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Chapitre 9

Non pulsated reacting flow

9.1 Reduction of chemical complexity

Fuel (Natural gas) and oxidiser (Air) used for the experiment contain many components. When reacting together, an extremely large number of intermediate species are formed. In order to transport a limited number of species and therefore decrease the computational cost, the strategy consists in two points:

- Finding an equivalent composition, in terms of density $\rho$ and calorific value $C_p$, of employed gases with a limited number of species (section 9.1.1).
- Creating a reduced chemical kinetic scheme which will produce similar flame speed $S_L$ and adiabatic flame temperature $T_{AD}$ (section 9.1.2).

9.1.1 Gases composition

Despite natural gas used in the experiment is mainly composed of methane, many other components (either reactive e.g. ethane, propane or neutral such as nitrogen) are present in it. The air is also a mixture of nitrogen, oxygen, argon and some carbon dioxide.

The analysis of natural gas and air composition was done by Nederlandse Gasunie. Consequently, a reduced composition (summarised in Tab. 9.1) has been proposed for both gases. Table 9.2 evidences the good agreement between the properties of the real composition and of the reduced composition for both air and natural gas.

Section 9.1.2 will demonstrate that a two-step reduced kinetic scheme can be built by adding only three other species as products: Carbon dioxide, Carbon monoxide and Water. Therefore, the only species which the LES code has to consider are: Methane, Oxygen, Nitrogen, Carbon dioxide, Carbon monoxide and Water.
9.1.2 Kinetic scheme for methane

Before simulating a reacting flow with AVBP and the DTFLES model, a reduced kinetic scheme adapted to the operating point must be sought. For the experiment installed in University of Twente where pure natural gas is injected into air at a globally lean regime, a two-step chemical scheme is fitted on the GRI-Mech V3 reference [60]. 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 \( \phi = 1.2 \), given a temperature of cold gases of 573 K and a pressure of \( 1.5 \cdot 10^5 \) Pa.

The fact that this mechanism is not valid above \( \phi = 1.2 \) means that regimes where multiple flamelets would burn in very rich conditions cannot be computed with this scheme. Section 9.2 will demonstrate that this is not the case in the present flow where intense premixing takes place before combustion and no rich flamelets are found.

---

\(^1\) properties are given at 1bar and 293.15K
9.1 Reduction of chemical complexity

In the detailed studies of Martin [111], many two-step schemes have been already fitted on the GRI-Mech reference using a genetic algorithm. The scheme named "2S.CH₄.CM2", which has been widely used in publications [186, 185], fulfils these specifications excepts for the pressure (2S.CH₄.CM2 was developed for atmospheric pressure). Therefore, the complete genetic fitting procedure is not required. By adjusting only the pre-exponential constant of the first reaction, the new two-step scheme "2S.CH₄.AS1" matches the GRI-Mech reference at 1.5 bar.

Fig. 9.1 displays the good agreement between GRI-Mech and 2S.CH₄.AS1 within the range of equivalence ratio considered for both adiabatic flame temperature $T_{AD}$, laminar flame speed $S_L$ but also flame thickness$^2 \delta_{Th}$.

![Graphs](image_url)

**Fig. 9.1 - Results of the fitting procedure of kinetic scheme 2S.CH₄.AS1. Cold gas temperature : 573 K. Pressure : 1.5 bar.**

$^2$evaluated from $\delta_{Th} = \frac{\theta_{2} - \theta_{1}}{\max(|\theta_{x-\phi}|)}$
9.2 Mixing analysis

9.2.1 Objectives of mixing studies

The objectives of this section are:

– To check if the structure of the fuel jets mixing in the air cross flow are properly captured by LES.
– To assess the efficiency of the mixing.
– To evaluate at which regime does the flame burn?

Sections 9.2.2 to 9.2.4 will answer each of these questions.

9.2.2 Unsteady behaviour: phenomenology

The natural gas is injected via four jets in the swirled cross flow. The topology of jets in cross flow has
been widely studied [61, 155]. Since the ratio of jet velocity over the cross flow velocity is of the order
of 0.3, the jet deeply penetrates the flow. The two typical counter-rotating vortices which fold the jet on
itself, as described by Fric [61], are clearly distinguishable in Fig. 9.2-a. In other words, the structure of
jets in cross flow seems to be well captured by LES.

The jets are also strongly affected by the swirling motion of the cross flow. This increases the resi-
dence time of fuel pockets in the mixing region (before reaching the chamber) and therefore improves
the quality of the mixing. However, some pockets of rich gases are still visible close to the beginning of
the chamber (Fig. 9.2-b).

Fig. 9.2 - a) Instantaneous structure of the fuel jets in the air cross flow and b) instantaneous cut of equivalence
ratio in longitudinal plane (see Fig. 8.1 for longitudinal plane location).
9.2.3 Mean behaviour

A brief study showing statistical data of the mixing is carried out in this section. The mean equivalence ratio in transverse plane displayed on Fig. 9.3-a exhibits a non symmetrical pattern (four richer zones) which correspond to the path of the fuel jets. It is also significantly higher near the central hub, where it reaches values close to the stoichiometry.

Fig. 9.3-b evaluates the quality of the mixing as well: RMS fluctuations of equivalence ratio never exceed 0.4. Moreover, the highest $\phi_{RMS}$ zones do not coincide with the highest $\phi$ zones, which tend to indicate that in the worst case, the flame should not be fed by a mixture richer than stoichiometry. This specific point is very qualitatively shown here and will be clarified in section 9.2.4. The main conclusion is that the mixing is not perfect which discredits the usual assumption of fully premixed flow.

![Fig. 9.3 - Mean a) and RMS b) values of equivalence ratio in transverse plane (see Fig. 8.1 for transverse plane location).](image)

9.2.4 Combustion regime

To evaluate precisely the composition of the mixture feeding locally the flame, the equivalence ratio $\phi$ is reconstructed through the mixture fraction $Z$. According to the development of Légier [95] we consider two mass fractions (reference states) :

The mass fraction of fuel at the fuel inlet$^3$ : $Y^0_F = 0.767$

The mass fraction of oxygen at the air inlet : $Y^0_O = 0.2315$

Let’s define the stoechiometric mixture fraction $Z_{ST}$ :

$$Z_{ST} = \frac{1}{1 + s \frac{Y^0_F}{Y^0_O}}$$

(9.1)

$^3$as indicated by University of Twente in their fuel composition, $Y^0_{CH_4} = 0.767$ due to the high amount of $N_2$ in natural gas.
where \( s \) is the stoechiometric ration for methane \((s = 4)\). The mixture fraction\(^4\) \( Z \) can be expressed in function of the local methane and oxygen mass fractions:

\[
Z = \frac{sY_F - Y_O + Y_O^0}{sY_F^0 + Y_O^0}
\]

(9.2)

The local equivalence ratio \( \phi \) (everywhere in the flow even in the burnt gases) can be expressed as:

\[
\phi = \frac{Y_F}{Y_O}
\]

(9.3)

where \( Y_F \) and \( Y_O \) correspond to the mixing lines \([147]\) so that \( Y_F = Y_F^0 Z \) and \( Y_O = Y_O^0 (1 - Z) \). Therefore:

\[
\phi = \frac{sY_F^0}{Y_O} \frac{Z}{(1 - Z)}
\]

(9.4)

which can be also written:

\[
\phi = \frac{Z}{(1 - Z)} \frac{(1 - Z_{ST})}{Z_{ST}}
\]

(9.5)

The crucial property of Eq. 9.5 is that \( \phi \) remains valid in the flame and in the burnt gases. In other words, it allows an identification of the equivalence ratio at which the flame locally burns or has burnt. Figure 9.4-a now displays an instantaneous scatter plot of local reaction rate versus local equivalence ratio computed through Eq. 9.5. Each point on Fig. 9.4-a represent a point of the LES. Keeping now only the points over a minimum reaction rate threshold, it is possible to reconstruct the distribution function of equivalence ratio, conditioned by reaction rate (Fig. 9.4-b).

**FIG. 9.4 - Instantaneous combustion regime**: Scatter plot of local reaction rate versus equivalence ratio \( a) \) and associated population density \( b) \) for case \( AD_{STEADY} \).

This "PDF"\(^5\) evidences two points:

\(^4\)also known as passive scalar.

\(^5\)the term Probability Density Function is abusively employed here.
The mixture feeding the flame is slightly more homogeneous than suggested by section 9.2.3: the variance of the PDF is very narrow. It assesses the quality of mixing, since very few points burn at equivalence ratio below 0.4 or above 0.7. The lack of precision of qualitative conclusions made in section 9.2.3 are due to the position of the transverse plane which was not close enough to the flame.

No point of the flame burns at the stoechiometry ($\phi = 1$). This clearly implies that no part of the flame at all is susceptible to burn in diffusion regime. The flame may burn sequentially pockets of gases richer and poorer than the global equivalence ratio $\phi_{\text{mean}}$, but the structure of the flame is always premixed.

### 9.3 Adiabatic reacting cases

#### 9.3.1 Objectives of unforced flow studies

The aims of unforced reacting flow adiabatic simulations are:

- to have a brief overview of reacting flow dynamics and compare with cold flow (section 9.3.3).
- to investigate the unsteady flame structure in the absence of forcing and the mechanisms controlling the flame (section 9.3.4).
- to validate reacting LES by comparing the flame mean position with experiment\(^6\) (section 9.3.5).

\(^6\)i.e. chemiluminescence $CH^*$ data

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[9.3 Adiabatic reacting cases]
9.3.2 Verification of thickened zone

The Dynamic Thickened Flame model presented in section 3.4.3 is built to use a variable thickening factor $F$, depending on the local mesh resolution and the presence of the flame. The first point is to check that the thickened zone closely surrounds the flame but also that $F$ remains small.

Figure 9.5-a presents the instantaneous distribution function of $F$, considering only reacting points.$^7$ Most of the reacting points are gathered around a thickening factor of $F = 25$, and no point in the flame is thickened more than 40. A similar distribution function of $F$ (Fig. 9.5-b) for non reacting points only evidences that very few non reacting points are submitted to thickening. The mixing which occurs upstream of the flame front is not affected by thickening: the DTFLES model does not modify mixing computations away from the flame.

9.3.3 Reacting flow dynamics

The topologies of unforced reacting flow and cold flow are very similar. Figure 9.6 compares the cold flow velocity profiles shown in Chap. 8.2 (case AD_COLD) with reacting ones (case AD_STEADY).

Three main differences are noticeable:

- Even though both cold and reacting flows have the same swirl number, the opening angle of the jet is clearly increased with combustion (Fig. 9.6-a). This general result has been already observed in [184].
- The flow is substantially accelerated by the thermal expansion due to the flame. It leads to a modification of the shape of lateral recirculation zone and higher velocities along the chamber walls (Fig. 9.6-a).
- The level of RMS fluctuations is significantly increased by the reaction (Fig. 9.6-b).

$^7$ the threshold is fixed at 10 mol.m$^{-3}$.s$^{-1}$
9.3 Adiabatic reacting cases

FIG. 9.6 - Comparison of axial velocity statistical profiles: a) mean values, b) RMS values; dotted line: cold flow (case AD_COLD); solid line: reacting flow (case AD_STEADY); dashed line: zero line.
9.3.4 Unsteady flame structure

Takeno index

A final verification of the combustion regime can be done using the Takeno index [212], which has been successfully employed in both DNS by Mizobuchi [118] and LES by Vervisch [207]. According to the notation of Vervisch [207], the Takeno index $N_{F,O}$ reads:

$$N_{F,O} = \frac{\nabla Y_F \cdot \nabla Y_O}{\|\nabla Y_F\| \|\nabla Y_O\|}$$

(9.6)

Figure 9.7 now presents the distribution function of $N_{F,O}$ considering once more only reacting points. Almost all points in the flame burn with $N_{F,O}$ close to 1, which adds another indication of the absence of diffusion flamelets.

