi imposantes ? Même si cette question n’appartient pas nécessaire au domaine de la mécanique des fluides elle est d’un intérêt vital pour l’avenir de la SGE.

Le travail accompli s’inscrit dans le projet Européen DESIRE. Les partenaires incluent Siemens PG, l’université de Twente (Hollande), le DLR Stuttgart (Allemagne), CIMNE (Espagne) et le CERFACS. Siemens PG a participé activement à cette étude en fournissant les géométries et en guidant notre recherche du point de vue applicatif. Des résultats expérimentaux dans une vraie turbine ou dans l’expérience développée pour le projet DESIRE par le DLR et Siemens ont été obtenus, mais la divulgation d’informations était très limitée. L’expérience pour le projet DESIRE est un brûleur triple du même type que la vraie turbine. Ceci constitue une première étape dans l’étude des interactions inter-brûleurs.


Le chapitre 1 décrit le code SGE AVBP ainsi que le solveur de Helmholtz AVSP. Le chapitre 2 présente les thématiques qui sont au centre de cette étude : les flammes pilotes, l’interaction entre brûleurs et les modes acoustiques azimutaux. Il décrit une méthode numérique (la méthode ESBAC) pour évaluer l’impact des modes azimutaux de chambre annulaire en ne considérant que un seul brûleur. Le chapitre 3 présente les résultats obtenus lors de l’étude de l’influence
APPENDIX A. PRÉSENTATION ÉTENDUE DE LA THÈSE

de la flamme pilote sur un brûleur. Les chapitres 4 et 5 abordent l’interaction entre brûleurs et l’interaction acoustique/flamme dans une chambre annulaire. Dans le chapitre 4, la méthode ESBAC est appliquée à un brûleur pour évaluer quel est le mécanisme affectant le plus la flamme dans un mode acoustique azimutal.
Dans le chapitre 5, une autre voie est empruntée. On étudie une configuration avec trois brûleurs. Un intérêt particulier est dirigé vers l’influence des brûleurs latéraux sur le brûleur central. Son comportement est notamment comparé à celui d’un brûleur équivalent périodique. L’analyse acoustique des deux configurations est effectuée et on étudie également la réponse forcée des flammes dans les deux configurations. Pour finir, la possible extension de la SGE vers une étude d’une turbine complète est démontrée.

Conclusion

Cette thèse c’est concentrée sur des thèmes peu ou pas abordés pour le moment:

- L’influence de la flamme pilote sur la stabilité de flamme.
- L’impact d’un mode acoustique azimutal sur les brûleurs dans un trubine à gaz annulaire
- Les effets des interactions entre des brûleurs voisins dans une configuration multi-brûleurs.

Dans un premier temps l’étude a démontré que la flamme pilote a une réelle importance dans la stabilité de la flamme. Une flamme pilote “riche” permet d’obtenir une flamme stable et robuste. Par contre si on baisse trop la quantité de carburant de la flamme pilote, le mélange est trop rapide et la limite de flammabilité est rapidement atteinte empêchant un accrochage efficace. La flamme oscille sans position déterminant ce qui peut être une source de bruit et qui peux provoquer des instabilités plus grave si le fluctuations de pression et de dégagement de chaleur sont en phase a un moment donné.

Les tests en laboratoire de turbines à gaz sont souvent effectués sur des brûleurs simplifiés. Dans le cas des turbines annulaires, un seul brûleur est considéré négligeant ainsi toute influence des autres brûleurs. L’étude à présenté que même si l’influence dans l’écoulement non réactif est négligeable, l’écoulement réactif est grandement affecté. Un mode naturel azimutal de la chambre est excité. Ce mode compromet la stabilisation de flamme et rend la configuration instable.
Une méthode numérique développée pendant cette thèse pour étudié l’influence d’un mode acoustique azimutal en n'étudiant que deux configurations à montré que l’influence des fluctuations de vitesse transverse est moins important que celle des fluctuations de débit. Malgré cela,
les fluctuations transverses affectent de façon importante l’interaction brûleur/brûleur ce qui vu les résultats précédents peu amener a une mauvaise estimation de la stabilité de la turbine.

Pour résumer, cette thèse montre la grande importance des interactions azimutales sur la stabilité des turbines. La puissance de calcul disponible actuellement nous permet de considérer des domaines plus précis mais aussi plus grand. L’étude démontre que même en ne considèrent que trois brûleurs sur vingt quatre, de nouvelles données sur la stabilité des flammes sont obtenues. Données qui sont impossible à récupérer en n’étudiant que un seul brûleur.
Pour étudier une turbine il est donc indispensable de considérer la plus grandes portion possible ce qui permettra de étudier des phénomènes base fréquence qui sont directement dépendant de la taille du domaine considéré. L’extension de la SGE vers des simulation de chambre complète est abordée également dans ce document et même si les besoins en ressources informatiques sont trop grand aujourd’hui, ils ne cessent de croître.
APPENDIX A. PRÉSENTATION ÉTENDUE DE LA THÈSE
Appendix B

Characteristic Wave Decomposition

B.1 Basic definitions

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>mass density</td>
<td>$\rho = \sum_k \rho_k$</td>
</tr>
<tr>
<td>mass fractions</td>
<td>$Y_k = \rho_k / \rho$</td>
</tr>
<tr>
<td>momentum</td>
<td>$m_1 = \rho u, \quad m_2 = \rho v, \quad m_3 = \rho w$</td>
</tr>
<tr>
<td>sensible energy</td>
<td>$e_{sk} = \int_0^T C_{vk}dT$</td>
</tr>
<tr>
<td>sensible enthalpy</td>
<td>$h_{sk} = \int_0^T C_{pk}dT$</td>
</tr>
<tr>
<td>sensible energy density</td>
<td>$\rho \bar{e}<em>s = \sum_k \rho_k e</em>{sk} = \rho \sum_k Y_k e_{sk}$</td>
</tr>
<tr>
<td>sensible enthalpy density</td>
<td>$\rho \bar{h}<em>s = \sum_k \rho_k h</em>{sk} = \rho \sum_k Y_k h_{sk}$</td>
</tr>
<tr>
<td>kinetic energy density</td>
<td>$\rho \bar{e}_c = \frac{1}{2} \rho (u^2 + v^2 + w^2) = \frac{1}{\rho} (m_1^2 + m_2^2 + m_3^2)$</td>
</tr>
<tr>
<td>total energy</td>
<td>$\varepsilon = \rho \bar{E} = \rho \bar{e}_c + \rho \bar{e}_s$</td>
</tr>
<tr>
<td>total enthalpy</td>
<td>$\mathcal{H} = \rho \bar{H} = \rho \bar{e}_c + \rho \bar{h}_s$</td>
</tr>
</tbody>
</table>

For each species:

$$r_k = C_{pk} - C_{vk} \quad \gamma_k = \frac{C_{pk}}{C_{vk}}$$

Mean (mixture) quantities are defined as:

$$\bar{C}_v = \sum_k Y_k C_{vk} \quad \bar{C}_p = \sum_k Y_k C_{pk} \quad \bar{r} = \sum_k Y_k r_k \quad \frac{1}{W} = \sum_k \frac{Y_k}{W_k} \quad \gamma = \frac{\bar{C}_p}{\bar{C}_v}$$

Finally, pressure is:

$$P = \sum_k \rho_k r_k T = \rho \bar{r} T$$
The fundamental relation between enthalpy and energy reads:

\[ \mathcal{H} = \mathcal{E} + P \]

It is useful to introduce two new parameters:

\[ \beta = \gamma - 1 \quad \text{et} \quad \chi_k = r_k T - \beta e_{sk} \]

and thus:

\[ \chi = \sum_k \chi_k Y_k = \bar{r} T - \beta \bar{e}_s = \beta (C_v T - \bar{e}_s) = -\beta \bar{e}_s^0 \]

where \( \bar{e}_s^0 \) is defined by \( \bar{e}_s^0 = \bar{e}_s - C_v T \) so that the sensible energy can be locally written as a linear function of temperature:

\[ \bar{e}_s = C_v T + \bar{e}_s^0 \]

Of course, \( C_v \) and \( \bar{e}_s^0 \) are not constant and \( \bar{e}_s \) is not a linear function of \( T \) over the whole range of temperature. However, this notation is useful to simply the coding in AVBP.

These are useful differential relations:

\[
\begin{align*}
    d\rho &= \sum_k d\rho_k \\
    dP &= \rho d\bar{r} + \sum_k r_k T d\rho_k \\
    dT &= \frac{1}{\rho \bar{r}} dP - \sum_k \frac{r_k T}{\rho \bar{r}} d\rho_k \\
    dm_1 &= \rho du + \sum_k ud\rho_k \\
    dm_2 &= \rho dv + \sum_k vd\rho_k \\
    dm_3 &= \rho dw + \sum_k wd\rho_k \\
    d(\rho e_c) &= \rho du + \rho vd \bar{v} + \rho dw + \sum_k e_c d\rho_k \\
    &= udm_1 + vdm_2 + wdm_3 - \sum_k e_c d\rho_k \\
    d(\rho \bar{e}_s) &= \rho C_v dT + \sum_k e_{sk} d\rho_k \\
    d\mathcal{E} &= \rho du + \rho vd + \rho dw + \sum_k (e_c + e_{sk}) d\rho_k + \rho C_v dT \\
    d\mathcal{E} &= udm_1 + vdm_2 + wdm_3 + \sum_k (-e_c + e_{sk}) d\rho_k + \rho C_v dT \\
    d\mathcal{E} &= \rho du + \rho vd + \rho dw + \sum_k (e_c + e_{sk} - \frac{r_k T}{\bar{r}}) d\rho_k + \frac{1}{\beta} dP
\end{align*}
\]
\[ d\varepsilon = u dm_1 + v dm_2 + w dm_3 + \sum_k (-e_c + e_{sk} - \frac{r_k}{\tau} C_v T_k) d \rho_k + \frac{1}{\beta} dP \]

\[ dT = \frac{1}{\rho C_v} \left( d\varepsilon - \rho u du - \rho v dv - \rho w dw - \sum_k (e_c + e_{sk}) d \rho_k \right) \]

\[ dT = \frac{1}{\rho C_v} \left( d\varepsilon - ud m_1 - v dm_2 - w dm_3 + \sum_k (e_c - e_{sk}) d \rho_k \right) \]

\[ dP = \beta \left( -\rho u du - \rho v dv - \rho w dw + d\varepsilon + \sum_k \left[ -e_c + \frac{\chi_k}{\beta} \right] d \rho_k \right) \]

\[ dP = \beta \left( -ud m_1 - v dm_2 - w dm_3 + d\varepsilon + \sum_k \left[ e_c + \frac{\chi_k}{\beta} \right] d \rho_k \right) \]

As from AVBPV5.1 the \( e_{sk} \) are tabulated in intervals of 100 \( K \) such that \( C_{vk} \) are piecewise constant.

**B.2 Governing equations**

This section explains how to recast the equations from the AVBP form (conservative fluxes in the global basis \( \vec{i}, \vec{j}, \vec{k} \)) to primitive variables in a normal \( \vec{n}, \vec{t}_1, \vec{t}_2 \) basis (where \( \vec{n} \) is the inward normal to the patch reference vector and \( \vec{t}_1, \vec{t}_2 \) the tangential ones). Then projection on a characteristic basis will be detailed. The key idea is to build three transformation matrices: the first, called \( M^{-1} \), allows the passage from conservative \( (U) \) to primitive variables \( (V) \), the second, called \( \Omega^{-1} \) the rotation to the basis normal to the wall \( (V_n) \) and the third, called \( L \) the characteristic decomposition \( (W) \). Then, these matrices are combined to give the global transformation. Table B.1 summarizes the whole procedure showing the three transformations.