Three-dimensional flame structure

Figure A.3 exhibits the instantaneous three-dimensional flame structure, materialised by an isosurface of temperature at 1200 K. Even though the flame is compact, it is strongly wrinkled by the turbulence. Some pockets of fresh gases are sometimes released and burn later. This source of unsteady heat release is one of the phenomena involved in the combustion instability chain.

Local one-dimensional flame structure

The flame structure can be locally compared to one-dimensional laminar flames. Profiles of temperature and reaction rate are extracted normally to the instantaneous 3D flame front. Figure 9.8 indicates the location of these 1D profiles superimposed on isolevels of reaction rate in longitudinal plane.

Figure 9.9 evidences that the instantaneous structure of the flame front computed with TFLES differs strongly for points a,b or c. This is expected since TFLES computes reaction rates explicitly as well
9.3 Adiabatic reacting cases

**Fig. 9.8 - Reaction rate in longitudinal plane and location of reacting 1D profiles displayed on Fig. 9.9.**

**Fig. 9.9 - Temperature and reaction rate 1D profiles at cuts a), b) and c) shown on Fig. 9.8.**

as local diffusion phenomena. Since the macroscopic stretch imposed at points a, b or c is different, the flame structure has to be different. The flame thickness for example is not the same for cut a, b or c.

What the TFLES model guarantees is that each flame element moves locally at the flame speed corresponding to the equivalence ratio and turbulence level. The flame structure itself obtained ultimately with the TFLES model has no physical meaning. It depends on the mesh for example: thicker flames are obtained in places where the mesh is coarse. Interpreting plots such as Fig. 9.9 is therefore a difficult exercise.
9.3.5 Comparison of mean flame position

Informations on the mean location of the flame are gathered on Fig. 9.10: heat release on a longitudinal cut in the central plane is first compared with an Abel transformation [1] of chemiluminescence $CH^*$ intensity (Fig. 9.10-a). Then, an integration over a line of sight is performed to relate the heat release to the raw $CH^*$ intensity (Fig. 9.10-b).

Both LES and experiment yield a very compact flame, with a length ($\approx 80$ mm) shorter than twice the diameter of the burner outlet. Despite the aberrations of Abel transformation [1] close to the axis, the opening angle shown by chemiluminescence is slightly larger than predicted by LES case AD_STEADY. Unfortunately, the bad quality of the $CH^*$ signal as well as the assumption of axisymmetry restricts this comparison to qualitative conclusions.

A possible way to improve LES results and especially the interaction between the flame and the outer recirculation zones is to take into account heat losses. This issue will be discussed in section 9.4.

9.4 Non adiabatic reacting cases

9.4.1 Heat losses computation

Heat losses are an important issue in combustion chambers since both the reaction rate and the acoustics of the chamber are strongly linked with temperature. Adiabatic walls can be a good assumption when the thermal barrier coating is efficient, e.g. when ceramic heat shield is employed on the chamber walls [186]. In the present test rig, the thin metallic liner surrounded by the cooling channel invalidates that assumption. Moreover, section 9.3 indicated that the simulated shape of the flame (e.g. opening angle) should be slightly improved to match perfectly the experiment (Fig. 9.10).

In the experiment, the heat loss to the cooling air can be calculated directly using the measured mass flow and temperatures at inlet and outlet. The total heat loss from the combustion chamber $Q_{Total}$ is the
sum of the heat loss to the cooling air $Q_1$ and to the surroundings $Q_2$ (via the pressure vessel). Based on the adiabatic flame temperature and the measured temperature at the combustion chamber outlet, the total heat loss from the combustion gases is estimated at approximately 27% of the burner total power, e.g. 34 kW. The heat transferred to the surroundings $Q_2$ is subsequently determined from the difference between the total heat loss and the heat taken by the cooling air:

$$Q_2 = Q_{Total} - Q_1 \quad (9.7)$$

In the LES, heat losses are computed by taking into account two phenomena (Fig. 9.11):

- Turbulent convection to the chamber walls. Heat transfer to the chamber walls is modelled using a law-of-the-wall function \[175\] (briefly presented in section 5.4). A simple conjugate approach \[201\] is used for conduction through the walls and convection through air in the cooling channel. A global heat resistance $R_w$ is used for these two mechanisms such that the heat flux $Q_w$ is\[^8\] :

$$Q_w = \frac{T_c - T_w}{R_w} \quad \text{with} \quad R_w = \frac{d_c}{\lambda_c N_u} + \frac{d_w}{\lambda_w} \quad (9.8)$$

where $T_w$, $d_w$ and $\lambda_w$ are respectively the temperature, thickness and conductivity of the wall, and $T_c$, $d_c$ and $\lambda_c$ are the temperature, the height and conductivity of the cooling channel air. The Nusselt number is given by a simple heat transfer correlation in the cooling channel:

$$N_u = 0.023 \quad Re^{4/5} \quad Pr^{1/3} \quad (9.9)$$

where $Re$ is the Reynolds number of the cooling flow ($Re = 5700$). In all presented results, $R_w$ is assumed to remain constant along the chamber wall and $T_c$ to rise linearly along the combustion chamber axis from\[^9\] 300 K to 575 K.

\[^8\]note that $Q_w$ is always negative, as well as all heat losses.

\[^9\]these values of cooling channel air temperature are provided by experimental measurements.
ON PULSATED REACTING FLOW

- Radiation to the walls. Assuming that gases are optically thin, radiation can be modelled as a volumetric sink term calculated with a Stefan-Boltzman law [7]:

\[
Q_r = -4\sigma(T^4 - T_s^4) \sum_{k=1}^{n} (Y_k a_{p,k})
\]

(9.10)

where \( T_s \) is the adjustable temperature of the surroundings (here \( T_s = 1500K \)), \( \sigma \) the Stefan-Boltzman constant, and \( Y_k \) and \( a_{p,k} \) are the mass fraction and Planck mean absorption coefficient for species \( k \). These coefficients are obtained using the RADCAL programme [69] and curve-fits provided by Gore et al [68]:

\[
a_{p,k} = \exp \left( C_0 + C_1 \ln(T) + C_2 [\ln(T)]^2 + C_3 [\ln(T)]^3 + C_4 [\ln(T)]^4 \right)
\]

(9.11)

with coefficients for \( CO_2 \) and \( H_2O \) from Tab. 9.3.

<table>
<thead>
<tr>
<th>Species</th>
<th>( C_0 )</th>
<th>( C_1 )</th>
<th>( C_2 )</th>
<th>( C_3 )</th>
<th>( C_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H_2O )</td>
<td>278.713</td>
<td>-153.240</td>
<td>32.1971</td>
<td>-3.00870</td>
<td>0.104055</td>
</tr>
<tr>
<td>( CO_2 )</td>
<td>969.86</td>
<td>-588.38</td>
<td>132.89</td>
<td>-13.182</td>
<td>0.48396</td>
</tr>
</tbody>
</table>

Tab. 9.3 - Coefficients for \( CO_2 \) and \( H_2O \) to obtain the Planck mean absorption coefficients.

9.4.2 Mean heat losses

Table 9.4 summarizes the measured mean heatfluxes in the experiment and the values resulting from the LES case HL_steady. The main objective of heat-loss treatment, which is to have the same global losses, is achieved despite the questionable accuracy of thermocouples measurements. The similar value of mean outlet temperature is a good hint that the enthalpy balance is approximately closed.

<table>
<thead>
<tr>
<th>Experiment</th>
<th>LES</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluxes</td>
<td></td>
</tr>
<tr>
<td>( Q_{Total} )</td>
<td>-34kW</td>
</tr>
<tr>
<td>( T_{Outlet} )</td>
<td>( \approx 1300K )</td>
</tr>
</tbody>
</table>

Tab. 9.4 - Evaluation of the heat losses measured in the experiment and modelled in the LES.
The global energy balance obtained by LES is illustrated in Fig. 9.12. Note that all of the fuel burns in the chamber, yielding an efficiency almost equal to 1.

Another validation of the heat losses evaluation can be done by comparing one-dimensional profiles of temperature at the wall $T_w$ and more precisely along a line in the middle of the bottom wall. $T_w$ is reconstructed from Eq. 9.8 by $T_w = T_c - Q_w R_w$. The only available experimental data is a rough evaluation of wall temperature for other operating conditions, i.e. at 1 bar and 5 bar using a Nusselt number approach. The predicted temperature remains within the range evaluated experimentally (Fig. 9.13-a) and the wall mean temperature nowhere exceeds 1200 K. Moreover, Fig. 9.13-b displays the wall heat flux along this line, which is clearly maximum in the closest region to the flame.

9.4.3 Instantaneous heat losses

The agreement on global heat losses values presented in section 9.4.2 seemed reasonable. Local heat fluxes at the wall are now investigated. Figure A.4 illustrates the instantaneous distribution of heat losses at the chamber bottom wall. Note that the losses are displayed as negative values here. Close to the flame, the losses can reach up to 50 kW/m$^2$, and the spatial variations are very intense. This point is a fundamental input for the evaluation of thermo-mechanical fatigue. The unsteadiness of this thermal load will be detailed in section 10.7.
9.4.4 Comparison with experimental data

As presented in section 9.3, Fig. 9.14 compares the field of heat release from LES case HL_STEADY with chemiluminescence $CH^*$. Comparing Fig. 9.14 (with heat losses) and 9.10 (adiabatic) shows that the effects of heat losses on the flame shape seem limited. Its length and opening angle look similar, but a quantitative comparison between the cases case HL_STEADY and case AD_STEADY is required for further investigation.

![Comparison of measured CH* intensity (Experimental result) with heat release (LES result of case HL_STEADY). (a) Cut in central plane. (b) Integration over line of sight.](image)

9.4.5 Influence of heat losses on the flow field

Comparing now mean axial velocity profiles confirms the negligible impact of heat losses on the global organisation of the flow field (Fig. 9.15-a). Even the RMS values are nearly the same (Fig. 9.15-b). As a matter of fact, the consequences of heat losses are limited to two effects:

- The first effect of heat loss wall treatment is to decrease the maximum temperature of 100 to 200 K, which has a small impact on velocities.
- A second (and main) effect is the modification of the acoustics of the chamber which will be introduced in the next sections.
FIG. 9.15 - Comparison of axial velocity statistical profiles: a) mean values, b) RMS values; dotted line: adiabatic reacting flow (case AD_STEADY); solid line: heatloss reacting flow (case HL_STEADY); dashed line: zero line.
9.5 Acoustic analysis using Helmholtz solver

Acoustic analysis is a powerful tool to understand the mechanisms leading to combustion instabilities [49, 185]. The acoustic eigenmodes of the setup can be computed using the 3D Helmholtz code AVSP [11, 12, 112, 113] presented in section 7.2. The field required for this analysis is the local mean speed of sound and is provided by a time-averaged solution of the reactive LES (cases AD_STEADY and HL_STEADY). Table 9.5 shows the lowest eigenfrequencies found numerically and compares them to the values measured in the experiment.