The model equations for solving the Boundary Conditions for \( U \) are the compressible 3D Euler equations written in conservative form:

\[
\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho uu + P)}{\partial x} + \frac{\partial \rho uv}{\partial y} + \frac{\partial \rho uw}{\partial z} = 0 \quad (B.1)
\]
APPENDIX B. CHARACTERISTIC WAVE DECOMPOSITION

<table>
<thead>
<tr>
<th>Conservative</th>
<th>Primitive</th>
<th>Primitive in a normal basis</th>
<th>Characteristic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\partial U$</td>
<td>$\partial V$</td>
<td>$\partial V_n$</td>
<td>$\partial W$</td>
</tr>
<tr>
<td>$\begin{pmatrix} \partial (\rho u) \ \partial (\rho v) \ \partial (\rho w) \ \partial (\rho E) \ \partial (\rho Y_k) \end{pmatrix}$</td>
<td>$M^{-1}$</td>
<td>$\Omega^{-1}$</td>
<td>$L$</td>
</tr>
<tr>
<td>$\begin{pmatrix} \partial u \ \partial v \ \partial P \end{pmatrix}$</td>
<td>$\partial (\rho Y_k)$</td>
<td>$\Omega$</td>
<td>$R$</td>
</tr>
</tbody>
</table>

$L_U \rightarrow R_U$

\[ \begin{align*}
\frac{\partial \rho v}{\partial t} + \frac{\partial \rho vu}{\partial x} + \frac{\partial (\rho vv + P)}{\partial y} + \frac{\partial \rho vw}{\partial z} &= 0 \\
\frac{\partial \rho w}{\partial t} + \frac{\partial \rho uw}{\partial x} + \frac{\partial \rho vw}{\partial y} + \frac{\partial (\rho ww + P)}{\partial z} &= 0 \\
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho Hu}{\partial x} + \frac{\partial \rho Hv}{\partial y} + \frac{\partial \rho Hw}{\partial z} &= 0 \\
\frac{\partial \rho_k}{\partial t} + \frac{\partial \rho_{ku}}{\partial x} + \frac{\partial \rho_{kv}}{\partial y} + \frac{\partial \rho_{kw}}{\partial z} &= 0
\end{align*} \] (B.2-5)

These equations can be re-written in matrix notation:

\[ \frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}_U}{\partial x} + \frac{\partial \vec{G}_U}{\partial y} + \frac{\partial \vec{H}_U}{\partial y} = 0 \] (B.6)

where $\vec{U}$ is the vector of conserved variables:

\[ \vec{U} = (m_1, m_2, m_3, \varepsilon, \rho_k)^t \] (B.7)

The fluxes in $x$, $y$ and $z$ directions are:

\[ \begin{align*}
\vec{F}_U &= (\rho uu + P, \rho vu, \rho uu + P, \rho Hu, \rho ku)^t \\
\vec{G}_U &= (\rho uv, \rho vv + P, \rho vw, \rho Hv, \rho kv)^t \\
\vec{H}_U &= (\rho uw, \rho vw + P, \rho ww + P, \rho Hw, \rho kw)^t
\end{align*} \] (B.8)

Table B.1: Summary of links between different set of variables and passage matrices involved in the wave decomposition process.
B.2. GOVERNING EQUATIONS

These equations can finally be written in quasi-linear form:

\[
\frac{\partial \tilde{U}}{\partial t} + A_U \frac{\partial \tilde{U}}{\partial x} + B_U \frac{\partial \tilde{U}}{\partial y} + C_U \frac{\partial \tilde{U}}{\partial y} = 0
\]

where \( A_U, B_U \) and \( C_U \) are the Jacobian matrices in the \( x, y \) and \( z \) directions:

\[
A_U = \frac{\partial \tilde{F}_U}{\partial \tilde{U}} \quad B_U = \frac{\partial \tilde{G}_U}{\partial \tilde{U}} \quad C_U = \frac{\partial \tilde{H}_U}{\partial \tilde{U}} \quad (B.9)
\]

The \( x \)-Jacobian matrix:

\[
A_U = \begin{pmatrix}
\frac{\partial F_{m1}}{\partial \tilde{m1}} & \frac{\partial F_{m1}}{\partial \tilde{m2}} & \frac{\partial F_{m1}}{\partial \tilde{m3}} & \frac{\partial F_{m1}}{\partial \tilde{m4}} & \frac{\partial F_{m1}}{\partial \tilde{m5}} \\
\frac{\partial F_{m2}}{\partial \tilde{m1}} & \frac{\partial F_{m2}}{\partial \tilde{m2}} & \frac{\partial F_{m2}}{\partial \tilde{m3}} & \frac{\partial F_{m2}}{\partial \tilde{m4}} & \frac{\partial F_{m2}}{\partial \tilde{m5}} \\
\frac{\partial F_{m3}}{\partial \tilde{m1}} & \frac{\partial F_{m3}}{\partial \tilde{m2}} & \frac{\partial F_{m3}}{\partial \tilde{m3}} & \frac{\partial F_{m3}}{\partial \tilde{m4}} & \frac{\partial F_{m3}}{\partial \tilde{m5}} \\
\frac{\partial F_{m4}}{\partial \tilde{m1}} & \frac{\partial F_{m4}}{\partial \tilde{m2}} & \frac{\partial F_{m4}}{\partial \tilde{m3}} & \frac{\partial F_{m4}}{\partial \tilde{m4}} & \frac{\partial F_{m4}}{\partial \tilde{m5}} \\
\frac{\partial F_{m5}}{\partial \tilde{m1}} & \frac{\partial F_{m5}}{\partial \tilde{m2}} & \frac{\partial F_{m5}}{\partial \tilde{m3}} & \frac{\partial F_{m5}}{\partial \tilde{m4}} & \frac{\partial F_{m5}}{\partial \tilde{m5}} \\
\end{pmatrix}
\]

Explicitely:

\[
A_U = \begin{pmatrix}
\frac{\partial \rho u u + \rho \sigma uu}{\partial \tilde{m1}} & \frac{\partial \rho u u + \rho \sigma uu}{\partial \tilde{m2}} & \frac{\partial \rho u u + \rho \sigma uu}{\partial \tilde{m3}} & \frac{\partial \rho u u + \rho \sigma uu}{\partial \tilde{m4}} & \frac{\partial \rho u u + \rho \sigma uu}{\partial \tilde{m5}} \\
\frac{\partial \rho \sigma uu}{\partial \tilde{m1}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m2}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m3}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m4}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m5}} \\
\frac{\partial \rho \sigma uu}{\partial \tilde{m1}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m2}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m3}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m4}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m5}} \\
\frac{\partial \rho \sigma uu}{\partial \tilde{m1}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m2}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m3}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m4}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m5}} \\
\frac{\partial \rho \sigma uu}{\partial \tilde{m1}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m2}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m3}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m4}} & \frac{\partial \rho \sigma uu}{\partial \tilde{m5}} \\
\end{pmatrix}
\]

so that:

\[
A_U = \begin{pmatrix}
2u - \beta u & -\beta v & -\beta w & \beta & -uu + \beta \sigma v + \chi_1 & \ldots & -uu + \beta \sigma v + \chi_N \\
v & u & 0 & 0 & -uv & \ldots & -uv \\
w & 0 & u & 0 & -uw & \ldots & -uw \\
Y - \beta uu & -\beta uv & -\beta uw & (1 + \beta)u & -uH + \beta \sigma v + u\chi_1 & \ldots & -uH + \beta \sigma v + u\chi_N \\
Y_1 & 0 & 0 & 0 & u - uY_1 & \ldots & u - uY_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
Y_N & 0 & 0 & 0 & -uY_N & \ldots & u - uY_N \\
\end{pmatrix}
\]
where $e_c$ is the kinetic energy and $H$, $\beta$ and $\chi$ are defined in the previous section (appendix B.1).

The $y$-Jacobian matrix:

$$B_U = \begin{pmatrix}
\frac{\partial G_{m1}}{\partial m_1} & \frac{\partial G_{m1}}{\partial m_2} & \frac{\partial G_{m1}}{\partial m_3} & \frac{\partial G_{m1}}{\partial m_4} & \frac{\partial G_{m1}}{\partial m_5} & \frac{\partial G_{m1}}{\partial p_k} \\
\frac{\partial G_{m2}}{\partial m_1} & \frac{\partial G_{m2}}{\partial m_2} & \frac{\partial G_{m2}}{\partial m_3} & \frac{\partial G_{m2}}{\partial m_4} & \frac{\partial G_{m2}}{\partial m_5} & \frac{\partial G_{m2}}{\partial p_k} \\
\frac{\partial G_{m3}}{\partial m_1} & \frac{\partial G_{m3}}{\partial m_2} & \frac{\partial G_{m3}}{\partial m_3} & \frac{\partial G_{m3}}{\partial m_4} & \frac{\partial G_{m3}}{\partial m_5} & \frac{\partial G_{m3}}{\partial p_k} \\
\frac{\partial G_{m4}}{\partial m_1} & \frac{\partial G_{m4}}{\partial m_2} & \frac{\partial G_{m4}}{\partial m_3} & \frac{\partial G_{m4}}{\partial m_4} & \frac{\partial G_{m4}}{\partial m_5} & \frac{\partial G_{m4}}{\partial p_k} \\
\frac{\partial G_{m5}}{\partial m_1} & \frac{\partial G_{m5}}{\partial m_2} & \frac{\partial G_{m5}}{\partial m_3} & \frac{\partial G_{m5}}{\partial m_4} & \frac{\partial G_{m5}}{\partial m_5} & \frac{\partial G_{m5}}{\partial p_k} \\
\frac{\partial G_{p_k}}{\partial m_1} & \frac{\partial G_{p_k}}{\partial m_2} & \frac{\partial G_{p_k}}{\partial m_3} & \frac{\partial G_{p_k}}{\partial m_4} & \frac{\partial G_{p_k}}{\partial m_5} & \frac{\partial G_{p_k}}{\partial p_k}
\end{pmatrix}$$

Explicitely:

$$B_U = \begin{pmatrix}
\frac{\partial \rho u}{\partial m_1} & \frac{\partial \rho u}{\partial m_2} & \frac{\partial \rho u}{\partial m_3} & \frac{\partial \rho u}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} \\
\frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} \\
\frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} \\
\frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} \\
\frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} \\
\frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k} & \frac{\partial \rho v}{\partial m_1} & \frac{\partial \rho v}{\partial m_2} & \frac{\partial \rho v}{\partial m_3} & \frac{\partial \rho v}{\partial p_k}
\end{pmatrix}$$

so that:

$$B_U = \begin{pmatrix}
v & u & 0 & 0 & \ldots & \ldots & -v u & \ldots & -v u \\
-v u & 2 v - \beta v & -\beta w & \beta & -v v + \beta e_c + \chi_1 & \ldots & -v v + \beta e_c + \chi N \\
0 & w & v & \beta & -v v & \ldots & -v w & \ldots & -v w \\
-\beta v u & H - \beta v v & -\beta w v & (1 + \beta)v & -v H + \beta v e_c + v \chi_1 & \ldots & -v H + \beta v e_c + v \chi N \\
0 & Y_1 & 0 & 0 & v - v Y_1 & \ldots & -v Y_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\
0 & Y N & 0 & 0 & -v Y N & \ldots & v - v Y N
\end{pmatrix}$$

The $z$-Jacobian matrix:
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Explicitly:

\[
C_U = \begin{pmatrix}
\frac{\partial H_{m_1}}{\partial m_1} & \frac{\partial H_{m_1}}{\partial m_2} & \frac{\partial H_{m_1}}{\partial m_3} & \frac{\partial H_{m_1}}{\partial E} & \frac{\partial \rho_k}{\partial H_{m_1}} \\
\frac{\partial H_{m_2}}{\partial m_1} & \frac{\partial H_{m_2}}{\partial m_2} & \frac{\partial H_{m_2}}{\partial m_3} & \frac{\partial H_{m_2}}{\partial E} & \frac{\partial \rho_k}{\partial H_{m_2}} \\
\frac{\partial H_{m_3}}{\partial m_1} & \frac{\partial H_{m_3}}{\partial m_2} & \frac{\partial H_{m_3}}{\partial m_3} & \frac{\partial H_{m_3}}{\partial E} & \frac{\partial \rho_k}{\partial H_{m_3}} \\
\frac{\partial H_{p_k}}{\partial m_1} & \frac{\partial H_{p_k}}{\partial m_2} & \frac{\partial H_{p_k}}{\partial m_3} & \frac{\partial \rho_k}{\partial H_{p_k}} & \frac{\partial \rho_k}{\partial \rho_k}
\end{pmatrix}
\]

so that

\[
C_U = \begin{pmatrix}
w & 0 & u & 0 & -wu & \ldots & -wu \\
0 & w & v & 0 & -wv & \ldots & -wv \\
-\beta u & -\beta v & 2w - \beta w & \beta & -ww + \beta e_c + \chi_1 & \ldots & -ww + \beta e_c + \chi_N \\
-\beta wu & -\beta wv & H - \beta w w & (1 + \beta)w & -wH + \beta ve_c + v \chi_1 & \ldots & -wH + \beta ve_c + v \chi_N \\
0 & 0 & Y_1 & 0 & w - wY_1 & \ldots & w - wY_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & Y_N & 0 & -wY_N & \ldots & w - wY_N
\end{pmatrix}
\]

The \( A_U, B_U \) and \( C_U \) Jacobian matrices are difficult to diagonalise. It is more convenient to reintroduce the primitive variables \( V \)

\[
V = (u, v, w, P, \rho_k)^t
\]

The \( M \) matrix allows to change from conserved variables \( U \) to primitive variables \( V \):

\[
\frac{\partial U}{\partial V} = M \cdot \frac{\partial V}{\partial V} \\
M = \frac{\partial U}{\partial V}
\]

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Obviously, the inverse relations hold:

\[ \partial V = M^{-1} \partial U \quad M^{-1} = \frac{\partial V}{\partial U} \]

The transformation matrices \( M \) and \( M^{-1} \) are:

\[
M = \begin{pmatrix}
0 & 0 & 0 & u & \ldots & u \\
0 & 0 & 0 & v & \ldots & v \\
0 & 0 & 0 & w & \ldots & w \\
\rho & 0 & 0 & 0 & \rho & \ldots & \rho \\
\rho u & \rho v & \rho w & 1 & \frac{e_c - \chi_1}{\beta} & \ldots & \frac{e_c - \chi_N}{\beta} \\
0 & 0 & 0 & 0 & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & 1
\end{pmatrix}
\]

\[
M^{-1} = \begin{pmatrix}
\frac{1}{\rho} & 0 & 0 & 0 & -\frac{u}{\rho} & \ldots & -\frac{u}{\rho} \\
0 & \frac{1}{\rho} & 0 & 0 & -\frac{v}{\rho} & \ldots & -\frac{v}{\rho} \\
0 & 0 & 1 & 0 & -\frac{w}{\rho} & \ldots & -\frac{w}{\rho} \\
\frac{1}{\rho} & 0 & 0 & 0 & -\frac{u}{\rho} & \ldots & -\frac{u}{\rho} \\
-\beta u & -\beta v & -\beta w & \beta & \beta e_c + \chi_1 & \ldots & \beta e_c + \chi_N \\
0 & 0 & 0 & 0 & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & 0 & \ldots & 1
\end{pmatrix}
\]

where \( e_c \) is the kinetic energy and \( H, \beta \) and \( \chi \) are defined as in the previous section (appendix B.1).