<table>
<thead>
<tr>
<th>Case</th>
<th>Eigenfrequencies (Hz)</th>
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</thead>
<tbody>
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<td>Helmholz solver</td>
<td>Adiabatic</td>
</tr>
<tr>
<td></td>
<td>72 131 272 298 487 705</td>
</tr>
<tr>
<td></td>
<td>Heat loss</td>
</tr>
<tr>
<td></td>
<td>64 128 250 294 443 642</td>
</tr>
<tr>
<td></td>
<td>298 487 705 926 1093</td>
</tr>
<tr>
<td>Experiment</td>
<td>Measured</td>
</tr>
<tr>
<td></td>
<td>62 171 270 433 625</td>
</tr>
<tr>
<td></td>
<td>820 1022</td>
</tr>
<tr>
<td>LES</td>
<td>Adiabatic</td>
</tr>
<tr>
<td></td>
<td>X X X X X 480 X 920</td>
</tr>
<tr>
<td></td>
<td>Heat loss</td>
</tr>
<tr>
<td></td>
<td>X X X X X 428 X 810</td>
</tr>
<tr>
<td></td>
<td>X</td>
</tr>
<tr>
<td>Mode</td>
<td>description</td>
</tr>
<tr>
<td></td>
<td>1/4 3/4 5/4 7/4 5/4</td>
</tr>
<tr>
<td></td>
<td>7/4 9/4 1/2</td>
</tr>
<tr>
<td></td>
<td>related to</td>
</tr>
<tr>
<td></td>
<td>S S S S C(a) C(b) C(c)</td>
</tr>
<tr>
<td></td>
<td>P</td>
</tr>
</tbody>
</table>

Tab. 9.5 - Eigenfrequencies computed by the Helmholtz code, measured in the experiment and in the LES. S for "full Setup", P for "Plenum" and C for "Chamber". Superscripts (a), (b) & (c) indicate that this mode is represented on Fig. 9.16-(a), (b) & (c) respectively.

Modes have been classified in three categories: the modes which correspond to eigen frequencies of the plenum (marked as "P" in the last line of Table 9.5), to eigenfrequencies of the chamber (marked "C") and to eigenfrequencies coupling the plenum and the chamber, thereby involving the full Setup (marked "S"). For modes "P" and "C", this partial decoupling is possible because the inlet section of the chamber...
acts essentially like a velocity node.

The agreement between the predicted eigenmodes frequencies and the measured results is quite good. Note that it is greatly improved by using the mean temperature field obtained from the LES case using heat loss (HL\textunderscore STEADY) instead of the adiabatic case (AD\textunderscore STEADY) which yields lower and more realistic temperature and sound speeds. However, the 171 Hz mode measured in the experiment is still difficult to link either with the 3 quarterwave or with the 5 quarterwave mode of the setup.

### 9.6 Unsteady modes in the unforced case

Not all modes (listed in Table 9.5) identified by the Helmholtz solver do necessarily occur in the LES or the experiment. In the experiment, a loud tonal noise appears after a certain heating time of the setup at the frequency of 433 Hz.

LES captures this instability too and Fig. 9.17 now demonstrates that the main peak at 433 Hz observed in the experiment is also predicted by LES in both cases AD\textunderscore STEADY and HL\textunderscore STEADY. Moreover, the Helmholtz analysis presented in section 9.5 reveals that this self-excited mode is an acoustic eigenmode. It corresponds to the 5/4 wave mode of the chamber itself ($\lambda = 4/5L$ where $L$ is the combustion chamber length $L = 1.93$ m).

The frequency of this mode is 487 Hz for the Helmholtz solver and 480 Hz in the LES code using adiabatic walls and no radiation (case AD\textunderscore STEADY). These values are too high compared to the 433 Hz frequency measured experimentally because the temperature field is overpredicted. When heat-losses are accounted for (case HL\textunderscore STEADY), the Helmholtz solver yields a frequency for the 5/4 wave mode of 443 Hz while the LES gives 428 Hz. Both values match the experimental value (433 Hz) within 3% (see Table 9.5).

![Figure 9.17](image-url) - Pressure spectra measured in the experiment (thin line) and computed with LES pressure signal (thick line) for cases AD\textunderscore STEADY and HL\textunderscore STEADY.
Figure 9.17 also exhibits that beyond the expected effect of heat losses on the prediction of self-excited mode frequency, the impact on the eigenmode amplitude is strong. Whereas the 480 Hz peak (Fig. 9.17, case AD,STEADY) is hardly distinguishable from the background noise (due to log scale), the corresponding 428 Hz peak (Fig. 9.17, case HL,STEADY) is much higher and closer to the measured level. In other words, by changing the mode frequency, the heat losses trigger a different flame response [179] and yield higher pressure fluctuations levels. This LES result demonstrates the impact of thermal boundary conditions on flame response.
Chapitre 10

Pulsated reacting cases

10.1 Phenomenology and forcing method

10.1.1 Phenomenology

A central question for modeling approaches is to know what induces an unsteady reaction rate (necessary to sustain the oscillations) when an acoustic wave enters the combustion chamber. This unsteady combustion process may be due to at least two main effects:

1. The formation of vortices in the combustion chamber (Fig. 10.1-a) : These vortices are usually triggered by strong acoustic waves propagating in the air passages. These structures capture large pockets of fresh gases which burn only later in a violent process leading to small scale turbulence and high reaction rates [64, 146].

2. The modification of the fuel and oxidizer flow rates when the acoustic wave propagates into the fuel and air feeding lines (Fig. 10.1-b). This can lead to local changes of the equivalence ratio and therefore to a modification of the burning rate when these pockets enter the chamber. If the burner operates in a very lean mode, this effect may be important since variations of inlet equivalence ratio may trigger localized extinction and strong combustion oscillations [31].

In non-premixed combustors, the second mechanism has been identified as a key element controlling combustor stability [100, 31]. According to Lieuwen, the mechanism is the following : even away from Lean or Rich Blow Off (LBO or RBO), equivalence ratio fluctuations produce heat-release oscillations which trigger combustion instabilities through pressure oscillations feedback. A direct proof of the importance of fuel injection on stability is that the location of fuel injectors often alters the stability of the system. The crucial role of fuel modulation can also be readily identified by considering active control examples in which a small modulation of the fuel lines feeding a combustor can be sufficient to alter the stability of the combustor [73, 114, 130, 148].
Even though the general idea of the mechanism proposed by Lieuwen is fairly clear, the details of the coupling phenomenon are unknown. For instance, real instability mechanisms are often a mixture of mechanisms 1 and 2 and not of only one of them. A possible method to gain more insights into this instability mechanism is to pulsate the fuel flow rate in a partially premixed combustor. Multiple studies have examined the behaviour of combustors submitted to a pulsation of the air stream to measure their transfer function [30, 64, 83]. Less data is available for fuel pulsation in partially premixed devices [13].

### 10.1.2 Forcing method

To study the flame transfer function, the reactants flow rate needs to be pulsated. Because of the acoustic decoupling system (Fig. 6.3-b), the air flow rate is difficult to force. Only the fuel line may be pulsated in the experiment.

In the LES, forcing the reacting flow is achieved by pulsating the fuel mass flow rate in the four fuel pipes (Fig. 6.3-a). Forcing is performed at 300 Hz for several amplitudes: 5, 10, 15, 30, 50, and 80 percent of the unforced mean mass flow rate. For all these amplitudes, the fuel pipes flows remain subsonic but the maximum Mach number can reach $M \approx 0.9$ in these pipes for case HL_FORCE80. The air flow rate provided by the "air supply room" remains constant, and is only affected by the flow modulations induced by acoustic waves propagation. Section 10.2 will show that these modulations are not negligible.

In the experiment, this fuel pulsator can have different forms. Some authors use a siren-like pulsator, i.e. with a rotating part [30, 62, 164]. An advantage of such a pulsator is its high maximum frequency of oscillation. The disadvantage is that the form of the excitation is fixed by the geometry of the siren, i.e. white noise excitation is not possible. Moreover, a sinus-like excitation would require a complex form of the rotating disc.
Another option is to use a control valve [13, 73]. This type of pulsator has a somewhat lower maximum frequency of oscillation but it can accept any excitation signal. Since the maximum frequency of excitation is still high enough for the experiments performed here, a D633-7320 MOOG control valve is used in this study. The maximum level of excitation by the MOOG valve depends on the frequency and the operating point [206]. At the operating point presented in section 6.3 and at the considered frequency of 300 Hz, the maximum forcing level is 12% of the mean fuel mass flow at the rim of the fuel pipes.

An overview of the different elements that play a role in the unsteady measurements is shown in Fig. 10.2. The MOOG valve is fed by an excitation signal $V'_{exc}$ leading to a displacement $\delta'$ of the MOOG’s piston. To obtain the fuel mass flow perturbation at the fuel nozzles, the transfer function $\frac{m'_{fuel}}{\delta'}$ has been determined in a separate experiment. Hence, the fuel mass flow perturbation can be determined from the measured piston displacement $\delta'$. The fuel mass flow perturbation will cause a heat release perturbation $Q'$, which can be detected by the laser measurements via the radical fields.

**Fig. 10.2 - Schematic layout of the method used in the unsteady measurements.**
10.2 Self amplification of excitation

A controversial question to understand excitation mechanisms when fuel flow rate is pulsated is the following: is the air flow rate remaining constant during fuel flow rate pulsation? This can be checked in the LES by evaluating the fuel and air mass flow rates at the mouth of the burner (through transverse plane, see Fig. 8.1).

\[ \phi = \frac{\dot{m}_F}{\dot{m}_A} \]  

(10.1)

Starting from the usual definition of equivalence ratio (Eq. 10.1), taking its logarithm and differentiating leads to:

\[ \frac{d\phi}{\phi} = \frac{d\dot{m}_F}{\dot{m}_F} - \frac{d\dot{m}_A}{\dot{m}_A} \]  

(10.2)

For small variations around a mean state, it can be assumed that:

\[ \phi \simeq \bar{\phi} \quad \dot{m}_F \simeq \bar{m}_F \quad \dot{m}_A \simeq \bar{m}_A \]  

(10.3)

Considering this, Eq. 10.2 yields:

\[ \phi' = \frac{\dot{m}_F'}{\dot{m}_F} - \frac{\dot{m}_A'}{\dot{m}_A} \]  

(10.4)

The equivalence ratio at the chamber inlet can be split in two parts (Eq. 10.4): the first corresponds to the contribution of instantaneous fuel flow rate to equivalence ratio fluctuations \( \dot{\phi}'_F \), and the second to the contribution of instantaneous air flow rate to equivalence ratio fluctuations \( \dot{\phi}'_A \). Eq. 10.4 is exact for small equivalence ratio perturbations but it can be considered as a reasonable first order evaluation of \( \dot{\phi}' \) for larger fluctuations (up to 30%). Figure 10.3 presents the two contributions \( \dot{\phi}'_F \) and \( \dot{\phi}'_A \) measured in the LES for two pulsation amplitudes: 15% and 30%.

Fig. 10.3 - Contribution of the fuel (thin line) and the air (thick line) fluctuations to equivalence ratio oscillations at the mouth of the burner for case AD_FORCE15 a) and case AD_FORCE30 b).
10.3 Unsteady modes in the forced case

After a time delay of two cycles, the acoustic waves produced by the flame and partially reflected at the end of the chamber clearly perturb the air flow rate. In other words, the \( X \% \) pulsation of the fuel line is seen by the flame as a \( 1.2 \cdot X \% \) equivalence ratio excitation. In the present situation and for a forcing frequency of 300 Hz, the air flow is also affected by the fuel flow modulation and amplifies its impact on the fluctuations of equivalence ratio at the burner inlet. This conclusion is not general (it depends on the air line impedance) but shows that this effect should be taken into account for modelling. Moreover, this conclusion does not necessarily implies that the response of the flame is not linear (see section 10.6).

10.3 Unsteady modes in the forced case

In forced cases as well, spectral analysis is required to highlight the link between acoustics and flame response. Figure 10.4 displays a typical pressure spectrum during forced operation at an excitation level of 15\% at 300 Hz (cases AD\_FORCE15 and HL\_FORCE15).

The self-excited mode at 433 Hz is still present and even increased by the forcing. As presented in section 9.6, taking into account wall heat losses improves the prediction of both frequency and amplitude of the 433 Hz eigenmode. Moreover, the forcing frequency (300 Hz) is also clearly noticeable on these spectra.

The order of magnitude of the broad band noise seems to be predicted quite correctly, but the reliability of this point must be considered with the greatest care because it was not checked in the present study.

In summary, this section demonstrates that LES captures with a reasonable accuracy the impact of forcing on the acoustic resonance of the test rig, but the exact phenomena leading to unsteady heat release and consequently to pressure fluctuations remains unclear. This will be investigated in section 10.4.
10.4 Phase-locked averaged analysis

10.4.1 Observed mechanism

LES results can be phase-averaged (here on 7 cycles) to isolate the flame response at 300 Hz. Figures 10.5 displays the shape and intensity of the flame in longitudinal plane at eight phases of the cycle for the adiabatic case AD_FORCE15. It also shows the evolution of pockets along the cycle which are richer than global equivalence ratio. These pockets are materialised by an isosurface of equivalence ratio at $\phi = 0.6$ (slightly richer than the mean $\phi = 0.55$).

![Phase locked heat release in the central plane and isosurface of equivalence ratio $\phi = 0.6$ for case AD_FORCE15.](image)

After a certain time lag, these pockets reach the reacting zone. The flame does not move significantly when it is reached by these pockets but the local heat release oscillates and triggers the pressure fluctuations feeding the 433 Hz acoustic mode (as described in section 10.3). The global heat release seems to be maximum around a phase of 225° but a quantitative analysis is required for greater accuracy.
10.4 Phase-locked averaged analysis

(Section 10.5).

10.4.2 Influence of heat losses

As presented in section 10.4.1, Fig. 10.6 displays the evolution of phase-locked heat release from LES case HL_FORCED15 along the cycle. Comparing Fig. 10.6 (with heat losses) and 10.5 (adiabatic) evidences that the effects of heat losses on the flame response are limited.

The same mechanism (convection of pockets richer than global equivalence ratio) is observed and the maximum heat release occurs at the same phase (225°).
### 10.5 Flame transfer function

#### 10.5.1 Definition of $n$ and $\tau$ for fuel pulsation

**Original definition**

In the original paper from Crocco [42], the flame transfer function was characterised by an interaction index $n$ and a delay $\tau$ between pressure fluctuations $P'$ due to acoustic waves in the premix passages and the reaction rate $\dot{\omega}_T$.

One issue for $n - \tau$ definition is normalisation: the obtained $n$ and $\tau$ are valid for a given burner and the comparison of $n$ between two burners is not easy. In recent studies, Kaufmann et al. [83] proposed the following normalisation of the flame transfer function for premix pulsation:

$$n e^{i\omega \tau} = \gamma - 1 \frac{S_F \gamma p_0}{\int \dot{\omega}_r(t) dV}$$

(10.5)

where $S_F$ is the forced surface, $u'_r(t)$ the velocity excitation (due to pulsation) and $\int \dot{\omega}_r(t) dV$ the resulting global heat release fluctuations.

**Low frequency asymptotic value**

In the low frequency limit ($\omega \to 0$), and for perfectly premixed flames, an estimate has been derived by Kaufmann et al. [83] for the limit value of the interaction index $n$. Such a derivation can be done for pure fuel pulsation as well.

The fuel mass flow rate fluctuations can be expressed as:

$$\dot{m}'_F = S_F \rho_F Y_F u'_F$$

(10.6)

Assuming that all fuel entering the domain burns, i.e. balancing fuel consumption with fuel supply, integral heat release fluctuations reads:

$$\int \dot{\omega}'_T dV = Q_{HR} \dot{m}'_F = Q_{HR} S_F \rho_F Y_F u'_F$$

(10.7)

where $Q_{HR}$ is the heat of reaction per unit mass of fuel and $S_F$ the surface of the fuel inlet.

Replacing in Eq. 10.5 integral heat release fluctuations by fuel consumption (Eq. 10.7) leads (for globally lean regime) to the low frequency limit interaction index $n(\omega \to 0)$:

$$n(\omega \to 0) = \frac{\gamma - 1}{\gamma p_0} Q_{HR} \rho_F Y_F$$

(10.8)

Eq. 10.8 demonstrates that the normalisation proposed by Kaufmann et al. [83] yields an interaction index $n$ degenerating, when $\omega \to 0$, towards values which are independent of the burner geometry. For
10.5 Flame transfer function

case AD_FORCE15, considering numerical data provided in Tab. 10.1, the limit interaction index \( n \) is:

\[ n(\omega \rightarrow 0) = 66 \quad (10.9) \]

### 10.5.2 Evaluation of \( n \) and \( \tau \) for fuel pulsation

The reference point from which excitation signal is extracted is located at the inlet of the fuel nozzle. Since all fuel jets are pulsated together, the forced surface \( S_F \) is four times the area of each fuel pipe (i.e. 3.14 mm\(^2\)). The required data for the computation of interaction index \( n \) is summarised on Tab. 10.1.

<table>
<thead>
<tr>
<th>( \gamma )</th>
<th>( \rho_F )</th>
<th>( Y_F )</th>
<th>( Q_{HR}^1 )</th>
<th>( S_F )</th>
<th>( p_0 )</th>
<th>( u_F'(t) )</th>
<th>( \int \omega_F'(t)dV )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.32</td>
<td>1.059 kg/m(^3)</td>
<td>0.767</td>
<td>50.1 ( \cdot 10^6 ) J/kg</td>
<td>1.25 ( \cdot 10^{-5} ) m(^2)</td>
<td>1.5 ( \cdot 10^5 ) Pa</td>
<td>35 m/s</td>
<td>20.5 ( \cdot 10^3 ) J/s</td>
</tr>
</tbody>
</table>

Tab. 10.1 - Required data for the computation of interaction index \( n \) (case AD_FORCE15).

The time delay can be obtained by extracting the angle of Eq. 10.5. In the case AD_FORCE15, \( \tau \) reads:

\[ \tau = 230^\circ \quad (10.10) \]

This confirms the approximate results obtained in section 10.4.

Considering Eq. 10.5 and the data provided in Tab. 10.1, the interaction index \( n \) computed is:

\[ n = 75 \quad (10.11) \]

This value is much higher than usually obtained when pulsating premix passages\(^2\) [83, 64]. The normalisation proposed by Kaufmann et al. [83] is adequate to compare interaction indexes \( n \) for air pulsation, but not appropriate to compare interaction indexes resulting from fuel pulsation with usual values from premix pulsation. However, the low frequency limit value \( (n(\omega \rightarrow 0) = 66) \), see Eq. 10.8) of interaction index is of the same order as computed value \( (n = 75) \) which confirms its validity.

### 10.5.3 Comparison with experiment

Instead of finding an adequate normalisation of the flame transfer function between \( u' \) and \( \int \omega'_F(t)dV \) in order to make it independent of the burner geometry (see section 10.5.2), another strategy is to investigate the transfer function between dimensionless fluctuations of velocity \( u'/\pi \) and dimensionless fluctuations of reaction rate \( Q'/Q \).

Figure 10.7 first compares the level of reaction rate fluctuations \( (Q'/Q) \) observed in the LES (case AD_FORCE15) with the fluctuations of \( CH^* \) radical \( (CH^*/CH^2) \) along the cycle. Heat release \( (Q) \) and \( CH^* \) emission are probably not linearly related for such a partially premixed flame so that comparing \( Q'/Q \) and \( CH^*/CH^2 \) is a challenging test. However, results show that both amplitude and phase are in quite good agreement, despite the limited number of cycles used in the LES phase-averaging procedure.

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\(^1\)\( Q_{HR} \) is reduced to \( 48.3 \cdot 10^6 \) J/kg when accounting for the 2\(^{nd} \) reaction equilibrium

\(^2\)are of the order of 5
10.6 Linearity of the flame response

Recent experimental results in studies of forced flames by Balachandran et al. [5, 6] show that beyond a certain pulsation amplitude, a saturation effect is observed. LES can be a good tool to investigate this point by evaluating the response of the flame up to high amplitude excitations where measurements can be either dangerous or even not feasible due to the limitations of the MOOG valve. Figure 10.8 presents the reaction rate fluctuation level for several pulsation amplitudes up to 80% and its evolution along the cycle.

The maximum of normalized global reaction rate fluctuations for each amplitude is plotted on Fig. 10.9-a as well as the integrated \( CH^* \) fluctuations for low pulsation amplitudes only. Fig. 10.9-b displays the phase corresponding to each maximum of global reaction rate fluctuations versus the pulsation amplitude.

No saturation effect is noticed here: the flame behaves linearly within the range considered (Fig. 10.9-a), which makes it suitable for low-order modelling. Moreover, the phase of maximum \( Q' \) is approximately constant (Fig. 10.9-b).

This major difference between the present results and [5, 6] may be due to the method used to pulsate the equivalence ratio: in Balachandran et al. [5, 6], the fuel flow rate is constant (fuel line choked)
10.7 Thermal load of the structure

10.7.1 Global heat fluxes fluctuations

In heavy duty gas turbines, the thermal load on the walls is an important issue: on one hand, the air used to cool down either the metallic liner or the tile-holders of ceramic heat-shield must be minimum to optimise the efficiency. On the other, even a temporary overheating may damage the structure and fluctuating heat load plays a crucial role in its long term fatigue. Therefore, the mean thermal balance is not sufficient to predict this. Unsteady heat losses must be investigated.

![Graph](image1)

**FIG. 10.9** - Dependence of a) normalized global reaction rate fluctuations and b) phase of maximum fluctuations upon the forcing amplitude.

and they pulsate the air flow. Therefore, both mechanisms (1) and (2) are involved (see section 10.1.1). Coherent structures (e.g. ring vortices) may wrinkle the flame and capture pockets of fresh gases [64]. In this study, since the momentum of the fuel jets is very small compared to the momentum of the air flow, only the second mechanism described in section 10.1.1 (Fig. 10.1-b) dominates. The modulation of fuel flow rate creates alternatively pockets of rich and poor mixture, which after a given convective time will excite the flame.

10.7 Thermal load of the structure

**FIG. 10.10** - Temporal evolution of a) global convective \(Q_w\) and b) radiative \(Q_r\) heat losses for cases HL_STEADY (thin line) and HL_FORCE15 (thick line).

![Graph](image2)
Figure 10.10 presents the temporal evolution of global heat losses (integrated over the hole chamber) in the LES for both forced (HL_FORCE15) and unforced (HL_STEADY) cases. The level of fluctuations of convective heat flux $Q_w$ (Fig. 10.10-a) as well as the radiative heat flux $Q_r$ (Fig. 10.10-b) are significantly increased by the forcing. The forcing frequency (300 Hz) is also clearly noticeable on these oscillations, which establishes the link between the instability and the fluctuating heat load.

### 10.7.2 Local heat fluxes fluctuations

The global information presented in section 10.7.1 is important as a stepstone towards the evaluation of the thermal load of the structure but it is not enough. A local analysis is required.

**Heat losses along the cycle**

A first analysis is performed using phase-locked averaging to quantify the evolution of thermal load on the structure along a cycle.

![Graph](image)

**Fig. 10.11 - Evolution of thermal load on the structure (bottom wall) for each phase of the cycle (case HL_FORCE15). White isoline corresponds to $Q_w = -45$ kW.**

Fig. 10.11 displays the heat flux at the bottom wall for eight phases of the cycle. The white isoline corresponds to $Q_w = -45$ kW/m$^2$. The phase at which the thermal load is the most intense$^{3}$ seems to be

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$^{3}$“intense” means “larger absolute value” since $Q_w$ is always negative
between 315° and 360°. Comparing Fig. 10.11 with Fig. 10.6 evidences that the phase at which the heat release is maximum (i.e. ≈ 230°) does not correspond to the phase at which the heat losses are maximum (i.e. ≈ 340°). This time delay (of the order of 1 ms) can be explained by the convective time required for the gases heated by the flame to reach the wall.