It is important to notice that the \( \partial \) operator is not applied to matrix \( M \). This means that the matrix does not change depending on the way variations are calculated and therefore on the choice of the formulation (i.e., Iwave) used for the characteristic decomposition. Now, Eq. (B.9) is multiplied by \( M^{-1} \):

\[
M^{-1} \frac{\partial M \partial V}{\partial t} + M^{-1} A U \frac{\partial M \partial V}{\partial x} + M^{-1} B U \frac{M \partial V}{\partial y} + M^{-1} C U \frac{M \partial V}{\partial z} = 0 \quad \text{(B.11)}
\]

to give the Euler equations written in quasi-linear form in primitive variables:

\[
\frac{\partial V}{\partial t} + A V \frac{\partial V}{\partial x} + B V \frac{\partial V}{\partial y} + C V \frac{\partial V}{\partial z} = 0 \quad \text{(B.12)}
\]

The Jacobians for primitive variables are then:
A.V. = M^{-1}.A_U.M \quad B.V. = M^{-1}.B_U.M \quad C.V. = M^{-1}.C_U.M \quad (B.13)

The primitive Jacobian matrices are thus:

\[
A.V. = \begin{pmatrix}
    u & 0 & 0 & \frac{1}{\rho} & 0 & \ldots & 0 \\
    0 & u & 0 & 0 & 0 & \ldots & 0 \\
    0 & 0 & u & 0 & 0 & \ldots & 0 \\
    \rho c^2 & 0 & 0 & u & 0 & \ldots & 0 \\
    \rho_1 & 0 & 0 & 0 & u & \ldots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    \rho_N & 0 & 0 & 0 & 0 & \ldots & u
\end{pmatrix}
\]

\[
B.V. = \begin{pmatrix}
    v & 0 & 0 & 0 & 0 & \ldots & 0 \\
    0 & v & 0 & \frac{1}{\rho} & 0 & \ldots & 0 \\
    0 & 0 & v & 0 & 0 & \ldots & 0 \\
    0 & \rho c^2 & 0 & v & 0 & \ldots & 0 \\
    0 & \rho_1 & 0 & 0 & v & \ldots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & \rho_N & 0 & 0 & 0 & \ldots & v
\end{pmatrix}
\]

\[
C.V. = \begin{pmatrix}
    w & 0 & 0 & 0 & 0 & \ldots & 0 \\
    0 & w & 0 & 0 & 0 & \ldots & 0 \\
    0 & 0 & w & \frac{1}{\rho} & 0 & \ldots & 0 \\
    0 & 0 & \rho c^2 & w & 0 & \ldots & 0 \\
    0 & 0 & \rho_1 & 0 & w & \ldots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & \rho_N & 0 & 0 & \ldots & w
\end{pmatrix}
\]

The next step is to write this system of equations in the basis associated to the boundary \((\vec{n},\vec{t}_1,\vec{t}_2)\). For simplicity the derivation is described first in two dimensions and then extended in 3D.

The transformation can be done in two steps: first, a change of coordinates \((x,y) \Rightarrow (X,Y)\) must be performed and second, the velocity must be expressed in this new orthogonal basis \(\vec{s} = u\vec{i} + v\vec{j} = u_n\vec{n} + u_t\vec{t}\).

Let \(\vec{p}\) be a generic space vector. It can be written as:

\[
\vec{p} = x\vec{i} + y\vec{j} = X\vec{n} + Y\vec{t} \quad (B.14)
\]
APPENDIX B. CHARACTERISTIC WAVE DECOMPOSITION

The vectors containing their coordinates are noted as:

\[ P_{(\vec{i}, \vec{j})} = \begin{pmatrix} x \\ y \end{pmatrix} \quad \text{and} \quad P_{(\vec{n}, \vec{t})} = \begin{pmatrix} X \\ Y \end{pmatrix} \]

(B.15)

These two vectors are linked by a rotation matrix \( \Omega_\Theta \) by:

\[ P_{(\vec{i}, \vec{j})} = \Omega_\Theta P_{(\vec{n}, \vec{t})} \]

(B.16)

where \( \Theta \) is the angle of rotation. The matrix \( \Omega_\Theta \) can be written as:

\[ \Omega_\Theta = \begin{pmatrix} \cos \Theta & \sin \Theta \\ -\sin \Theta & \cos \Theta \end{pmatrix} = \begin{pmatrix} n_x & t_x \\ n_y & t_y \end{pmatrix} \]

(B.17)

where \( \vec{n} = n_x \vec{i} + n_y \vec{j} \) and \( \vec{t} = t_x \vec{i} + t_y \vec{j} \).

The matrix \( \Omega_\Theta \) is orthogonal:

\[ \Omega_\Theta^{-1} = \Omega_\Theta^T = \Omega_{-\Theta} \]

(B.18)

An interesting property is that:

\[ d\vec{p} = dx\vec{i} + dy\vec{j} = dX\vec{n} + dY\vec{t} \]

(B.19)

and thus:

\[ \begin{pmatrix} dx \\ dy \end{pmatrix} = \Omega_\Theta \begin{pmatrix} dx \\ dy \end{pmatrix} \quad \text{or} \quad dP_{(\vec{i}, \vec{j})} = \Omega_\Theta dP_{(\vec{n}, \vec{t})} \]

(B.20)

One can thus write for any scalar field \( Z \):

\[ dZ = \frac{\partial Z}{\partial x} dx + \frac{\partial Z}{\partial y} dy = (\nabla Z)_{(\vec{i}, \vec{j})} dP_{(\vec{i}, \vec{j})} \]

(B.21)

and

\[ dZ = \frac{\partial Z}{\partial X} dX + \frac{\partial Z}{\partial Y} dY = (\nabla Z)_{(\vec{n}, \vec{t})} dP_{(\vec{n}, \vec{t})} \]

(B.22)

with:

\[ (\nabla Z)_{(\vec{i}, \vec{j})} = \left( \frac{\partial Z}{\partial x}, \frac{\partial Z}{\partial y} \right) \quad \text{and} \quad (\nabla Z)_{(\vec{n}, \vec{t})} = \left( \frac{\partial Z}{\partial X}, \frac{\partial Z}{\partial Y} \right) \]

(B.23)

This finally gives:

\[ (\nabla Z)_{(\vec{i}, \vec{j})} = (\nabla Z)_{(\vec{n}, \vec{t})} \Omega_\Theta^{-1} \]

(B.24)

or explicitly

\[ \begin{cases} \frac{\partial Z}{\partial x} = n_x \frac{\partial Z}{\partial X} + t_x \frac{\partial Z}{\partial Y} \\ \frac{\partial Z}{\partial y} = n_y \frac{\partial Z}{\partial X} + t_y \frac{\partial Z}{\partial Y} \end{cases} \]

(B.25)
Eq. (B.12) can be recast in the \((\vec{n}, \vec{t})\) basis:

\[
\frac{\partial V}{\partial t} + (A V n_x + B V n_y) \frac{\partial V}{\partial X} + (A V t_x + B V t_y) \frac{\partial V}{\partial Y} = 0 \tag{B.26}
\]

The final transformation is to make a new change of variable:

\[
V_{2D} = \Omega_{V_{2D}} V_{n2D} \tag{B.27}
\]

with:

\[
V_{n2D} = (u_n, u_t, P, \rho_1, \ldots, \rho_N)^T \tag{B.28}
\]

being the primitive variables with the velocity now written in the \((\vec{n}, \vec{t})\) basis. The matrix \(\Omega_{V_{2D}}\) is thus:

\[
\Omega_{V_{2D}} = \begin{pmatrix}
    n_x & t_x & 0 & 0 & \cdots & 0 \\
    n_y & t_y & 0 & 0 & \cdots & 0 \\
    0 & 0 & 1 & 0 & \cdots & 0 \\
    0 & 0 & 0 & 1 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix} \tag{B.29}
\]

The inverse matrix is just:

\[
\Omega_{V_{2D}}^{-1} = \Omega_{V_{2D}}^T = \begin{pmatrix}
    n_x & n_y & 0 & 0 & \cdots & 0 \\
    t_x & t_y & 0 & 0 & \cdots & 0 \\
    0 & 0 & 1 & 0 & \cdots & 0 \\
    0 & 0 & 0 & 1 & \cdots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix} \tag{B.30}
\]

In three dimensions two vectors are linked by a rotation matrix \(\Omega_{\Theta_1, \Theta_2, \Theta_3}\) by:

\[
P_{(i,j,k)} = \Omega_{\Theta_1, \Theta_2, \Theta_3} P_{(\vec{i}, \vec{j}, \vec{k})} \tag{B.31}
\]

where \(\Theta_1, \Theta_2, \Theta_3\) are the angles of rotation around the three axis \((\vec{i}, \vec{j}, \vec{k})\). The matrix \(\Omega_{\Theta}\) can be written as the product of three bi-dimensionnal rotation matrices:

\[
\Omega_{\Theta_1, \Theta_2, \Theta_3} = \begin{pmatrix}
    \cos \Theta_1 & \sin \Theta_1 & 0 \\
    -\sin \Theta_1 & \cos \Theta_1 & 0 \\
    0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
    \cos \Theta_2 & 0 & \sin \Theta_2 \\
    0 & 1 & 0 \\
    -\sin \Theta_2 & 0 & \cos \Theta_2
\end{pmatrix} \begin{pmatrix}
    1 & 0 & 0 \\
    0 & \cos \Theta_3 & \sin \Theta_3 \\
    0 & -\sin \Theta_3 & \cos \Theta_3
\end{pmatrix}
\]
In summary, the matrix $\Omega_V$ allows to change from variables $V$ in $(\vec{i}, \vec{j}, \vec{k})$ frame to variables $V_n$ in $(\vec{n}, \vec{t}_1, \vec{t}_2)$ frame. The link between $V_n$ and $V$ is:

$$ V = \Omega_V V_n $$  \hspace{1cm} (B.32)

with

$$ V_n = (u_n, u_{t_1}, u_{t_2}, P, \rho_1, \ldots, \rho_N)^T $$  \hspace{1cm} (B.33)

These are the same variables as $V$ except for the velocity which is now written in the $(\vec{n}, \vec{t}_1, \vec{t}_2)$ basis. The matrix $\Omega_V$ is thus:

$$ \Omega_V = \begin{pmatrix}
  n_x & t_{1x} & t_{2x} & 0 & 0 & \cdots & 0 \\
  n_y & t_{1y} & t_{2y} & 0 & 0 & \cdots & 0 \\
  n_z & t_{1z} & t_{2z} & 0 & 0 & \cdots & 0 \\
  0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix} $$  \hspace{1cm} (B.34)

The inverse matrix is just:

$$ \Omega_V^{-1} = \Omega_V^T = \begin{pmatrix}
  n_x & n_y & n_z & 0 & 0 & \cdots & 0 \\
  t_{1x} & t_{1y} & t_{1z} & 0 & 0 & \cdots & 0 \\
  t_{2x} & t_{2y} & t_{2z} & 0 & 0 & \cdots & 0 \\
  0 & 0 & 0 & 1 & 0 & \cdots & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \cdots & 1
\end{pmatrix} $$  \hspace{1cm} (B.35)

The calculation of the terms of this matrix can be found in AVBP normals\_bface.F and tangential\_F routines.

As before, the change of variables in Eq. (B.26) is performed by multiplying by $\Omega_V^{-1}$:

$$ \Omega_V^{-1} \frac{\partial V_n}{\partial t} + \Omega_V^{-1} A_n \frac{\partial V_n}{\partial X} + \Omega_V^{-1} B_n \frac{\partial V_n}{\partial Y} + \Omega_V^{-1} C_n \frac{\partial V_n}{\partial Z} = 0 $$  \hspace{1cm} (B.36)

where

$$ A_n = A_V n_x + B_V n_y + C_V n_z $$

$$ B_n = A_V t_{1x} + B_V t_{1y} + C_V t_{1z} $$

$$ C_n = A_V t_{2x} + B_V t_{2y} + C_V t_{2z} $$
or, in a more compact form:

$$ \frac{\partial V_n}{\partial t} + N \frac{\partial V_n}{\partial X} + T_1 \frac{\partial V_n}{\partial Y} + T_2 \frac{\partial V_n}{\partial Z} = 0 $$  \hspace{1cm} (B.37)
with:

\[
N = \Omega_V^{-1} A_n \Omega_V \tag{B.38}
\]

and

\[
T_1 = \Omega_V^{-1} B_n \Omega_V \tag{B.39}
\]

\[
T_2 = \Omega_V^{-1} C_n \Omega_V \tag{B.40}
\]

The matrix \( N \), contains the normal Jacobian in primitive variables and can now be diagonalised to decompose the system into characteristic waves:

\[
D = L.N.L^{-1} = L.N.R \tag{B.41}
\]

\[
N = L^{-1}.D.L = R.D.L \tag{B.42}
\]

\( D \) is the diagonal matrix that contains the eigenvalues of the system, \( L \) is the matrix composed of the left eigenvectors (ordered in rows) and \( R \) is the matrix of right eigenvectors (ordered in columns)

\[
L = \begin{pmatrix}
1 & 0 & 0 & \frac{1}{\rho c} & 0 & \ldots & 0 \\
-1 & 0 & 0 & \frac{1}{\rho c} & 0 & \ldots & 0 \\
0 & 1 & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & -\frac{\gamma}{c^2} & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & -\frac{\gamma}{c^2} & 0 & \ldots & 1 \\
\end{pmatrix}
\]

and

\[
R = \begin{pmatrix}
\frac{1}{\tau} & -\frac{1}{\tau} & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 1 & 0 & \ldots & 0 \\
0 & 0 & 0 & \frac{\rho c}{\tau} & \frac{\rho c}{\tau} & 0 & \ldots & 0 \\
0 & 0 & 0 & \frac{\rho c}{\tau} & \frac{\rho c}{\tau} & 0 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\rho_n & \rho_n & \rho_n & \rho_n & \rho_n & \ldots & 1 \\
\end{pmatrix} \tag{B.43}
\]

\[
D = \begin{pmatrix}
\ddot{u} \cdot \ddot{n} + c & \ddot{u} \cdot \ddot{n} - c & 0 \\
\ddot{u} \cdot \ddot{n} & \ddot{u} \cdot \ddot{n} & 0 \\
\ddot{u} \cdot \ddot{n} & \ddot{u} \cdot \ddot{n} & 0 \\
\ddot{u} \cdot \ddot{n} & \ddot{u} \cdot \ddot{n} & \ddots \\
\ddot{u} \cdot \ddot{n} & \ddot{u} \cdot \ddot{n} & \ddot{u} \cdot \ddot{n} \\
\end{pmatrix}
\]

It must be noticed that three eigenvectors are associated to the same eigenvalue \( \ddot{u} \cdot \ddot{n} \). This means that the choice of right and left eigenvectors is not unique because every linear combination of these three eigenvectors is still an eigenvector of the system. More details on this issue
can be found in section B.3 related to the actual coding. In this derivation only the normal Jacobi-
ian has been diagonalised, this means that the flow is decomposed into waves travelling nor-
mally to the boundary. However, no unique direction of propagation exists in multidimensional
problems, because the jacobian matrices $N$, $T_1$ and $T_2$ are not simultaneously diagonalizable.
Fortunately, the boundary condition analysis only requires that any one coordinate direction be
diagonalizable at a time, and this may always be done. So, even tangent jacobian matrices can,
in theory, be decomposed into waves propagating in the two tangent directions. This appoach
is useful for the treatment of edge and corners even if the implementation is somehow cumber-
some. In AVBP, the decomposition is performed only for the direction normal to the boundary
since most important physical aspects of the flow (i.e. acoustics) can be taken into account in
this way.

The transformation into characteristic variables $\partial W$ can be recast as

\[
\begin{align*}
\partial W &= L \partial V_n \\
\partial V_n &= L^{-1} \partial W = R \partial W \\
\end{align*}
\]

(B.44)

So, multiplying Eq. B.37 by $L$ gives:

\[
L \frac{\partial V_n}{\partial t} + LL^{-1} DL \frac{\partial V_n}{\partial X} + LT_1 L^{-1} L \frac{\partial V_n}{\partial Y} + LT_2 L^{-1} L \frac{\partial V_n}{\partial Z} = 0
\]

(B.45)

that leads to

\[
\frac{\partial W}{\partial t} + D \frac{\partial W}{\partial X} + LT_1 L^{-1} \frac{\partial W}{\partial Y} + LT_2 L^{-1} \frac{\partial W}{\partial Z} = 0
\]

(B.46)

$L$ and $L^{-1}$ perform the passage from the variations of primitive variables to the variations of the
characteristic variables without making any assumptions on how to calculate these variations.
This is very important since it allows the use of different formulations for describing physical
quantities variations.

Now that we have obtained the variation of characteristic variables $\partial W$ from the variation of
primitive variables in a local normal basis $\partial V_n$ we can start going back. Reminding that

\[
D = L.N.R \\
N = \Omega V^{-1} A_n.\Omega V
\]

we obtain for $D$

\[
D = L.\Omega V^{-1}.A_n.\Omega V.R
\]

(B.47)

and defining now

\[
L_V = L.\Omega V^{-1} \\
R_V = \Omega V.R
\]
as

\[ L_V = \begin{pmatrix}
    n_x & n_y & n_z & \frac{1}{\rho c} & 0 & \ldots & 0 \\
    -n_x & -n_y & -n_z & \frac{1}{\rho c} & 0 & \ldots & 0 \\
    t_{1x} & t_{1y} & t_{1z} & 0 & 0 & \ldots & 0 \\
    t_{2x} & t_{2y} & t_{2z} & 0 & 0 & \ldots & 0 \\
    0 & 0 & 0 & -\frac{\rho}{c^2} & 1 & \ldots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & -\frac{\rho}{c^2} & 0 & \ldots & 1
\end{pmatrix} \]

\[ R_V = \begin{pmatrix}
    \frac{1}{\rho c} & -n_x & t_{1x} & t_{2x} & 0 & \ldots & 0 \\
    \frac{1}{\rho c} & -n_y & t_{1y} & t_{2y} & 0 & \ldots & 0 \\
    \frac{1}{\rho c} & -n_z & t_{1z} & t_{2z} & 0 & \ldots & 0 \\
    \rho & \rho & 0 & 0 & 0 & \ldots & 0 \\
    \rho & \rho & 0 & 0 & 1 & \ldots & 0 \\
    \rho & \rho & 0 & 0 & 0 & \ldots & 1
\end{pmatrix} \]

characteristic variables can be obtained directly from primitive variables in a global basis using the following relations:

\[ \partial W = L_V \partial V \]
\[ \partial V = R_V \partial W \]

In the same way, reminding that:

\[ A_V = M^{-1} A_U M \]  \hspace{1cm} (B.48)

we can define the following matrices

\[ L_U = L_V M^{-1} \]
\[ R_U = M R_V \]

\[ L_U = \begin{pmatrix}
    -\frac{\beta u - cn_x}{\rho c} & -\frac{\beta v - cn_y}{\rho c} & -\frac{\beta w - cn_z}{\rho c} & \frac{\beta}{\rho c} & \frac{\beta}{\rho c} (\frac{\beta e + \chi_1}{c^2} - \frac{\beta}{c} \bar{u}) & \ldots & \frac{\beta}{\rho c} (\frac{\beta e + \chi_N}{c^2} - \frac{\beta}{c} \bar{u}) \\
    -\frac{\beta u + cn_x}{\rho c} & -\frac{\beta v + cn_y}{\rho c} & -\frac{\beta w + cn_z}{\rho c} & \frac{\beta}{\rho c} & \frac{\beta}{\rho c} (\frac{\beta e + \chi_1}{c^2} + \frac{\beta}{c} \bar{u}) & \ldots & \frac{\beta}{\rho c} (\frac{\beta e + \chi_N}{c^2} + \frac{\beta}{c} \bar{u}) \\
    \frac{n_x}{\rho} & \frac{n_y}{\rho} & \frac{n_z}{\rho} & 0 & -\frac{\bar{u}}{c} & \ldots & -\frac{\bar{u}}{c} \\
    \frac{n_x}{\rho} & \frac{n_y}{\rho} & \frac{n_z}{\rho} & 0 & -\frac{\bar{u}}{c} & \ldots & -\frac{\bar{u}}{c} \\
    \frac{\beta u Y_1}{c^2} & \frac{\beta v Y_1}{c^2} & \frac{\beta w Y_1}{c^2} & -\frac{\beta Y_1}{c^2} & -Y_1 (\frac{\beta e + \chi_1}{c^2}) + 1 & \ldots & -Y_1 (\frac{\beta e + \chi_N}{c^2}) \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    \frac{\beta u Y_N}{c^2} & \frac{\beta v Y_N}{c^2} & \frac{\beta w Y_N}{c^2} & -\frac{\beta Y_N}{c^2} & -Y_N (\frac{\beta e + \chi_1}{c^2}) & \ldots & -Y_N (\frac{\beta e + \chi_N}{c^2}) + 1
\end{pmatrix} \]  \hspace{1cm} (B.49)
APPENDIX B. CHARACTERISTIC WAVE DECOMPOSITION

\[ R_U = \begin{pmatrix}
\frac{\rho}{p_x}(u + cn) & \frac{\rho}{p_x}(u - cn) & \rho \tau_1 & \rho \tau_2 & u & \ldots & u \\
\frac{\rho}{p_x}(v + cn) & \frac{\rho}{p_x}(v - cn) & \rho \tau_1 & \rho \tau_2 & v & \ldots & v \\
\frac{\rho}{p_x}(w + cn) & \frac{\rho}{p_x}(w - cn) & \rho \tau_1 & \rho \tau_2 & w & \ldots & w \\
\frac{\rho}{p_x} e_c + c u \bar{n} + \frac{c^2}{p} \bar{z} & \frac{\rho}{p_x} (e_c - c u \bar{n} + \frac{c^2}{p} \bar{z}) & \rho u \bar{r}_1 & \rho u \bar{r}_2 & e_c - \frac{c}{p} & \ldots & e_c - \frac{c}{p} \\
\rho \frac{\rho}{p_x} & \rho \frac{\rho}{p_x} & 0 & 0 & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
\rho \frac{\rho}{p_x} & \rho \frac{\rho}{p_x} & 0 & 0 & 0 & \ldots & 1 \\
\end{pmatrix} \]

The following relations allow the passage from conserved variables in a global basis to characteristic variables.

\[ \partial W = L_U \partial U \]
\[ \partial U = R_U \partial W \]

The following relations show wave definitions (\(\partial W\) with the notation used for primitive and conservative variables. Moreover, some useful identities obtained with the following inverse relations are detailed.

\[ \partial V = R_V \partial W \quad \partial U = R_U \partial W \]  

(B.51)

In primitive variables, we have:

\[
\begin{align*}
\partial W^1 &= + \tilde{n} \partial \tilde{u} + \frac{1}{p_c} \partial P \\
\partial W^2 &= - \tilde{n} \partial \tilde{u} + \frac{1}{p_c} \partial P \\
\partial W^3 &= + \tilde{n} \partial \bar{u} \\
\partial W^4 &= + \tilde{n} \partial \bar{u} \\
\partial W^{4+k} &= - \frac{c}{\tilde{n}} \partial P + \partial \rho \end{align*}
\]

\[ \lambda^1 = \tilde{u} \bar{n} + c \]
\[ \lambda^2 = \tilde{u} \bar{n} - c \]
\[ \lambda^3 = \bar{u} \tilde{n} \]
\[ \lambda^{4+k} = \bar{u} \tilde{n} \]

While in conserved variables:

\[
\begin{align*}
\partial W^1 &= - \frac{1}{p_c} (\beta \bar{u} - c \bar{n}) \partial \rho \bar{u} + \frac{1}{p_c} \partial \mathcal{E} + \sum_k \frac{1}{p} \left( - \tilde{u} \bar{n} + \frac{\beta e_c + \chi_c}{c} \right) \partial \rho_k \\
\partial W^2 &= - \frac{1}{p_c} (\beta \bar{u} + c \bar{n}) \partial \rho \bar{u} + \frac{1}{p_c} \partial \mathcal{E} + \sum_k \frac{1}{p} \left( + \tilde{u} \bar{n} + \frac{\beta e_c + \chi_c}{c} \right) \partial \rho_k \\
\partial W^3 &= \frac{1}{p} \bar{e}_1 \partial \rho \bar{u} - \sum_k \frac{\bar{e}_1}{p} \partial \rho_k \\
\partial W^4 &= \frac{1}{p} \bar{e}_2 \partial \rho \bar{u} - \sum_k \frac{\bar{e}_2}{p} \partial \rho_k \\
\partial W^{4+k} &= \frac{\beta y_c}{c} \partial \rho \bar{u} - \frac{\beta y_c}{c} \partial \mathcal{E} + \partial \rho_k - \frac{y_c}{c} \sum_j (\beta e_c + \chi_j) \partial \rho_j \\
\end{align*}
\]

One can also find the entropy wave \(\partial W^S\) by adding all the species waves \(W^{4+k}\). \(\partial W^S\) is a linear combination of eigenvectors that have the same eigenvalue \(\tilde{u} \bar{n}\) and thus this pseudo-wave is also convected at the speed \(\tilde{u} \bar{n}\).

\[ \partial W^S = \sum_j \partial W^{4+k} = \partial \rho - \frac{\partial P}{c^2} \]

\[ \lambda^S = \tilde{u} \bar{n} \]