Unsteady heat losses at the wall

Another way to evaluate the fluctuation of heat flux at the wall is to observe the temporal evolution of $Q_w$ at several points of the bottom wall along the chamber axis. Fig. 10.12 shows the location of probes a), b), c) and d) superimposed on a sketch of the flame front location.

![Fig. 10.12 - Location of the heat flux probes employed in Fig. 10.13.](image)

**Fig. 10.13 - Temporal evolution local convective ($Q_w$) heat losses at a) $x = 50$ mm, b) $x = 100$ mm, c) $x = 200$ mm and d) $x = 300$ mm for case HL_FORCE15. The probes are located on Fig. 10.12.**
Fig. 10.13-a) to d) respectively present the results obtained from probes a) to d). The liner is submitted to very large thermal load: The maximum value of mean heat flux is $-47 \text{ kW/m}^2$ (probe b) and the RMS fluctuations can reach up to $15 \text{ kW/m}^2$ (probe a). Comparing all graphs of Fig. 10.13 leads to three conclusions:

- The mean value of $|Q_w|$ decreases along the chamber axis, as shown qualitatively on Fig. A.4 (instantaneous view of flame and heat fluxes).
- The closest probe to the flame (probe a) is not submitted to the most intense mean heat fluxes: Actually, probe b) which is in the stream of the swirled jet experiences a slightly larger mean thermal load.
- The fluctuations (RMS) of heat flux, which are the source of thermo-mechanical fatigue, are larger at probe a) than at probe b). In other words, the highest RMS fluctuations of heat flux are not necessarily correlated with the highest mean thermal load.

This section demonstrated that LES is able to capture the local unsteadiness of heat fluxes at the wall when forcing the fuel flow rate. In addition to the noise level inside the combustion chamber (section 10.8), this can constitute a fundamental input data for a structure code.

However in the conjugate approach presented in section 9.4, no thermal inertia of the wall [201] is accounted for. This possible improvement in modelling the heat transfer between the chamber and the cooling channel may have an impact on the heat flux fluctuations and therefore change the input of thermo-mechanical fatigue evaluation.

### 10.8 Mechanical load of the structure

#### 10.8.1 Prototype of fluid / structure coupling

The cases HL_STEADY and HL_FORCE15 are selected as inputs for building the fluid / structure prototype. The unsteady LES pressure field is transmitted to the structure code ANSYS used at University of Twente with the following procedure:

1. The LES signal is sampled at 6.6 kHz at the walls during a simulated time of 21 ms (Total 140 samples).
2. These samples are interpolated for each wall of the chamber on a coarse structured grid with elements size of $10 \times 10 \text{ mm}$ (i.e. a mesh size of $182 \times 16$ for each wall).
3. The signal is reproduced periodically as long as needed and transmitted to ANSYS.

For this first prototype, only the pressure field is involved in the coupling. No information on heat fluxes, which would be necessary for the evaluation of thermo-mechanical fatigue, is exchanged.
10.8 Mechanical load of the structure

10.8.2 Coupling results

All structure computations with ANSYS (using LES dataset as input) and laser vibrometer measurements presented in this section have been done by Huls et al. at University of Twente [79] and are useful to illustrate the comparison between experiment (pressure sensor / vibrometer) and LES coupled with ANSYS.

Results in the unforced case

The wall pressure fluctuation signal extracted from the LES is first compared without pulsation (case HL_STEADY) with temporal signal extracted from the "kulite" pressure sensor at the same location (Fig. 10.14-a). Both LES and pressure sensor reveal the 433 Hz eigenfrequency (investigated in section 9.5). Moreover, both signals match quite well in terms of amplitude. Of course, no phase information can be obtained since the signals were not phase-locked.

![Pressure fluctuations comparison](image)

**Fig. 10.14 - a) Pressure fluctuations at the wall and b) resulting displacement of the structure for case HL_STEADY. Thick line: results from LES signal; Thin line: results from a) "kulite" sensor or b) vibrometer.**

Fig. 10.14-b compares the resulting liner displacement velocities computed with ANSYS [79] from the LES pressure signal and measured by laser vibrometer. Since the agreement on the pressure field was quite good (Fig. 10.14-a), the displacement velocities from AVBP / ANSYS and vibrometer naturally match as well.

It confirms that the key element in the coupling procedure is the accuracy of the pressure signal at the wall. The structure code is less critical in predicting correctly structure displacement velocities.
Results in the forced case

The results presented in the last paragraph on the unforced case (HL_STEADY) were encouraging. Fig. 10.15 now displays the same graphs for forced case HL_FORCE15. Comparing Fig. 10.15-a and Fig. 10.14-a corroborates that the pressure fluctuations are increased by forcing (as shown on pressure spectra in section 10.3). The agreement between LES and measurements, in terms of both amplitude and frequency of pressure oscillations, is quite good. The displacement velocities from AVBP/ANSYS and vibrometer measurements match reasonably well (Fig. 10.15-b). Note that the signals were not phase-locked either.

![Graphs showing pressure fluctuations and displacement velocities for forced case HL_FORCE15.](image)

**FIG. 10.15 - a) Pressure fluctuations at the wall and b) resulting displacement of the structure for case HL_FORCE15. Thick line : results from LES signal ; Thin line : results from a) "kulite" sensor or b) vibrometer.**

The main objective of this section was to achieve a first prototype of fluid / structure coupling. The feasibility has been evidenced and results shown here seem promising. The level of agreement between vibrometer measurements and AVBP coupled to ANSYS appears to be good enough to evaluate the impact of combustion instabilities on the structure fatigue. However, the reliability has not been demonstrated and should be investigated on other (and simpler) cases.
Conclusion générale

Computations of a partially premixed lab-scale burner are carried out using LES for both non-pulsated and pulsed cases. State-of-the-art techniques are gathered to overcome the difficulties of combustion instabilities simulations (i.e. thermal law of the wall, characteristic boundary conditions, high order schemes on unstructured meshes). These methods are applied on the geometrically complex experimental setup specifically developed for the DESIRE project at University of Twente.

For the non reacting flow, detailed comparisons of LES / experiment are successfully performed in terms of mean and RMS velocities which validate the accuracy of LES. Moreover, cold flow simulations exhibit the impact of wall function on the flow field.

For the reacting flow, several classical questions are investigated :
– A self-amplification effect of the equivalence ratio excitations due to reflected acoustic waves perturbing the air flow rate is revealed.
– No saturation of the flame response to large pulsation amplitude is noticeable : the flame behaves linearly within the range of observation considered (up to 80%).

Many issues are determined as step-stones towards fluid / structure coupling and clarified :
– The mechanism leading from equivalence ratio fluctuations to heat release oscillations is characterized using phase-locked average analysis.
– The loud tonal noise appearing in the unforced reacting case (self excited mode) is explained by the joint use of LES solver AVBP and Helmholtz solver AVSP. This mode predicted by LES is in good agreement with the experimental spectra in terms of both frequency and amplitude.
– A first evaluation of the impact of combustion instability on the heat load at the chamber walls is achieved.

Finally, a prototype of fluid / structure coupling between AVBP and ANSYS is presented. The results are encouraging but further investigation on other cases must be done to assess the reliability of predictions.

More generally, this study demonstrated that LES is able to capture the specific role of equivalence ratio fluctuations in phenomena leading to combustion instabilities and their consequences on the chamber structure.
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Annexes
Annexe A

Planches en couleur

A.1 Écoulement à froid

FIG. A.1 - Champ instantané de vitesse axiale $u$ et iso-contour $u = 0$ dans le plan longitudinal avec le schéma TTGC. Fermeture de la zone de recirculation centrale.
FIG. A.2 - Champ instantané de vitesse axiale $u$ et iso-contour $u = 0$ dans le plan longitudinal avec le schéma TTGC. a) loi de parois ; b) murs non glissants.
A.2 Écoulement à chaud

FIG. A.3 - Instantaneous view of the flame (isosurface of temperature at $T = 1000\,\text{K}$, colored by axial velocity) and of the methane jets (isosurface of fuel mass fraction at $Y_{CH_4} = 0.1$, colored in blue).

FIG. A.4 - Instantaneous view of the flame, methane jets, pressure and heat losses at the walls.
A.3 Influence de l’injection pilote

Fig. A.5 - Visualisation du front de flamme instantané par une isosurface de température $T = 2/3 \cdot T_{\text{ref}}$ (colorée par la vitesse axiale), et isosurface stoechiométrique ($\phi = 1$, colorée en bleu) pour les cas a) 2% et b) 6%. Figure couleur reproduite de l’annexe C.
Annexe B

Characteristic wave decomposition

B.1 Basic definitions

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></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>$m_1 = \rho u, m_2 = \rho v, m_3 = \rho w$</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>$\rho e_s = \sum_k \rho_k e_{sk} = \rho \sum_k Y_k e_{sk}$</td>
</tr>
<tr>
<td>sensible enthalpy density</td>
<td>$\rho h_s = \sum_k \rho_k h_{sk} = \rho \sum_k Y_k h_{sk}$</td>
</tr>
<tr>
<td>kinetic energy density</td>
<td>$\rho e_c = \frac{1}{2}\rho (u^2 + v^2 + w^2) = \frac{1}{\rho} (m_1^2 + m_2^2 + m_3^2)$</td>
</tr>
<tr>
<td>total energy</td>
<td>$\mathcal{E} = \rho \mathcal{E} = \rho e_c + \rho e_s$</td>
</tr>
<tr>
<td>total enthalpy</td>
<td>$\mathcal{H} = \rho \mathcal{H} = \rho e_c + \rho h_s$</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 :

$$\overline{C_v} = \sum_k Y_k C_{vk} \quad \overline{C_p} = \sum_k Y_k C_{pk} \quad \overline{\tau} = \sum_k Y_k r_k \quad \frac{1}{\overline{W}} = \sum_k \frac{Y_k}{W_k} \quad \overline{\gamma} = \frac{\overline{C_p}}{\overline{C_v}}$$

Finally, pressure is :

$$P = \sum_k \rho_k r_k T = \rho \overline{\tau} T$$

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:

\[ \chi = \sum_k \chi_k Y_k = r T - \beta \bar{e} = \beta (C_v T - \bar{e}) = -\beta e_0^s \]

where \( e_0^s \) is defined by \( e_0^s = e_s - C_v T \) so that the sensible energy can be locally written as a linear function of temperature:

\[ e_s = C_v T + e_0^s \]

Of course, \( C_v \) and \( e_0^s \) are not constant and \( e_s \) 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:

\[ d\rho = \sum_k d\rho_k \quad dP = \frac{\rho}{\rho^*}dT + \sum_k r_k T d\rho_k \quad dT = \frac{1}{\rho^*}dP - \sum_k \frac{r_k T}{\rho^*}d\rho_k \]

\[ dm_1 = \rho du + \sum_k u d\rho_k \quad dm_2 = \rho dv + \sum_k v d\rho_k \quad dm_3 = \rho dw + \sum_k w d\rho_k \]

\[ d(\rho v_c) = \rho v_u dT + \sum_k e_{sk} d\rho_k \quad d(\rho h_s) = \rho C_v dT + \sum_k h_{sk} d\rho_k \]

\[ dE = \rho v_u du + \rho v_d dv + \rho v_d dw + \sum_k (e_c + e_{sk}) d\rho_k + \rho C_v dT \]

\[ dE = u dm_1 + v dm_2 + w dm_3 + \sum_k (-e_c + e_{sk}) d\rho_k + \rho C_v dT \]

\[ dE = \rho v_u du + \rho v_d dv + \rho v_d dw + \sum_k (e_c + e_{sk}) d\rho_k - \frac{r_k}{\rho^*} C_v T d\rho_k + \frac{1}{\beta}dP \]

\[ dE = u dm_1 + v dm_2 + w dm_3 + \sum_k (-e_c + e_{sk}) d\rho_k - \frac{r_k}{\rho^*} C_v T d\rho_k + \frac{1}{\beta}dP \]

\[ dT = \frac{1}{\rho C_v} \left( dE - \rho v_u du - \rho v_d dv - \rho v_d dw - \sum_k (e_c + e_{sk}) d\rho_k \right) \]

\[ dT = \frac{1}{\rho C_v} \left( dE - u dm_1 - v dm_2 - w dm_3 + \sum_k (e_c - e_{sk}) d\rho_k \right) \]

\[ dP = \beta \left( -\rho v_u du - \rho v_d dv - \rho v_d dw + dE + \sum_k \left[ -e_c + \frac{\chi_k}{\beta} \right] d\rho_k \right) \]

\[ dP = \beta \left( -u dm_1 - v dm_2 - w dm_3 + dE + \sum_k \left[ +e_c + \frac{\chi_k}{\beta} \right] d\rho_k \right) \]

As from AvBPV5.1 the \( e_{sk} \) are tabulated in intervals of 100 \( K \) such that \( C_{vk} \) are piecewise contant.
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.