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We also have the following inverse relations:
\[
\begin{align*}
\partial (\bar{u}, \bar{n}) & = \frac{1}{2} (\partial W^1 - \partial W^2) \\
\partial (\bar{u}, \bar{n}_1) & = \partial W^3 \\
\partial (\bar{u}, \bar{n}_2) & = \partial W^4 \\
\partial u & = \frac{1}{2} n_1 (\partial W^1 - \partial W^2) + t_1 x \partial W^3 + t_2 x \partial W^4 \\
\partial v & = \frac{1}{2} n_1 (\partial W^1 - \partial W^2) + t_1 y \partial W^3 + t_2 y \partial W^4 \\
\partial w & = \frac{1}{2} n_2 (\partial W^1 - \partial W^2) + t_1 z \partial W^3 + t_2 z \partial W^4 \\
\partial P & = \frac{1}{2} \rho c (\partial W^1 + \partial W^2) \\
\partial \rho_k & = \frac{1}{2} \rho c (\partial W^1 + \partial W^2) + \partial W^{4+k} \\
\partial \rho & = \frac{1}{2} \rho (\partial W^1 + \partial W^2) + \partial W^S \\
\partial Y_k & = \frac{1}{2} \rho (\partial W^{4+k} - Y_k \partial W^S) \\
\partial \tau & = \frac{1}{2} \rho \left( \sum_k \eta_k (\partial W^{4+k} - \tau \partial W^S) \right) \\
\partial T & = \frac{1}{2} \rho \left( \partial W^1 + \partial W^2 \right) - \sum_j \frac{r_j T}{\rho} \partial W^{4+j} \\
\partial \rho u & = \rho (u+c_n) \partial W^1 + \rho (u-c_n) \partial W^2 + \rho t_1 x \partial W^3 + \rho t_2 x \partial W^4 + u \partial W^S \\
\partial \rho v & = \rho (v+c_n) \partial W^1 + \rho (v-c_n) \partial W^2 + \rho t_1 y \partial W^3 + \rho t_2 y \partial W^4 + v \partial W^S \\
\partial \rho w & = \rho (w+c_n) \partial W^1 + \rho (w-c_n) \partial W^2 + \rho t_1 z \partial W^3 + \rho t_2 z \partial W^4 + w \partial W^S \\
\end{align*}
\]

B.3. SOME HINTS ON THE ACTUAL CODING

This chapter is intended for users who want to look into the eigvec_array.F file. It describes the passage matrix \( L_{AB}^{AVBP} \) and \( R_{AB}^{AVBP} \) coded into eigvec_array.F. As said before these matrices allow for the base change from conservative \((U)\) into characteristic \((W)\) variables and vice versa. Conservative variables transported in AVBP are \( U = (\rho, \rho u, \rho v, \rho w, \rho \beta, \rho \nu) \). Since \( \rho = \sum_k \rho_k \), the system is then overdefined because we have both the entropy wave \((\rho)\) and all the species waves \((\rho_k)\). Waves in the following matrices are ordered with the strength notation, this is the reason why \( L_{AB}^{AVBP} \) and \( R_{AB}^{AVBP} \) detailed here look different from \( L_U \) and \( R_U \) (eqs. B.49 and B.50).

\[
L_{AB}^{AVBP} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & \ldots & 0 \\
0 & -\bar{t}_1 & \bar{t}_1 & 0 & 0 & \ldots & -\bar{u}_1 \bar{n}_1 \\
0 & \bar{t}_2 & -\bar{t}_2 & \bar{t}_2 & 0 & \ldots & -\bar{u}_2 \bar{n}_2 \\
0 & \bar{t}_1 & -\bar{t}_1 & \bar{t}_1 & 0 & \ldots & -\bar{u}_1 \bar{n}_1 \\
0 & -\bar{u}_1 & \bar{u}_1 & \bar{u}_1 & 0 & \ldots & -\bar{u}_1 \bar{n}_1 \\
0 & \bar{u}_2 & -\bar{u}_2 & \bar{u}_2 & 0 & \ldots & -\bar{u}_2 \bar{n}_2 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\
0 & \bar{u}_N & -\bar{u}_N & \bar{u}_N & 0 & \ldots & -\bar{u}_1 \bar{n}_1 \\
\end{pmatrix}
\]
APPENDIX B. CHARACTERISTIC WAVE DECOMPOSITION

\[
R_{AVBP}^U = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
0 & \rho t_1x & \rho t_2x & \frac{\rho}{\rho_t} (u + cn_x) & \frac{\rho}{\rho_t} (u - cn_x) & u & \cdots & u \\
0 & \rho t_1y & \rho t_2y & \frac{\rho}{\rho_t} (v + cn_y) & \frac{\rho}{\rho_t} (v - cn_y) & v & \cdots & v \\
0 & \rho t_1z & \rho t_2z & \frac{\rho}{\rho_t} (w + cn_z) & \frac{\rho}{\rho_t} (w - cn_z) & w & \cdots & w \\
0 & \rho \vec{u} \cdot \vec{i}_1 & \rho \vec{u} \cdot \vec{i}_2 & \frac{\rho}{\rho_t} (e_c + c\vec{u} \cdot \vec{n} + \frac{c^2 - Z}{\beta} \vec{n}) & \frac{\rho}{\rho_t} (e_c - c\vec{u} \cdot \vec{n} + \frac{c^2 - Z}{\beta} \vec{n}) & e_c - \frac{\beta}{\rho_t} \vec{n} & \cdots & e_c - \frac{\beta}{\rho_t} \vec{n} \\
0 & 0 & 0 & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & 1 & \cdots & 0 \\
0 & 0 & 0 & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & \frac{\rho}{\rho_t} & 0 & \cdots & 1 \\
\end{pmatrix}
\]

In this formulation the "global" entropy wave has been removed (the first row and column are zero!). Now the entropy wave can truly be recast by summing all the species waves. This formulation can be considered as a first step towards the harder task of taking away the density equation everywhere in AVBP (now density is calculated and then overwritten by the sum of \( \rho_k \)). In AVBP 5.5, by switching the flag (called man_flag) present in bcsubsonic.F it is possible to choose between this new non-overdefined formulation and the old one. First tests show no important differences between the two forms at least as far as mass is conserved.

As said in the previous section three eigenvectors are associated to the same eigenvalue. This means that the choice of right and left eigenvectors is not unique because every linear combination of these three eigenvectors is still an eigenvector of the system. Hirsch [35] defined an adapted set of eigenvectors which did not require the calculation of the orthonormal basis \( (\vec{n}, \vec{t}_1, \vec{t}_2) \). The disadvantage is that entropic and shear waves are mixed, leading to problems to impose boundary conditions. In AVBP, to have separated waves, the approach of M. Manna (PhD Thesis 1992) is followed. In this derivation an if statement is introduced in the construction of the orthonormal basis giving:

for \( |n_z| > 0.7 \)

\[
\vec{t}_1 = \frac{1}{\sqrt{n_x^2 + n_y^2}} \begin{pmatrix}
0 \\
-n_z \\
n_y \\
\end{pmatrix} \quad \vec{t}_2 = \frac{1}{\sqrt{n_x^2 + n_y^2}} \begin{pmatrix}
n_z^2 + n_y^2 \\
-n_x n_y \\
-n_x n_z \\
\end{pmatrix} \quad (B.52)
\]

for \( |n_z| \leq 0.7 \)

\[
\vec{t}_1 = \frac{1}{\sqrt{n_x^2 + n_y^2}} \begin{pmatrix}
n_y \\
-n_z \\
0 \\
\end{pmatrix} \quad \vec{t}_2 = \frac{1}{\sqrt{n_x^2 + n_y^2}} \begin{pmatrix}
n_z n_x \\
n_z n_y \\
n_z^2 + n_y^2 \\
\end{pmatrix} \quad (B.53)
\]

This approach is not used for 2D cases since there is no ambiguity in the basis definition. The orthonormal basis is calculated in the tangential.F file.
B.4 Link between AVBP formulation and original NSCBC

This section presents some theory about the NSCBC method [75]. Following the development of Poinsoit [75] we can introduce the $L$ notation for wave amplitude variations:

$$L = \lambda \frac{\partial W}{\partial n}$$

(B.54)

The link between $L$ and $\partial W$ formulations is detailed in table B.2. To recast the original notation of Poinsoit, acoustic waves should be multiplied by $\rho c$ and species waves by $c^2$.

<table>
<thead>
<tr>
<th>Type</th>
<th>Way</th>
<th>NSCBC MS [64]</th>
<th>AVBP V5.X</th>
<th>Annex B</th>
</tr>
</thead>
<tbody>
<tr>
<td>acoustic wave</td>
<td>out</td>
<td>$-L_2 \Delta t$</td>
<td>strength(5)</td>
<td>$\partial W^2$</td>
</tr>
<tr>
<td>entropy wave</td>
<td>in</td>
<td>$-L_S \Delta t$</td>
<td>strength(1)</td>
<td>$\partial W^s$</td>
</tr>
<tr>
<td>transverse shear</td>
<td>in</td>
<td>$-L_{t1} \Delta t$</td>
<td>strength(2)</td>
<td>$\partial W^3$</td>
</tr>
<tr>
<td>transverse shear</td>
<td>in</td>
<td>$-L_{t2} \Delta t$</td>
<td>strength(3)</td>
<td>$\partial W^4$</td>
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<td>in</td>
<td>$-L_+ \Delta t$</td>
<td>strength(4)</td>
<td>$\partial W^1$</td>
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<tr>
<td>species waves</td>
<td>in</td>
<td>$-L_k \Delta t$</td>
<td>strength(5+k)</td>
<td>$\partial W^{4+k}$</td>
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<tr>
<th>Type</th>
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<th>AVBP V5.X</th>
<th>Annex B</th>
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<td>strength(4)</td>
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<td>entropy wave</td>
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<td>transverse shear</td>
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<td>$\partial W^4$</td>
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<tr>
<td>acoustic wave</td>
<td>out</td>
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<td>strength(5)</td>
<td>$\partial W^1$</td>
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<td>$-L_k \Delta t$</td>
<td>strength(5+k)</td>
<td>$\partial W^{4+k}$</td>
</tr>
</tbody>
</table>

Table B.2: Correspondance between notations in the NSCBC_Ms paper [64], the $\partial W$ notation and the strength in the AVBP implementation (in 3D).

Values for the amplitude variations in the spatial form are:

$$\begin{pmatrix} L_+ \\ L_- \\ L_{t1} \\ L_{t2} \\ L_k \end{pmatrix} = \begin{pmatrix} (u_n + c) \left( \frac{\partial u_n}{\partial n} + \frac{1}{\rho c} \frac{\partial P}{\partial n} \right) \\ (u_n - c) \left( -\frac{\partial u_n}{\partial n} + \frac{1}{\rho c} \frac{\partial P}{\partial n} \right) \\ \frac{\partial u_n}{\partial n} \\ \frac{\partial u_n}{\partial n} \\ u_n \left( \frac{\partial \rho_k}{\partial n} - \frac{\gamma c^2}{c^2} \frac{\partial P}{\partial n} \right) \end{pmatrix}$$

(B.55)
APPENDIX B. CHARACTERISTIC WAVE DECOMPOSITION

with the associated propagation velocities

\[
\begin{pmatrix}
\lambda_+ \\
\lambda_- \\
\lambda_{t1} \\
\lambda_{t2} \\
\lambda_k
\end{pmatrix} =
\begin{pmatrix}
u_n + c \\
u_n - c \\
u_n \\
u_n \\
u_n
\end{pmatrix}
\]  
(B.56)

The acoustic waves \( \mathcal{L}_+ \) and \( \mathcal{L}_- \) are convected respectively at the velocity \( u_n + c \) and \( u_n - c \). All other waves are convected with the flow at the velocity \( u_n \). The waves \( \mathcal{L}_{t1} \) and \( \mathcal{L}_{t2} \) are shear waves. The remaining waves \( \mathcal{L}_k \) (for \( k = 1 \) to \( N \)) are species waves. The entropy wave \( \mathcal{L}_S \) is not explicitely used but can be constructed simply by adding all \( N \) species waves:

\[
\mathcal{L}_S = \sum_{k=1}^{N} \mathcal{L}_k = u_n \left( -\frac{1}{c^2} \frac{\partial P}{\partial n} + \frac{\partial \rho}{\partial n} \right)
\]  
(B.57)

The central idea of characteristic methods for boundary conditions is to identify the outgoing and incoming waves crossing a boundary. The outgoing waves carry information from the interior of the domain and must be kept as computed by the numerical scheme. However, the incoming waves carry information coming from the outside (i.e. controlled by the boundary condition). They cannot be computed from interior points data \([75]\). The principle of NSCBC is to infer the amplitude of the incoming waves from the amplitude of the outgoing waves using appropriate LODI (Local One Dimensional Inviscid) relations \([75]\). These LODI relations are obtained by writing (B.37) near the boundary as if the flow were locally inviscid and one-dimensional (in the direction normal to the boundary) giving:

\[
\frac{\partial V_n}{\partial t} + N \frac{\partial V_n}{\partial n} = 0
\]  
(B.58)

where

\[
N \frac{\partial V_n}{\partial n} = \begin{pmatrix}
\frac{u_n \frac{\partial u_n}{\partial n} + \frac{1}{\rho} \frac{\partial P}{\partial n}}{u_n \frac{\partial u_n}{\partial n}} \\
\frac{u_n \frac{\partial u_1}{\partial n}}{u_n \frac{\partial u_n}{\partial n}} \\
\frac{u_n \frac{\partial u_2}{\partial n}}{u_n \frac{\partial u_n}{\partial n}} \\
\frac{u_n \frac{\partial u_3}{\partial n} + \rho c^2 \frac{\partial u_n}{\partial n}}{u_n \frac{\partial u_n}{\partial n}} \\
\frac{\rho \frac{\partial \rho}{\partial n}}{\rho \frac{\partial \rho}{\partial n}} \\
\frac{\frac{\partial \rho}{\partial n}}{\frac{\partial \rho}{\partial n}}
\end{pmatrix} = \begin{pmatrix}
\frac{1}{2} (\mathcal{L}_+ - \mathcal{L}_-) \\
\mathcal{L}_{t1} \\
\mathcal{L}_{t2} \\
\frac{\partial \rho}{\partial n} (\mathcal{L}_+ + \mathcal{L}_-) \\
\frac{\partial \rho}{\partial n} \mathcal{L}_k
\end{pmatrix}
\]  
(B.59)

At this point, the physical behaviour of the boundary must be taken into account to find which LODI relation should be used in order to assess the entering wave(s). Some examples of useful LODI relations are given below, using standard notations (\( M_n \) is the local Mach number in direction \( n \); \( M_n = u_n / c \) and \( \beta = \gamma - 1 \) :
B.4. LINK BETWEEN AVBP FORMULATION AND ORIGINAL NSCBC

\[ \frac{\partial P}{\partial t} + \frac{bc}{2} (L_+ + L_-) = 0 \]
\[ \frac{\partial u_1}{\partial t} + \frac{1}{2} (L_+ - L_-) = 0 \]
\[ \frac{\partial u_2}{\partial t} + L_1 = 0 \]
\[ \frac{\partial p_k}{\partial t} + \frac{p_k}{2} (L_+ + L_-) + L_k = 0 \]
\[ \frac{\partial Y_k}{\partial t} + \frac{1}{p} (L_k - Y_k L_S) = 0 \]
\[ \frac{\partial T}{\partial t} + \beta T \frac{c}{2} (L_+ + L_-) - \frac{T}{p} \sum r_k L_k = 0 \]
\[ \frac{\partial p_u_n}{\partial t} + L_+ (\frac{p}{2} (\gamma M_n + 1)) + L_- (\frac{p}{2} (\gamma M_n - 1)) + \frac{p c M_n}{T} \frac{\partial T}{\partial t} = 0 \]
\[ \frac{\partial p_u_n}{\partial t} + L_+ (\frac{p}{2} (M_n + 1)) + L_- (\frac{p}{2} (M_n - 1)) + c M_n L_S = 0 \]

Additional LODI equations can be written for enthalpy, entropy, momentum or for normal gradients, by combining the previous relations. These LODI relations can be used to set the incoming wave amplitude as a function of the outgoing waves and the variations on the boundary. For example on fixed velocity inlet, the second LODI relation suggests that the incoming wave \( L_+ \) must be equal to \( L_- \).
Appendix C

Publications

The work performed during this Phd is the object of three publications. The first two papers are on the final stages of reviewal for the Proceedings of the combustion institute. The third was presented in the Complex Effects using Large Eddy simulation conference in Limassol, Cyprus.

C.1 Large Eddy Simulation and acoustic analysis of multi-burner combustors
Large Eddy Simulation and acoustic analysis of multi-burner combustors

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Colloquium: 11. IC ENGINE AND GAS TURBINE COMBUSTION
Short title: Burner/burner interactions
Total length of paper: 5045 words
Abstract: Gas turbine chambers contain multiple burners mounted around the turbine axis. To understand turbulent combustion in these devices, most experimental and numerical studies are performed on simplified geometries, usually limited to single burner configurations. Such geometrical simplifications allow faster computations and cheaper experiments but may miss important phenomena such as burner-to-burner interactions or azimuthal instability modes. To address this issue, this study describes a Large Eddy Simulation (LES) of two research set-ups: the first one contains one single turbulent swirled burner while the second one contains three neighbouring burners. LES results show that the cold flow features in both set-ups are very similar so that studying non-reactive flows in a single burner is probably adequate. However, the unsteady activity in the reactive case in both set-ups is very different: in the triple-burner set-up, a complex acoustic mode develops while it is not present in the single burner configuration. This result suggests that certain unsteady phenomena (and especially combustion instabilities) occurring in multi-burner systems can not be studied in single-burner set-ups.

Keywords: burner / burner interactions, swirled combustion, gas turbines

1 Introduction

In the highly competitive field of power generation, gas turbines have gained an increasing role over the years. New emission regulations and growing energy demand increase the weight on the research and development of gas turbine. Substantial advances have been made and ever more complex designs have been developed to meet the increasingly stringent regulations. Unfortunately, new designs sometimes are subject to combustion instabilities [1, 2, 3, 4]. Experimental tests must be conducted to evaluate the risk and impact of such phenomena on the machines. Building a full combustor for each test is unpractical and simplifications are necessary. Because of the azimuthal periodicity of these chambers and of the obvious building and computational cost reduction, laboratory studies as well as Large Eddy Simulation (LES) are often performed on combustors containing only one burner. This configuration is assumed to be representative of all the burners in the machine. The impact of this simplification on the results is not clear and raises various questions for turbulent combustion models: in single burner set-ups, the flame interacts with walls while they interact with other flames in the real chamber. These burner / burner interactions are known to be the source of increased turbulence and sometimes even instabilities [2, 5, 6]. Moreover, the acoustics of single burner set-ups...
and of full chambers are also obviously different. Knowing whether results (for combustion stability for example) obtained on single burner devices can be safely extrapolated to full gas turbines engines is a critical question which has been rarely studied up to now. In this paper, a first step in this direction is performed by using LES to investigate the differences between the reacting flow in a single and in a triple-burner set-up. By comparing the flows in these two set-ups, LES provides a direct investigation of the 'single-burner' simplification. The analysis is performed for the non-reacting and the reacting cases, both for mean flow and for unsteady activity (RMS Pressure and flame dynamics). The LES code is described first followed by the target configurations description. Cold flow, averaged reacting flow and unsteady combustion are then analyzed.

2 LES and Numerical models

Recent studies using LES have shown the accuracy of this approach for reacting flows (see reviews in [4] or [7]). LES is able to predict mixing [8, 9, 10], stable flame behaviour [11, 12, 13] and flame acoustic interaction [14]. It is also used for flame transfer function evaluation [15]. Here a fully compressible unstructured explicit code is used to solve the multi-species Navier-Stokes equations with realistic thermochemistry on unstructured grids. Multiple validations of the LES tool have been published [16, 14, 8] and are not included in the present paper. The classical Smagorinsky approach [17] is used to model the sub-grid stresses. A one-step methane/air scheme fitted on the Gri-mech 3.0 reference [18] is used. Turbulence/flame interaction is accounted for with the Dynamic Thickened Flame model (DTF) [19, 20]. The boundary conditions are based on a multi-species extension of the NSCBC approach [21]. All wall boundaries use a logarithmic law-of-the-wall formulation. In this compressible solver, acoustic waves are explicitly resolved: the time step is limited by the acoustic CFL condition and a high-order spatial and temporal scheme is used to propagate acoustics with precision [22] so that flame/ acoustics interaction is captured correctly.

3 Target configurations

The study focuses on a single burner and a triple burner segment of a typical annular combustion chamber (Fig. 1). Each burner has two co-rotating co-axial swirlers, the premix passage swirler and the pilot passage swirler (Fig. 2). The premix passage swirler contains 24 vanes. For each vane, methane is injected through 10 small holes located on
the upper face of the swirler blades. Combined with the swirl, this ensures an efficient mixing so that it is assumed for LES that a perfect mixture enters the premix passage (with an equivalence ratio of 0.56) [23]. The inner swirler contains 8 vanes. The pilot fuel is injected upstream of the vanes. For LES, the swirler vanes are not considered: appropriate profiles of velocity and species mass fractions matching experimental data are imposed at both inlets. These profiles correspond to jets of methane distributed in a pure air flow. The single burner case has periodic side walls whereas the triple burner side boundary conditions are adiabatic walls.

4 Results and discussions

All variables presented in this study are normalized by reference parameters. The reference length is the burner diameter \(D\) (Fig. 2). All velocities are normalized by the bulk velocity \(U_b\) obtained by \(U_b = \frac{\dot{m}}{\rho \cdot S}\) where \(\dot{m}\) is the total flow rate, \(\rho\) is the fresh gas density and \(S = \pi \cdot (\frac{D}{2})^2\). Pressure fluctuations are normalized by a reference pressure \(\rho \cdot U_b^2\).

4.1 Cold Flow Results

Swirled flows have been used for a long time in gas turbines [24, 25]. They offer an attractive alternative to flame holders for flame stabilization through the use of recirculation zones. However swirl flows can also lead to the creation of precessing structures also called precessing vortex cores (PVCs) [14, 26]. Figure 3 shows instantaneous views of the LES results for the single periodic (a) and the triple burner cases (b). For the single burner set-up a PVC at 300\(Hz\) is observed at the end of the burner. The Strouhal number for this PVC is \(St = \frac{f \cdot D}{U_b} = 0.41\) which is typical for this type of flow [25, 26]. This observation confirms many similar results obtained both numerically and experimentally [14]. In the triple burner set-up, three PVCs at 300\(Hz\) appear (one on each burner). In both cases the PVCs are visualized using a low pressure isosurface. In the triple burner set-up, all PVC’s precess in the same direction but are not phase-locked: each burner seems to feature a PVC that is independent of its neighbours.

Figures 4a and 4b show profiles of averaged axial velocity and pressure fluctuations for the single burner (solid line) and the central burner of the triple burner case (circles) for the non-reacting case. Profiles are extracted at five locations on a horizontal plane along the axis of the burner (Fig. 2). Even though small differences are observed, it is clear that not only the mean flow (identified through the mean axial velocity, Fig. 4a but also the unsteady flow (identified
through the RMS pressure, Fig. 4b are very similar in both burners. Studying a non-reacting flow, using a single burner set-up seems therefore sufficient: this confirms the validity of experiments and computations performed on single burner geometries for cold flow studies.

4.2 Reacting Flow

The cold flow observations suggest that the triple burner configuration produces very similar flow patterns even in terms of acoustic and unsteady activity. The situation is different for reacting cases as shown in the following section. Figure 5 shows the flame zone visualized by a $1000 K$ temperature isosurface in the single burner case (a) and the triple burner case (b). All flames are anchored near the inner hub. Figure 6a displays profiles of averaged axial velocity on the same cuts as in Fig. 4. Here again, the average velocity profiles are very similar, showing that the jet opening and the central recirculation zones are the same in both geometries. However the unsteady pressure fields are very different (Fig. 6b): predicted pressure fluctuations are much larger in the three-burner case than in the single burner case and exhibit a different structure. The geometry change alone, does not account for this difference. Spectral analysis of the pressure signals at the center of each sector of the triple burner set-up (Fig. 7) reveals a 370 Hz component which is present only on the side sectors. The central sector seems unaffected. This 370 Hz component is also absent in the single burner LES pressure signal. To understand why this mode appears only in the three burner set-up, an acoustic analysis of both configurations is performed in the next section.

5 Acoustic analysis

Acoustic solvers are often used in combustion chambers to determine the frequencies and the structure of modes which can be excited for a given geometry [5, 27]. This analysis is used here for both configurations. The outlet impedance of the set-ups is set identically for all cases (Velocity node). All inlets for both geometries are also treated as velocity nodes. A finite element solver is used on the geometries of both set-ups used in LES. The sound speed field is obtained from time-averaged LES data. The resulting first eigen-frequencies for both cases are listed in Table 1. Some eigen-values (1 and 3) match in both configurations: 129 Hz and 560 Hz are possible eigen-frequencies of both set-ups. Since the triple burner contains three single burners side by side, both configurations are expected to share certain modes. LES reveals that these modes are not excited in either configuration. However the triple burner has
a 371Hz eigen-value which is not present in the one sector configuration and which matches the LES data of Fig. 7.

The excitation of this 370 Hz eigen-mode may explain the differences observed in the reacting LES of the two set-ups. Indeed the 370 Hz is not a mode of the single burner set-up and does not appear in the acoustic analysis of the single burner geometry of Table 2. In the triple burner, the 370 Hz mode is predicted by both the acoustic solver and the LES. The presence of this acoustic mode yields important consequences for flame stabilization in the triple set-up. Figure 8 shows the flame structure at $t=\frac{T}{4}$ (Fig. 8a), $t=\frac{T}{2}$ (Fig. 8b) and $t=\frac{3T}{4}$ (Fig. 8c) where $T$ is the period of the 370Hz mode. At $t=\frac{T}{4}$, the left and central flame are attached to their respective inner hubs but the right flame is lifted away from this position. At $t=\frac{T}{2}$ all flames are attached to their inner hub. Finally, at $t=\frac{3T}{4}$ the right flame re-attaches while the left flame detaches itself from the inner hub. Flame anchoring is no longer guaranteed for the side burners in the triple burner set-up. The central flame seems unaffected by the phenomena. This is explained by the structure of the 370Hz mode (Tab. 2 eigen-mode 2). The central burner is located at a pressure node for this mode. Therefore it is not subject to strong acoustic perturbations. However the two side burners are located near pressure anti-nodes. Since the pressure oscillates for these two side burners, the flow rate going through them also fluctuates. The typical velocity fluctuations at the side burner mouths can reach up to 20 % of the bulk velocity. These oscillations are quite sufficient to induce intermittent lift-offs.

The single burner simulation is unable to reproduce this behaviour since 370 Hz is not an acoustic eigen-frequency for a one sector configuration. Performing a single burner study would yield incomplete data on the stability of the entire chamber as well as on the stabilization of the flames.