<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>(\partial(\rho u))</td>
<td>(M^{-1})</td>
<td>(\Omega V^{-1})</td>
<td>(L)</td>
</tr>
<tr>
<td>(\partial(\rho v))</td>
<td>(\rightarrow)</td>
<td>(\rightarrow)</td>
<td>(\leftarrow)</td>
</tr>
<tr>
<td>(\partial(\rho w))</td>
<td>(\leftarrow)</td>
<td>(\leftarrow)</td>
<td>(\rightarrow)</td>
</tr>
<tr>
<td>(\partial\rho E)</td>
<td>(M)</td>
<td>(\Omega_V)</td>
<td>(R)</td>
</tr>
<tr>
<td>(\partial(\rho Y_k))</td>
<td>(\Omega V)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[
\begin{align*}
\frac{\partial W_1}{\partial t} &= \frac{\partial u_n}{\partial t} + \frac{\partial P}{\partial x} \\
\frac{\partial W_2}{\partial t} &= -\frac{\partial u_n}{\partial t} + \frac{\partial P}{\partial x} \\
\frac{\partial W_3}{\partial t} &= \frac{\partial u_1}{\partial t} \\
\frac{\partial W_4}{\partial t} &= \frac{\partial u_2}{\partial t} \\
\frac{\partial W_{4+k}}{\partial t} &= -\frac{\partial Y_k}{\partial x} \frac{\partial P}{\partial t} + \frac{\partial \rho_k}{\partial t}
\end{align*}
\]

Tab. B.1 - Summary of links between different set of variables and passage matrices involved in the wave decomposition process.

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

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{\partial (u u + P)}{\partial x} + \frac{\partial (p w)}{\partial y} + \frac{\partial (p w w)}{\partial z} &= 0 \quad (B.1) \\
\frac{\partial v}{\partial t} + \frac{\partial (u v u + P)}{\partial x} + \frac{\partial (p v w)}{\partial y} + \frac{\partial (p w w)}{\partial z} &= 0 \quad (B.2) \\
\frac{\partial w}{\partial t} + \frac{\partial (u w u + P)}{\partial x} + \frac{\partial (p v w)}{\partial y} + \frac{\partial (p w w + P)}{\partial z} &= 0 \quad (B.3) \\
\frac{\partial \rho E}{\partial t} + \frac{\partial (H u u + P)}{\partial x} + \frac{\partial (H v v + P)}{\partial y} + \frac{\partial (H w w + P)}{\partial z} &= 0 \quad (B.4) \\
\frac{\partial \rho k}{\partial t} + \frac{\partial (K u u)}{\partial x} + \frac{\partial (K v v)}{\partial y} + \frac{\partial (K w w)}{\partial z} &= 0 \quad (B.5)
\end{align*}
\]
These equations can be re-written in matrix notation:

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial \vec{F}_U}{\partial x} + \frac{\partial \vec{G}_U}{\partial y} + \frac{\partial \vec{H}_U}{\partial y} = 0$$  \hspace{1cm} (B.6)$$

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

$$\vec{U} = (m_1, m_2, m_3, E, \rho_k)^t$$  \hspace{1cm} (B.7)$$

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

$$\vec{F}_U = (\rho uu + P, \rho vu, \rho wu, \rho Hu, \rho_k u)^t$$
$$\vec{G}_U = (\rho uv, \rho vv + P, \rho wv, \rho Hv, \rho_k v)^t$$
$$\vec{H}_U = (\rho uw, \rho vw, \rho ww + P, \rho Hw, \rho_k w)^t$$  \hspace{1cm} (B.8)$$

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

$$\frac{\partial \vec{U}}{\partial t} + A_U \frac{\partial \vec{U}}{\partial x} + B_U \frac{\partial \vec{U}}{\partial y} + C_U \frac{\partial \vec{U}}{\partial y} = 0$$  \hspace{1cm} (B.9)$$

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

$$A_U = \frac{\partial \vec{F}_U}{\partial \vec{U}} \hspace{1cm} B_U = \frac{\partial \vec{G}_U}{\partial \vec{U}} \hspace{1cm} C_U = \frac{\partial \vec{H}_U}{\partial \vec{U}}$$  \hspace{1cm} (B.10)$$

The $x$-Jacobian matrix:

$$A_U = \begin{pmatrix}
\frac{\partial F_{m_1}}{\partial m_1} & \frac{\partial F_{m_1}}{\partial m_2} & \frac{\partial F_{m_1}}{\partial m_3} & \frac{\partial F_{m_1}}{\partial E} & \frac{\partial F_{m_1}}{\partial \rho_k} \\
\frac{\partial F_{m_2}}{\partial m_1} & \frac{\partial F_{m_2}}{\partial m_2} & \frac{\partial F_{m_2}}{\partial m_3} & \frac{\partial F_{m_2}}{\partial E} & \frac{\partial F_{m_2}}{\partial \rho_k} \\
\frac{\partial F_{m_3}}{\partial m_1} & \frac{\partial F_{m_3}}{\partial m_2} & \frac{\partial F_{m_3}}{\partial m_3} & \frac{\partial F_{m_3}}{\partial E} & \frac{\partial F_{m_3}}{\partial \rho_k} \\
\frac{\partial F_E}{\partial m_1} & \frac{\partial F_E}{\partial m_2} & \frac{\partial F_E}{\partial m_3} & \frac{\partial F_E}{\partial E} & \frac{\partial F_E}{\partial \rho_k} \\
\frac{\partial F_{\rho_k}}{\partial m_1} & \frac{\partial F_{\rho_k}}{\partial m_2} & \frac{\partial F_{\rho_k}}{\partial m_3} & \frac{\partial F_{\rho_k}}{\partial E} & \frac{\partial F_{\rho_k}}{\partial \rho_k}
\end{pmatrix}$$

Explicitly:

$$A_U = \begin{pmatrix}
\frac{\partial (\rho uu + P)}{\partial m_1} & \frac{\partial (\rho uu + P)}{\partial m_2} & \frac{\partial (\rho uu + P)}{\partial m_3} & \frac{\partial (\rho uu + P)}{\partial E} & \frac{\partial (\rho uu + P)}{\partial \rho_k} \\
\frac{\partial \rho uv}{\partial m_1} & \frac{\partial \rho uv}{\partial m_2} & \frac{\partial \rho uv}{\partial m_3} & \frac{\partial \rho uv}{\partial E} & \frac{\partial \rho uv}{\partial \rho_k} \\
\frac{\partial \rho uw}{\partial m_1} & \frac{\partial \rho uw}{\partial m_2} & \frac{\partial \rho uw}{\partial m_3} & \frac{\partial \rho uw}{\partial E} & \frac{\partial \rho uw}{\partial \rho_k} \\
\frac{\partial (\rho vv + P)}{\partial m_1} & \frac{\partial (\rho vv + P)}{\partial m_2} & \frac{\partial (\rho vv + P)}{\partial m_3} & \frac{\partial (\rho vv + P)}{\partial E} & \frac{\partial (\rho vv + P)}{\partial \rho_k} \\
\frac{\partial \rho pw}{\partial m_1} & \frac{\partial \rho pw}{\partial m_2} & \frac{\partial \rho pw}{\partial m_3} & \frac{\partial \rho pw}{\partial E} & \frac{\partial \rho pw}{\partial \rho_k} \\
\frac{\partial \rho ph}{\partial m_1} & \frac{\partial \rho ph}{\partial m_2} & \frac{\partial \rho ph}{\partial m_3} & \frac{\partial \rho ph}{\partial E} & \frac{\partial \rho ph}{\partial \rho_k} \\
\frac{\partial (\rho wv)}{\partial m_1} & \frac{\partial (\rho wv)}{\partial m_2} & \frac{\partial (\rho wv)}{\partial m_3} & \frac{\partial (\rho wv)}{\partial E} & \frac{\partial (\rho wv)}{\partial \rho_k} \\
\frac{\partial \rho hw}{\partial m_1} & \frac{\partial \rho hw}{\partial m_2} & \frac{\partial \rho hw}{\partial m_3} & \frac{\partial \rho hw}{\partial E} & \frac{\partial \rho hw}{\partial \rho_k} \\
\frac{\partial \rho_k u}{\partial m_1} & \frac{\partial \rho_k u}{\partial m_2} & \frac{\partial \rho_k u}{\partial m_3} & \frac{\partial \rho_k u}{\partial E} & \frac{\partial \rho_k u}{\partial \rho_k} \\
\frac{\partial \rho_k w}{\partial m_1} & \frac{\partial \rho_k w}{\partial m_2} & \frac{\partial \rho_k w}{\partial m_3} & \frac{\partial \rho_k w}{\partial E} & \frac{\partial \rho_k w}{\partial \rho_k}
\end{pmatrix}$$

so that:
CHARACTERISTIC WAVE DECOMPOSITION

\[ A_U = \begin{pmatrix}
2u - \beta u & -\beta v & -\beta w & \beta & -uu + \beta e_c + \chi_1 & \ldots & -uu + \beta e_c + \chi_N \\
v & u & 0 & 0 & -uv & \ldots & -uv \\
w & 0 & u & 0 & -uw & \ldots & -uw \\
H - \beta uu & -\beta vw & -\beta uw & (1 + \beta)u & -uH + \beta ue_c + u\chi_1 & \ldots & -uH + \beta ue_c + u\chi_N \\
Y_1 & 0 & 0 & 0 & u - uY_1 & \ldots & -uY_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
Y_N & 0 & 0 & 0 & -uY_N & \ldots & u - uY_N
\end{pmatrix}\]

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:

$$
B_U = \begin{pmatrix}
\frac{\partial G_m}{\partial m_1} & \frac{\partial G_m}{\partial m_2} & \frac{\partial G_m}{\partial m_3} & \frac{\partial G_m}{\partial E} & \frac{\partial G_m}{\partial \rho_k} \\
\frac{\partial G_m}{\partial m_1} & \frac{\partial G_m}{\partial m_2} & \frac{\partial G_m}{\partial m_3} & \frac{\partial G_m}{\partial E} & \frac{\partial G_m}{\partial \rho_k} \\
\frac{\partial G_m}{\partial \rho_k} & \frac{\partial G_m}{\partial \rho_k} & \frac{\partial G_m}{\partial \rho_k} & \frac{\partial G_m}{\partial \rho_k} & \frac{\partial G_m}{\partial \rho_k}
\end{pmatrix}
$$