6 Conclusion

While real gas turbines can contain ten to thirty burners mounted in annular combustion chambers, most experimental and numerical studies of gas turbine combustion chambers are performed on isolated burners installed in specific laboratory set-ups: this geometrical simplification can have important consequences on the validity of the results and their possible extrapolation from laboratory scale to full gas turbine combustors. The present study shows that a single burner set-up and a triple burner set-up provide very similar results for non-reacting flows but that differences are present for reacting cases. When combustion is activated, a strong unstable mode involving the transverse azimuthal acoustic mode of the triple burner set-up is excited while the single-burner configuration remains stable. This numeri-
cal test should be followed by an experimental investigation (which would be expensive) but it is sufficient to suggest that single-burner results must be used with care to study full combustor stability and that additional studies are needed to understand the dynamics of flames in multi-burner configurations.

Acknowledgements

This work was carried out with the support of Siemens PG in the framework of EC project DESIRE (Design and Demonstration of Highly Reliable Low NOx Combustion Systems for Gas Turbines, contract number NNE5/388/2001). Computer support comes from CINES (Centre informatique National de l’Enseignement Superieur), French national computing center.

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Figure 1: Full Burner, single and triple burner configurations.

Figure 2: Burner geometry and location of the different cuts used for analysis.

Table 1: Lowest eigen-frequencies (Hz) for one and three burner set-ups

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<th>Three Burner</th>
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<td>128</td>
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<tr>
<td>2</td>
<td>371</td>
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</tr>
<tr>
<td>3</td>
<td>560</td>
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Figure 3: Precessing structure a) single burner, b) triple burner.

Figure 4: a) Mean axial velocity b) Pressure fluctuations: single burner (solid line) vs central burner of the triple set-up (circles).

Figure 5: Flame (1000K isosurface): a) Single burner b) Triple burner.
Figure 6: a) Mean axial velocity b) Pressure fluctuations: single burner (solid line) vs central burner of the triple set-up (circles).

Figure 7: Pressure spectra in the center of each sector of the triple burner case (LES result)
Figure 8: Flame (1000K isosurface) at: a. $t=T/4$ b. $t=T/2$ c. $t=3T/4$
Table 2: Eigen-modes for both configurations (Helmholtz analysis). $P_{RMS}$ fields on the walls.

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<td>2</td>
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<td>3</td>
<td><img src="image5" alt="Single Burner 3" /></td>
<td><img src="image6" alt="Triple Burner 3" /></td>
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C.2 Large Eddy Simulation of piloting effects on turbulent swirling flames
Large Eddy Simulation of piloting effects on turbulent swirling flames

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December 2, 2005

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Colloquium: 13. Co-chair papers (Turbulent Flames)

Short title: Swirl flames piloting

Total length of paper: 4710 words

Abstract: Pilot flames, created by additional injectors of pure fuel, are often used in turbulent burners to enhance flame stabilisation and reduce combustion instabilities. The exact mechanisms through which these additional rich zones modify the flame anchoring location and the combustion dynamics are often difficult to identify, especially when they include unsteady hydrodynamic motion. This study presents Large Eddy Simulations (LES) of the reacting flow within a large-scale gas turbine burner for two different cases of piloting, where either 2 or 6 percent of the total methane used in the burner is injected through additional pilot flame lines. For each case, LES shows how the pilot fuel injection affects both flame stabilisation and flame stability. The 6 percent case leads to a stable flame and limited hydrodynamic perturbations in the initial flame zone. The 2 percent case is less stable, with a small-lift-off of the flame and a Precessing Vortex Core (PVC) in the cold stabilisation zone. This PVC traps some of the lean cold gases issuing from the pilot passage stream, changes the flame stabilisation point and induces instability.

Keywords: Combustion instabilities; Partially premixed; Swirled; Large Eddy Simulations

1 Introduction

Modern heavy duty gas turbines usually operate in lean premixed regimes to satisfy emissions regulations and can be very sensitive to combustion instabilities [1–3]. In most cases, flame stabilisation is provided by swirl injectors. A key zone of the chamber controlling instabilities is the burner outlet section where swirl is very intense and must provide flame stabilisation. In these regions, the natural unstable modes of swirling flows (Precessing Vortex Cores or PVCs [4–8]) can interact with stabilisation and lift-off phenomena [9–12] to produce undesired oscillations.

A method to encourage robust stabilisation is to use small pilot flames in these regions, usually by adding pure fuel injection. This leads to increased $NO_x$ levels and therefore a compromise between stabilisation and pollution levels must be sought. Furthermore, stabilisation is a difficult task because its basic mechanisms in a piloted swirled zone are not well understood. Proof of the importance of fuel injection are observed in active control examples in which a small modulation of flow rate in the fuel lines feeding the pilot flame can be sufficient to alter the stability of the combustor [13–15].

Large Eddy Simulation (LES) is becoming a standard tool to study the dynamics of turbulent flames [16–18]. The objective of this paper is to use LES (section 2) to compare two different cases of piloting in a gas turbine burner.
Either 2 or 6 percent of the total methane used in the burner is injected additionally through pilot fuel lines. The burner is described in section 3. The 6% pilot fuel case leads to a robust and stabilized flame while the 2% case induces a small lift-off zone of the flame where a PVC can develop and lead to flame oscillations (section 4).

Because of the complexity of the burner, no detailed measurements are available. However, observations in the atmospheric test rig confirm LES predictions: the 2% leads to a more unstable flame than the 6% case.

2 Numerical approach used in Large Eddy Simulations

A fully compressible explicit code is used to solve the multi-species Navier-Stokes equations on hybrid grids [8, 19, 20]. Subgrid stresses are described by the classical Smagorinsky model [21]. A two-step chemical scheme is fitted for lean regimes on the GRI-Mech V3 reference [20]. The objective of the fit procedure is that the two-step mechanism and the GRI mechanism must produce the same flame speeds and maximum temperatures for laminar premixed one-dimensional flames for equivalence ratios ranging between $\phi = 0.4$ and $\phi = 1.2$.

The flame / turbulence interaction is modeled by the Dynamic Thickened Flame (DTF) model [22] which accounts for both mixing and combustion, and is crucial in partially premixed flames.

The explicit Lax-Wendroff numerical scheme uses second-order spatial accuracy and second-order time accuracy. The boundary condition treatment is based on a multi-species extension [19] of the NSCBC method [23], for which the acoustic impedance is controlled to minimise the unwanted reflections [24]. The adiabatic walls are handled using a logarithmic law-of-the-wall formulation which is known to perform well with the classical Smagorinsky model [25]. Typical runs are performed on a grid composed of 1.4 million tetrahedra on parallel architectures. Multiple validations of this LES tool are available for non-reacting [26, 27] and reacting flows [8, 20, 28, 29].

3 Target configuration

The test geometry is an axisymmetric combustion chamber (Fig. 1-a), with a 3MW full scale burner inlet (Fig. 1-b). This burner is composed of two coaxial swirlers:

- The premix passage swirler contains 24 vanes. Methane is injected through 10 small holes on each vane, ensuring efficient mixing and delivering approximately 90% of the total mass flow rate. In the LES, this flow is
assumed to be fully premixed.

- The pilot passage swirler (detailed in the upper part of Fig. 1-b) delivers the remaining 10% of the flow rate (pure air). The central hub is connected to 8 vanes. Four additional tubes are inserted between the 8 vanes to inject the methane used for piloting.

The computational domain includes all pilot passage vanes as well as the pilot fuel tubes, but not the premix passage vanes. Appropriate profiles of velocity and species are imposed to mimic the inlet experimental data [20] downstream of the premix passage vanes (Fig. 2).

The investigated cases correspond to test rig operating points only (experimental combustion chamber at atmospheric pressure) and not to real gas turbine operating conditions (annular chamber at high pressure). The two operating points simulated in this study (2% and 6%) only differ by the fuel mass flow rates in the pilot fuel inlets:

- In the pilot passage stream, the fuel delivered by pilot injection leads to a global equivalence ratio of $\phi = 0.36$ (case 6%) and $\phi = 0.12$ (case 2%), of which the latter is outside the flammability limits. However, the very heterogeneous mixture may allow combustion to develop locally in rich pockets or in diffusion flamelets, depending on the mixing efficiency.

- In the premix passage stream, the imposed profiles in both cases correspond to a perfectly premixed flow with an equivalence ratio of $\phi = 0.53$.

4 Results and discussions

In swirling flows, the general mechanism leading to flame stabilisation is well known [8, 20]: a central core of hot gases is maintained along the burner axis by the strong recirculation zone induced by swirl. This section shows how this classical stabilisation mechanism is affected by the pilot flames. Figures 3 and 5 respectively present statistical profiles (time averaged and RMS values) of temperature and axial velocity in the central plane. The axial location of these profiles is shown on Fig. 2. Velocity, temperature and location along axis are normalised respectively by references $U_{\text{ref}}, T_{\text{ref}}$ and the pilot passage radius $R$.

In the 6% pilot fuel case, the flame is clearly anchored on the central hub of the pilot passage, and the temperature fluctuations remain small (Fig. 3-b): burnt gases are found along the axis from $x = 0$ to $x = 2R$. Flame lift-off appears
in the 2% case (Fig. 3-a). The gases between $x = 0$ and $x = 2R$ are cold. Hot pockets begin to appear after $x = 2R$ but they are very intermittent, as demonstrated by the very large values of the RMS temperature (error bars on Fig. 3-a).

A clearer understanding of the differences between the two cases can be gained by plotting isosurfaces of temperature and stoichiometric equivalence ratio (Fig. 4). For the 6% case, the hot zone ($T = 2/3 \cdot T_{ref}$) is directly connected to the pilot passage hub (Fig. 4-b). For the 2% case, the flame is stabilised on a ‘finger’ of burnt gases which is rotating around the x-axis (Fig. 4-a), thereby inducing the large RMS fluctuations of temperature seen in Fig. 3-a.

The axial velocity fields (Fig. 5) also present significant differences. For the 6% case, a very large zone with small velocities (mean as well as RMS) develops between $x = 0$ and $x = 3R$ (Fig. 5-b). This zone contains the hot gases (Fig. 3-b) which provide stabilisation. The 2% case (Fig. 5-a) is characterised by a more intense recirculation (see for example cuts at $x = 2R$ or $x = 3R$) and a much higher level of RMS velocities. This zone (between $x = 0$ and $x = 3R$) contains cold gases (Fig. 3-a) which experience intense fluctuations. Even when the temperature increases (downstream of $x = 3R$), the velocity RMS values (Fig. 5-a) remain much higher for the 2% than for the 6% case, confirming that the 2% flame is not only lifted but also more hydrodynamically unstable.

Instantaneous combustion regimes can be visualised by scatter plots of reaction rate versus local mixture fraction $Z$ (Fig. 6). In both cases, most reacting points are located very close to the global mixture fraction of the combustor $Z_{mean}$, but in the 6% case, combustion also takes place at richer regimes, even slightly above stoichiometric ($Z_{st}$), yielding higher maximum heat release. These points correspond to the roughly stoichiometric mixture issuing from the four pilot fuel jets after it has mixed with the premix passage air and passed through the vanes. By burning vigourously, these zones provide the robust stabilisation observed in Fig 4-b. For the 2% case, almost no combustion takes place above the mean mixture fraction $Z_{mean}$, indicating that the fuel injected in the pilot lines mixes too fast and cannot produce any significant diffusion flame zones which could provide stabilisation.

Typical instantaneous fields of equivalence ratio are displayed on Fig. 7. While the 6% case remains roughly axisymmetric and stoichiometric near the pilot passage hub, the 2% case in this zone has an asymmetric pattern below the flammability limit ($\phi < 0.4$), which rotates around the x-axis.

The near stoichiometric zone of Fig. 7-b for the 6% case is the source of the robust stabilisation of this regime: this allows the flame to propagate back to the burner and anchor to the hub. On the other hand, for the 2% case (Fig. 7-a), mixing between the pilot fuel and the pilot passage air is too fast and leads to a mixture at the pilot passage mouth.
which is too lean for flame propagation. Figure 7 also shows a zone within which the flow is reversed. This central recirculation zone is delimited by the white isoline \( U = 0 \). Note that the 6% case exhibits a smaller zone of reversed flow (as expected from the mean velocity profiles of Fig. 5) than the 2% case. Obviously, having reversed flow is not a sufficient criterion for stabilisation: having robust burning pilot flames is more important (as for the 6% case). For the 2% case, the absence of combustion in this zone leads to a lean cold region in which even reversed flow can not anchor the flame.

The existence of such a lean and cold zone leads to the formation of a PVC [4–8]. This PVC only occurs in the 2% case and precesses at 408Hz. The drastic change of velocity field near the pilot passage mouth for this case presented on Fig. 5 is one of the factors which most probably facilitate its development.

A specific feature of the 2% case is the correlation between the lean jet of methane and cold air issuing from the pilot passage and the low pressure zone due to the PVC structure. Figure 8 displays fields of pressure, temperature and local equivalence ratio (reconstructed through the mixture fraction) for both pilot fuel cases in a transverse plane at \( x = 3R \).

The low pressure regions are a good indicator of the PVC presence (Fig. 8-a), and are well correlated with the cold (Fig. 8-b) and lean (Fig. 8-c) regions for the 2% case. The PVC appears to capture some of the lean cold gases produced by the pilot passage and prevents their mixing with the surrounding products. This observation is consistent with detailed mixing studies of jet / vortex interaction which show that mixing can be strongly decreased within vortex structures [30].

The flame then features a cold non-reacting "finger-like" rotating structure protruding within the stabilisation zone (illustrated by Fig. 4-a and sketched on Fig. 9). This is clearly not favorable either for flame stabilisation nor for thermoacoustic stability: RMS pressure levels for the 2% case can be as high as 6000 Pa (170 dB) on the axis and the noise is radiated to 2000 Pa (160 dB) at the wall while they do not exceed 500 Pa for the 6% case. For the 6% case, the situation is very different: a PVC is not observed (Fig. 8-a’), less cold gas reaches the plane at \( x = 3R \) (Fig. 8-b’) and lean gases are not found around the axis (Fig. 8-c’).

The mechanism leading to the PVC formation in the 2% case is purely due to hydrodynamic and combustion effects but not to acoustic coupling. A basic proof of the absence of acoustic coupling can be assessed by comparing the acoustic eigenfrequencies of the combustion chamber with the precessing frequency of the PVC (408 Hz).
5 Conclusions

This study presents Large Eddy Simulations (LES) of piloting effects in a full-scale gas turbine burner. By computing explicitly all details of the pilot passage zone where pure pilot methane is injected upstream of the vanes, LES provides new insights on the key mechanisms that control flame stability. When enough methane is injected in the pilot zone (in the 6% case), a roughly stoichiometric zone is formed at the burner mouth, allowing flame propagation within this zone and preventing the formation of a Precessing Vortex Core (PVC). On the other hand, when the flow rate of pilot fuel is too small (in the 2% case), the mixture issuing from the pilot passage is too lean, preventing flame stabilisation and leading to the formation of a PVC containing lean cold gases which diminishes the effect of piloting even more. Obviously, between the 2% and 6% piloting cases, a bifurcation takes place in the basic flow structure. The significant effects of this bifurcation captured by LES coincide with observations on stability limits in the atmospheric test rig. However, these conclusions are only valid for this experimental range and cannot be extended straightforward to real gas turbine operating conditions.

Acknowledgements

This work was carried out with the support of Siemens PG in the framework of EC project DESIRE.

Most numerical simulations have been conducted on the computers of CINES, the French national computing center, on a SGI origin 3800.

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HIGHLY PARALLEL LARGE EDDY SIMULATIONS OF MULTIBURNER CONFIGURATIONS IN INDUSTRIAL GAS TURBINES

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Keywords: LES, Multi-Burner

Abstract. Recent advances in computer science and highly parallel algorithms make Large Eddy Simulation (LES) an efficient tool for the study of complex flows. The available resources allow today to tackle full complex geometries that can not be installed in laboratory facilities. The present paper demonstrates that the state of the art in LES and computer science allows simulations of combustion chambers with one, three or all burners and that results may differ considerably from one configuration to the other. Computational needs and issues for such simulations are discussed. A single burner periodic sector and a triple burner sector of an annular combustion chamber of a gas turbine are investigated to assess the impact of the periodicity simplification. Cold flow results validate this approach while reacting simulations underline differences in the results. The acoustic response of the set-up is totally different in both cases so that full geometry simulations seem a requirement for combustion instability studies.

1 INTRODUCTION

In the highly competitive field of power generation, gas turbines have gained an increasing role over the years. New emission regulations and growing energy demand increase the weight on the research and development of the manufacturers of such machinery. Outstanding advances have been made and ever more complex designs have been developed to meet the increasingly stringent needs. Unfortunately sometimes the new designs are subject to combustion instabilities [2, 4, 11]. Experimental tests must be conducted to evaluate the risk and impact of such phenomena on the machines. Building a full burner for each test is unpractical and geometric simplifications must be made leading to approximations in the results. Numerical tools, who do not have this limitation, are an attractive alternative to experimental set-ups especially Large Eddy Simulation (LES).

Recent studies using Large Eddy Simulation (LES) have shown the accuracy of this approach in comparison with experimental data. LES is able to predict mixing [12], stable flame behaviour [13] and flame acoustic interaction [14]. It is also used for flame transfer function evaluation [8]. The objective of the present paper is to demonstrate the necessity to investigate full burner configurations for instability studies. Technical difficulties encountered for full burner LES are discussed. The interest of such simulations is shown by an a posteriori study of the flow for a single and a triple burner configurations. Note that the current work is part of the european project DESIRE with the support of SIEMENS PG.

2 TARGET CONFIGURATION AND LES MODELS

To demonstrate the feasibility and usefulness of multi-burner and full burner simulations, LES of an annular combustion chamber are performed. The injection system consists of two co-rotating partially premixed swirlers. The swirler vanes are not simulated and appropriate boundary conditions are set to mimic the vane effects on the flow.

LES is carried out with a parallel solver called AVBP, simulating the full compressible Navier Stokes equations on structured, unstructured or hybrid grids. The sub-grid scale influence is modeled with the standard Smagorinsky model [15]. A one step chemical scheme for methane matching the behaviour of the GRI-mech 3.0 scheme [5] at the target conditions is employed to represent the chemistry. The Thickened Flame Model (TFLES) ensures that the flame is properly solved on the grid [3, 9]. Finally all simulations employ the Lax-Wendroff numerical scheme.
3 COMPUTATIONAL ISSUES

When dealing with very large configurations, computer related issues rapidly arise. In order to perform a full burner LES, one needs to adapt the available tools. The potential difficulties are divided in three themes:

- Mesh generation
- Fast and efficient LES
- Post-processing of the results

Generating a mesh for the calculation is by far the most time consuming and remains a critical point in numerical simulations. The difficulty is greatly increased when trying to build a mesh for a full set-up. The memory requirements become important (over five gigabytes of RAM for a $5 \times 10^6$ cells mesh) and powerful computers are needed. Most designs have a natural geometric periodicity and the most practical solution to generate the mesh is to create a single periodic mesh and then duplicate it as many times as needed to build the full model.

A full twenty four burner set-up was meshed using this procedure (cf. Figure 1). The resulting computational domain has over forty million cells and requires three hundred Megabytes.

![Figure 1: Full burner set-up: 40 Million Tetrahedras](image)

In order to perform a fast and efficient LES for such a large mesh, a large number of processors is required. However using a large number of processors means decomposing the computational domain into a large number of parts. Since message passing communications are proportional to the quantity of domains, the code must not suffer any degradation in performance by increasing the number of processors. Figure 2 shows the ideal behaviour (black line) compared to the behaviour of AVBP for a five million cells LES (squares) and for a forty million cells case (circles). A close to optimal result is observed even for up to 5000 processors.

\[\text{Figure 2: Performance comparison for different mesh sizes and number of processors.}\]

The tests were performed on a Bluegene supercomputer from IBM.
Once LES is performed, a lot of data has been generated (over 20 gigabytes for the five million cells case). Memory limitations encountered during mesh generation are also present during the post-processing step. Retrieving such large quantities of data from a computer center to a visualization post can also be troublesome. Remote visualization applications are a potential solution and offer an interesting way to reduce post-processing time.

4 RESULTS AND DISCUSSION

To evaluate the possible benefits from multi-burner simulations compared to a simulation using a simplified geometry, a single burner (cf. Figure 3a) and a triple burner LES (cf. Figure 3b) are presented. The single burner side boundary conditions are periodic whereas the triple burner’s are simple walls. Details of the computational domain are given on Figure 4.
In the following the unsteady and averaged behaviours of the configurations are discussed. The single periodic and the central burner of the triple set-up are compared to assess the impact of the periodicity. Results show that the main hydrodynamic features remain the same but some substantial differences are observed in the reacting cases.

### 4.1 Cold Flow Results

Swirled flows have been used for a long time in gas turbines [1, 6, 13]. Their main objective is to create a central recirculation zone to anchor the flame without flame holders. Precessing structures, also called precessing vortex cores (PVC), are commonly observed for this type of flows and are usually located right at the outlet of the injector system. Figure 5 shows instantaneous views of the LES results for the single periodic burner (a) and for the triple burner (b). On the top part of each figure different velocity components are displayed. The central
recirculation zone is visible in the axial velocity component snapshot. For the periodic sector, a precessing vortex core rotating in the same direction as the imposed swirl is evidenced using a low pressure isosurface near the axial hub. Spectral analysis in the axial swirler region of the radial velocity component reveals that the PVC revolves at $300Hz$ (cf. Figure 6a). In the triple burner case, pressure isosurfaces reveal the existence of a PVC for each burner. They are located at the exit of the corresponding burner as observed in the single sector configuration. Spectral analysis of the central burner PVC confirms that the precession motion is also at $300Hz$ (cf. Figure 6b).

From the instantaneous behaviour we can conclude that the periodicity simplification seems to have no impact on LES results. The averaged quantities must be checked to enforce this conclusion: Figures 7a and 7b show the averaged axial velocity and the pressure fluctuations for the single burner (black line) and the central burner of the triple case (dashed line) for the non-reacting case. Profiles are extracted at different locations on a horizontal plane along the axis of the burner. The results match quite well even for pressure fluctuations. The main hydrodynamic features of the flow seem to be identical in the non-reacting cases for the single and triple sector.
4.2 Reacting Flow

The cold flow observations suggest that the triple burner LES offers no additional information compared to the periodic LES. The situation is different for reacting cases as shown in the following section.

Figure 8: Flame (1000K isosurface) and velocity components (reaction rate, black contours): a) periodic burner b) triple burner.

The recirculation zones observed in the cold flow simulations suggested that the flame should attach near the axial hub and at the burner outlet. Figure 8a) and 8b) show the flame zone represented by a one thousand Kelvin temperature isosurface. The different velocity components are shown at the top of the Figures in addition to a reaction rate iso-contour. The flame is anchored in both configurations and for all burners by the central recirculation zone as expected. The position of the central recirculation zone seems unaffected by the presence of the flame.

Using the coherent structure detection criterium from Hussain [7], a PVC is evidenced in the reacting case for the single burner (Fig. 9a). Its revolving movement matches the swirl’s. Spectral analysis of the radial velocity component reveals that the precessing structure’s frequency is 780Hz (cf. Figure 9b). Which differs from the one observed in the cold flow results. Since the presence of the flame disrupts considerably the near axial hub region this is expected. The structure is also present in the triple sector case.

Figure 9: Single periodic burner: a) flame (1000K transparent isosurface) and Q criterion (solid isosurface) b) power spectrum in the axial region.
The observations of the unsteady solutions highlight no clear difference between the two configurations. Figure 10a) shows that the mean axial velocity matches well for both simulations. As was the case in the non-reacting flow (cf. Figure 7a), the match is quite good. The mean temperature profiles also match reasonably well (cf. Figure 10b). However, pressure and temperature fluctuations differ greatly (cf. Figure 11). Predicted pressure fluctuations are two times higher in the three sector case than in the single sector case. The presence of the side burners modifies temperature fluctuations. Since pressure and heat release (therefore temperature fluctuations) are closely linked to the acoustic behavior of the set-up, acoustic analysis is required to evaluate the impact of the differences and their origin.

![Figure 10: a) Mean axial velocity b) mean temperature field: single burner (black line) vs central burner of the triple set-up (dashed line).](image)

![Figure 11: a) Pressure fluctuations b) temperature fluctuations: single burner (black line) vs central burner of the triple set-up (dashed line).](image)

5 ACOUSTIC DESCRIPTION

Eigen-value solvers are useful tools for visualizing and analyzing the possible acoustic modes present in a set-up. To conduct the acoustic analysis a Helmholtz solver [10] using the averaged speed of sound distribution from the reacting LES is used. The eigen-frequencies obtained for both cases are displayed in Table 1.
Table 1: Eigen-frequencies for one and three sectors

Some eigen values match in both configurations (cf. table 2). Since the triple burner contains three single burners side by side this is no surprise. However the triple burner has a 370Hz eigen-value which is not present in the one sector configuration (cf. Table 2 eigen-frequencies number 2).

Table 2: Eigen-modes for both configurations (Helmholtz analysis)

The excitation of the 370Hz eigen mode explains the differences observed in the reacting LES. Spectral analysis of the LES pressure field in the middle of each sector composing the triple burner yields a dominant harmonic at 370Hz for the side burners (cf. Figure 12). This frequency matches very well mode 2 as predicted by the Helmholtz solver (cf. table 2). The single burner simulation is unable to reproduce the right behavior for the reacting case since 370Hz is not a eigen-frequency for a one sector configuration. Therefore for combustion instability studies, considering a full burner LES may be necessary.

Figure 12: Pressure spectra in the center of each sector of the triple burner case (LES result)
6 CONCLUSION

The feasibility of full burner LES is demonstrated. The methodology and challenges behind such simulations are enumerated and possible solutions are given. To assess the benefits from full burner simulations compared to simplified configurations, a single periodic burner LES and a triple burner LES were performed. The periodic simplification seems to be adapted to cold flow studies. However, to retrieve the correct acoustic behaviour of the set-up for combustion instability studies, considering the full geometry seems paramount.

ACKNOWLEDGEMENTS

This work is funded by the European Community through project DESIRE (Design and Demonstration of Highly Reliable Low NOx Combustion Systems for Gas Turbines, contract n° NNE5/388/2001). The authors would like to thank CINES (Centre informatique National de l’Enseignement Supérieur), French national computing center, for their help and support. They are also indebted to IBM for the opportunity to use their latest Bluegene machine.

REFERENCES

Bibliography


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