Explicitly:

$$
B_U = \begin{pmatrix}
\frac{\partial P_m}{\partial m_1} & \frac{\partial P_m}{\partial m_2} & \frac{\partial P_m}{\partial m_3} & \frac{\partial P_m}{\partial E} & \frac{\partial P_m}{\partial \rho_k} \\
\frac{\partial P_m}{\partial m_1} & \frac{\partial P_m}{\partial m_2} & \frac{\partial P_m}{\partial m_3} & \frac{\partial P_m}{\partial E} & \frac{\partial P_m}{\partial \rho_k} \\
\frac{\partial P_m}{\partial \rho_k} & \frac{\partial P_m}{\partial \rho_k} & \frac{\partial P_m}{\partial \rho_k} & \frac{\partial P_m}{\partial \rho_k} & \frac{\partial P_m}{\partial \rho_k}
\end{pmatrix}
$$

so that:

$$
B_U = \begin{pmatrix}
v & u & 0 & 0 & -vu & \cdots & -vu \\
-\beta u & 2v - \beta v & -\beta w & \beta & -vw + \beta e_c + \chi_1 & \cdots & -vw + \beta e_c + \chi_N \\
0 & w & v & 0 & -vw & \cdots & -vw \\
-\beta vu & H - \beta vv & -\beta vw & (1 + \beta)v & -vH + \beta ve_c + v\chi_1 & \cdots & -vH + \beta ve_c + v\chi_N \\
0 & Y_1 & 0 & 0 & v - vY_1 & \cdots & v - vY_1 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & Y_N & 0 & 0 & -vY_N & \cdots & v - vY_N
\end{pmatrix}
$$
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The $z$-Jacobian matrix:

$$
C_U = \begin{pmatrix}
\frac{\partial H_{m1}}{\partial m1} & \frac{\partial H_{m1}}{\partial m2} & \frac{\partial H_{m1}}{\partial m3} & \frac{\partial H_{m1}}{\partial E} & \frac{\partial H_{m1}}{\partial \rho_k} \\
\frac{\partial H_{m2}}{\partial m1} & \frac{\partial H_{m2}}{\partial m2} & \frac{\partial H_{m2}}{\partial m3} & \frac{\partial H_{m2}}{\partial E} & \frac{\partial H_{m2}}{\partial \rho_k} \\
\frac{\partial H_{m3}}{\partial m1} & \frac{\partial H_{m3}}{\partial m2} & \frac{\partial H_{m3}}{\partial m3} & \frac{\partial H_{m3}}{\partial E} & \frac{\partial H_{m3}}{\partial \rho_k} \\
\frac{\partial H_{p1}}{\partial m1} & \frac{\partial H_{p1}}{\partial m2} & \frac{\partial H_{p1}}{\partial m3} & \frac{\partial H_{p1}}{\partial E} & \frac{\partial H_{p1}}{\partial \rho_k} \\
\frac{\partial H_{p2}}{\partial m1} & \frac{\partial H_{p2}}{\partial m2} & \frac{\partial H_{p2}}{\partial m3} & \frac{\partial H_{p2}}{\partial E} & \frac{\partial H_{p2}}{\partial \rho_k}
\end{pmatrix}
$$

Explicitely:

$$
C_U = \begin{pmatrix}
\frac{\partial \rho u}{\partial m1} & \frac{\partial \rho u}{\partial m2} & \frac{\partial \rho u}{\partial m3} & \frac{\partial \rho w}{\partial \rho k} \\
\frac{\partial \rho v}{\partial m1} & \frac{\partial \rho v}{\partial m2} & \frac{\partial \rho v}{\partial m3} & \frac{\partial \rho w}{\partial \rho k} \\
\frac{\partial \rho}{\partial m1} & \frac{\partial \rho}{\partial m2} & \frac{\partial \rho}{\partial m3} & \frac{\partial \rho w}{\partial \rho k} \\
\frac{\partial \rho H}{\partial m1} & \frac{\partial \rho H}{\partial m2} & \frac{\partial \rho H}{\partial m3} & \frac{\partial \rho w}{\partial \rho k} \\
\frac{\partial \rho w}{\partial m1} & \frac{\partial \rho w}{\partial m2} & \frac{\partial \rho w}{\partial m3} & \frac{\partial \rho w}{\partial \rho k}
\end{pmatrix}
$$

so that

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

The $A_U$, $B_U$ and $C_U$ Jacobian matrices are difficult to diagonalise. It is more convenient to reintroduce the primitive variables $\mathbf{V}$

$$ \mathbf{V} = (u, v, w, P, \rho_k)^T $$

The $M$ matrix allows to change from conserved variables $\mathbf{U}$ to primitive variables $\mathbf{V}$:

$$ \partial \mathbf{U} = M \partial \mathbf{V} \quad \quad M = \frac{\partial \mathbf{U}}{\partial \mathbf{V}} $$

Obviously, the inverse relations hold:

$$ \partial \mathbf{V} = M^{-1} \partial \mathbf{U} \quad \quad M^{-1} = \frac{\partial \mathbf{V}}{\partial \mathbf{U}} $$

The transformation matrices $M$ and $M^{-1}$ are:

$$ M = \begin{pmatrix} \frac{\partial m_1}{\partial u} & \frac{\partial m_1}{\partial v} & \frac{\partial m_1}{\partial w} & \frac{\partial m_1}{\partial P} & \frac{\partial m_1}{\partial \rho} & \cdots & \frac{\partial m_1}{\partial \rho} \\ \frac{\partial m_2}{\partial u} & \frac{\partial m_2}{\partial v} & \frac{\partial m_2}{\partial w} & \frac{\partial m_2}{\partial P} & \frac{\partial m_2}{\partial \rho} & \cdots & \frac{\partial m_2}{\partial \rho} \\ \frac{\partial m_3}{\partial u} & \frac{\partial m_3}{\partial v} & \frac{\partial m_3}{\partial w} & \frac{\partial m_3}{\partial P} & \frac{\partial m_3}{\partial \rho} & \cdots & \frac{\partial m_3}{\partial \rho} \\ \frac{\partial m_4}{\partial u} & \frac{\partial m_4}{\partial v} & \frac{\partial m_4}{\partial w} & \frac{\partial m_4}{\partial P} & \frac{\partial m_4}{\partial \rho} & \cdots & \frac{\partial m_4}{\partial \rho} \\ \frac{\partial m_5}{\partial u} & \frac{\partial m_5}{\partial v} & \frac{\partial m_5}{\partial w} & \frac{\partial m_5}{\partial P} & \frac{\partial m_5}{\partial \rho} & \cdots & \frac{\partial m_5}{\partial \rho} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial m_N}{\partial u} & \frac{\partial m_N}{\partial v} & \frac{\partial m_N}{\partial w} & \frac{\partial m_N}{\partial P} & \frac{\partial m_N}{\partial \rho} & \cdots & \frac{\partial m_N}{\partial \rho} \end{pmatrix} = \begin{pmatrix} \rho & 0 & 0 & 0 & u & \cdots & u \\ 0 & \rho & 0 & 0 & v & \cdots & v \\ 0 & 0 & \rho & 0 & w & \cdots & w \\ \rho u & \rho v & \rho w & \frac{1}{\beta} & c_e - \frac{\chi_1}{\beta} & \cdots & c_e - \frac{\chi_N}{\beta} \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} $$

$$ M^{-1} = \begin{pmatrix} \frac{\partial n_1}{\partial u} & \frac{\partial n_1}{\partial v} & \frac{\partial n_1}{\partial w} & \frac{\partial n_1}{\partial P} & \frac{\partial n_1}{\partial \rho} & \cdots & \frac{\partial n_1}{\partial \rho} \\ \frac{\partial n_2}{\partial u} & \frac{\partial n_2}{\partial v} & \frac{\partial n_2}{\partial w} & \frac{\partial n_2}{\partial P} & \frac{\partial n_2}{\partial \rho} & \cdots & \frac{\partial n_2}{\partial \rho} \\ \frac{\partial n_3}{\partial u} & \frac{\partial n_3}{\partial v} & \frac{\partial n_3}{\partial w} & \frac{\partial n_3}{\partial P} & \frac{\partial n_3}{\partial \rho} & \cdots & \frac{\partial n_3}{\partial \rho} \\ \frac{\partial n_4}{\partial u} & \frac{\partial n_4}{\partial v} & \frac{\partial n_4}{\partial w} & \frac{\partial n_4}{\partial P} & \frac{\partial n_4}{\partial \rho} & \cdots & \frac{\partial n_4}{\partial \rho} \\ \frac{\partial n_5}{\partial u} & \frac{\partial n_5}{\partial v} & \frac{\partial n_5}{\partial w} & \frac{\partial n_5}{\partial P} & \frac{\partial n_5}{\partial \rho} & \cdots & \frac{\partial n_5}{\partial \rho} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{\partial n_N}{\partial u} & \frac{\partial n_N}{\partial v} & \frac{\partial n_N}{\partial w} & \frac{\partial n_N}{\partial P} & \frac{\partial n_N}{\partial \rho} & \cdots & \frac{\partial n_N}{\partial \rho} \end{pmatrix} = \begin{pmatrix} \frac{1}{\rho} & 0 & 0 & 0 & -\frac{u}{\rho} & \cdots & -\frac{u}{\rho} \\ 0 & \frac{1}{\rho} & 0 & 0 & -\frac{v}{\rho} & \cdots & -\frac{v}{\rho} \\ 0 & 0 & \frac{1}{\rho} & 0 & -\frac{w}{\rho} & \cdots & -\frac{w}{\rho} \\ -\beta u & -\beta v & -\beta w & \beta & \beta e_e + \chi_1 & \cdots & \beta e_e + \chi_N \\ 0 & 0 & 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} $$

where $e_e$ 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. $I$wave) used for the characteristic decomposition. Now, Eq. (B.9) is multiplied by $M^{-1}$:

$$ M^{-1} \frac{\partial \mathbf{V}}{\partial t} + M^{-1} A_U \frac{\partial \mathbf{V}}{\partial x} + M^{-1} B_U \frac{\partial \mathbf{V}}{\partial y} + M^{-1} C_U \frac{\partial \mathbf{V}}{\partial z} = 0 $$

(B.11)

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

$$ \frac{\partial \mathbf{V}}{\partial t} + A \frac{\partial \mathbf{V}}{\partial x} + B \frac{\partial \mathbf{V}}{\partial y} + C \frac{\partial \mathbf{V}}{\partial z} = 0 $$

(B.12)

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The Jacobians for primitive variables are then:

\[ A_V = M^{-1}.A_U.M \quad B_V = M^{-1}.B_U.M \quad C_V = M^{-1}.C_U.M \] (B.13)

The primitive Jacobian matrices are thus:

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

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

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

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 \(\vec{s} = u \vec{n} + v \vec{t}\).

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

\[ \vec{p} = x \vec{i} + y \vec{j} = X \vec{n} + Y \vec{t} \] (B.14)
B.2 Governing equations

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:

\[ \Omega^{-1}_\Theta = \Omega^T_\Theta = \Omega_{-\Theta} \]  

(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:

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

(B.23)

This finally gives:

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

(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:
\[
\frac{\partial V}{\partial t} + (A_V n_x + B_V n_y) \frac{\partial V}{\partial x} + (A_V t_x + B_V t_y) \frac{\partial V}{\partial y} = 0
\]  

The final transformation is to make a new change of variable:
\[
V_{2D} = \Omega_{V_{2D}} V_{n_{2D}}
\]
with:
\[
V_{n_{2D}} = (u_n, u_t, P, \rho_1, \ldots, \rho_N)^T
\]  

being the primitive variables with the velocity now written in the \((\vec{n}, \vec{t})\) basis. The matrix \(\Omega_{V_{2D}}\) is thus:
\[
\Omega_{V_{2D}} = \begin{pmatrix}
n_x & t_x & 0 & 0 & \ldots & 0 \\
n_y & t_y & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & \ldots & 0 \\
0 & 0 & 0 & 1 & \ldots & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & 0 & \ldots & 1
\end{pmatrix}
\]  

The inverse matrix is just:
\[
\Omega_{V_{2D}}^{-1} = \Omega_{V_{2D}}^T
\]

In three dimensions two vectors are linked by a rotation matrix \(\Omega_{\Theta_1, \Theta_2, \Theta_3}\) by:
\[
P_{(i, j, k)} = \Omega_{\Theta_1, \Theta_2, \Theta_3} P_{(\vec{i}, \vec{j}, \vec{k})}
\]
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-dimensional 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:
\[
V = \Omega_V V_n
\]
with

\[ V_n = (u_n, u_{t1}, u_{t2}, P, \rho_1, \ldots, \rho_N)^T \]  (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:

\[
\Omega_V = \begin{pmatrix}
  n_x & t_{1x} & t_{2x} & 0 & 0 & \ldots & 0 \\
  n_y & t_{1y} & t_{2y} & 0 & 0 & \ldots & 0 \\
  n_z & t_{1z} & t_{2z} & 0 & 0 & \ldots & 0 \\
  0 & 0 & 0 & 1 & 0 & \ldots & 0 \\
  0 & 0 & 0 & 0 & 1 & \ldots & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \ldots & 1
\end{pmatrix}  
\]  (B.34)

The inverse matrix is just:

\[
\Omega_V^{-1} = \Omega_V^T = \begin{pmatrix}
  n_x & n_y & n_z & 0 & 0 & \ldots & 0 \\
  t_{1x} & t_{1y} & t_{1z} & 0 & 0 & \ldots & 0 \\
  t_{2x} & t_{2y} & t_{2z} & 0 & 0 & \ldots & 0 \\
  0 & 0 & 0 & 1 & 0 & \ldots & 0 \\
  0 & 0 & 0 & 0 & 1 & \ldots & 0 \\
  \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & 0 & 0 & 0 & \ldots & 1
\end{pmatrix}  
\]  (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 \( \Omega_V^{-1} \):

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

where

\[
A_n = A_V n_x + B_V n_y + C_V n_z \\
B_n = A_V t_{1x} + B_V t_{1y} + C_V t_{1z}  \\
C_n = A_V t_{2x} + B_V t_{2y} + C_V t_{2z}  
\]  (B.37)

or, in a more compact form:

\[
\frac{\partial V_n}{\partial t} + N \frac{\partial V_n}{\partial X} + T_1 \frac{\partial V_n}{\partial Y} + T_2 \frac{\partial V_n}{\partial Z} = 0  
\]  (B.38)

with:

\[
N = \Omega_V^{-1} A_n \Omega_V  
\]  (B.39)

and

\[
T_1 = \Omega_V^{-1} B_n \Omega_V  \\
T_2 = \Omega_V^{-1} C_n \Omega_V 
\]  (B.40)

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

$$D = L.N.L^{-1} = L.N.R$$ \hspace{1cm} (B.42)

$$N = L^{-1}.D.L = R.D.L$$ \hspace{1cm} (B.43)

$D$ 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)

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

and

$$R = \begin{pmatrix}
\frac{1}{\rho c^2} & \frac{\rho c}{\rho c^2} & 0 & 0 & 0 & \ldots & 0 \\
0 & 0 & 1 & 0 & 0 & \ldots & 0 \\
0 & 0 & 0 & 1 & 0 & \ldots & 0 \\
\frac{\rho c}{\rho c^2} & \frac{\rho c^2}{\rho c^2} & 0 & 0 & 0 & \ldots & 0 \\
\frac{\rho c^2}{\rho c^2} & \frac{\rho c^3}{\rho c^2} & 0 & 0 & 0 & \ldots & 1
\end{pmatrix} \hspace{1cm} (B.44)$$

It must be noticed that three eigenvectors are associated to the same eigenvalue $\vec{u}.\vec{n}$. 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. In this derivation only the normal Jacobian has been diagonalised, this means that the flow is decomposed into waves travelling normally 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 approach is useful for the treatment of edge and corners even if the implementation is somehow cumbersome. 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

$$\begin{cases}
\partial W = L\partial V_n \\
\partial V_n = L^{-1}\partial W = R\partial W
\end{cases} \hspace{1cm} (B.45)$$
B.2 Governing equations

So, multiplying Eq. B.38 by $L$ gives:

$$L \frac{\partial V_n}{\partial t} + LL^{-1}DL \frac{\partial V_n}{\partial x} + LT_1L^{-1}L \frac{\partial V_n}{\partial y} + LT_2L^{-1}L \frac{\partial V_n}{\partial z} = 0$$  \hspace{1cm} (B.46)

that leads to

$$\frac{\partial W}{\partial t} + D \frac{\partial W}{\partial x} + LT_1L^{-1} \frac{\partial W}{\partial y} + LT_2L^{-1} \frac{\partial W}{\partial z} = 0$$  \hspace{1cm} (B.47)

$L$ 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 (see sections 5.2.2 and 5.2.3).

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

$$D = L.N.R$$
$$N = \Omega_V^{-1}.A_n.\Omega_V$$  \hspace{1cm} (B.48)

we obtain for $D$

$$D = L.\Omega_V^{-1}.A_n.\Omega_V.R$$  \hspace{1cm} (B.49)

and defining now

$$L_V = L.\Omega_V^{-1}$$
$$R_V = \Omega_V.R$$  \hspace{1cm} (B.50)

as

$$L_V = \begin{pmatrix}
    n_x & n_y & n_z & \frac{1}{\rho c} & 0 & \ldots & 0 \\
    -n_x & -n_y & -n_z & \frac{1}{\rho c} & 0 & \ldots & 0 \\
    t_{1x} & t_{1y} & t_{1z} & 0 & 0 & \ldots & 0 \\
    t_{2x} & t_{2y} & t_{2z} & 0 & 0 & \ldots & 0 \\
    0 & 0 & 0 & -\frac{Y_1}{\rho^2} & 1 & \ldots & 0 \\
    \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
    0 & 0 & 0 & -\frac{Y_N}{\rho^2} & 0 & \ldots & 1
\end{pmatrix}$$

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

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

$$\frac{\partial W}{\partial t} = L_V \frac{\partial V}{\partial t}$$
$$\frac{\partial V}{\partial t} = R_V \frac{\partial W}{\partial t}$$  \hspace{1cm} (B.51)
CHARACTERISTIC WAVE DECOMPOSITION

In the same way, reminding that:

\[ A_V = M^{-1} A_U M \]  
\[ \text{(B.52)} \]

we can define the following matrices

\[ L_U = L_V M^{-1} \]
\[ R_U = M R_V \]  
\[ \text{(B.53)} \]

\[ L_U = \begin{pmatrix}
-\frac{\beta u - c n_x}{\rho c} & -\frac{\beta v - c n_y}{\rho c} & -\frac{\beta w - c n_z}{\rho c} & \frac{\beta}{\rho} \left( \frac{\beta c + \chi_1}{c^2} - \frac{\bar{u}_t}{c} \right) & \cdots & \frac{\beta}{\rho} \left( \frac{\beta c + \chi_N}{c^2} - \frac{\bar{u}_t}{c} \right) \\
-\frac{\beta u - c n_x}{\rho c} & -\frac{\beta v - c n_y}{\rho c} & -\frac{\beta w - c n_z}{\rho c} & \frac{\beta}{\rho} \left( \frac{\beta c + \chi_1}{c^2} + \frac{\bar{u}_t}{c} \right) & \cdots & \frac{\beta}{\rho} \left( \frac{\beta c + \chi_N}{c^2} + \frac{\bar{u}_t}{c} \right) \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & \cdots & 0 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & \cdots & 0 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & \cdots & 0 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & \cdots & 0 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & \cdots & 0
\end{pmatrix} \]  
\[ \text{(B.54)} \]

\[ R_U = \begin{pmatrix}
\frac{\rho}{c^2} (u + c n_x) & \frac{\rho}{c^2} (u - c n_x) & \rho t_{1x} & \rho t_{2x} & u & \cdots & u \\
\frac{\rho}{c^2} (v + c n_y) & \frac{\rho}{c^2} (v - c n_y) & \rho t_{1y} & \rho t_{2y} & v & \cdots & v \\
\frac{\rho}{c^2} (w + c n_z) & \frac{\rho}{c^2} (w - c n_z) & \rho t_{1z} & \rho t_{2z} & w & \cdots & w \\
\frac{\rho}{c^2} (e_c + c u . \bar{n} + \frac{c^2 - \chi}{\beta}) & \frac{\rho}{c^2} (e_c - c u . \bar{n} + \frac{c^2 - \chi}{\beta}) & \rho u . t_1 & \rho u . t_2 & e_c & \frac{\chi_1}{\beta} & \cdots & e_c - \frac{\chi_N}{\beta} \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & 0 & 1 & \cdots & 0 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & 0 & 0 & \cdots & 1 \\
\frac{\rho}{c^2} & \frac{\rho}{c^2} & 0 & 0 & 0 & \cdots & 1
\end{pmatrix} \]  
\[ \text{(B.55)} \]

The following relations

\[ \frac{\partial W}{\partial U} = L_U \frac{\partial U}{\partial W} \]
\[ \text{(B.56)} \]

allow the passage from conserved variables in a global basis to characteristic variables.
B.2 Governing equations

The following relations show wave definitions (\(\partial W\) with the notation used in section 5.2) for primitive and conservative variables. Moreover, some useful identities obtained with the following inverse relations are detailed.

\[
\partial V = R_V \partial W \quad \partial U = R_U \partial W \quad (B.57)
\]

In primitive variables, we have:

\[
\begin{align*}
\partial W^1 &= +\tilde{u} \cdot \tilde{u} + \frac{1}{\rho c^2} \partial P \\
\partial W^2 &= -\tilde{u} \cdot \tilde{u} + \frac{1}{\rho c^2} \partial P \\
\partial W^3 &= +t_1 \partial \tilde{u} \\
\partial W^4 &= +\bar{t}_2 \partial \tilde{u} \\
\partial W^{4+k} &= -\frac{Y_k}{c^2} \partial P + \partial \rho_k \\
\lambda^1 &= \tilde{u} \cdot \tilde{u} + c \\
\lambda^2 &= \tilde{u} \cdot \tilde{u} - c \\
\lambda^3 &= \tilde{u} \cdot \tilde{u} \\
\lambda^4 &= \tilde{u} \cdot \tilde{u} \\
\lambda^{4+k} &= \tilde{u} \cdot \tilde{u} 
\end{align*}
\]

While in conserved variables:

\[
\begin{align*}
\partial W^1 &= -\frac{1}{\rho c^2}(\beta \tilde{u} - c \tilde{n}) \cdot \partial \rho \tilde{u} + \frac{\beta}{\rho} \partial \mathcal{E} + \sum_k \frac{1}{\rho} \left(\frac{-\tilde{u} \cdot \tilde{u} + \beta \varepsilon_k c}{c} \right) \partial \rho_k \\
\partial W^2 &= -\frac{1}{\rho c^2}(\beta \tilde{u} + c \tilde{n}) \cdot \partial \rho \tilde{u} + \frac{\beta}{\rho} \partial \mathcal{E} + \sum_k \frac{1}{\rho} \left(\frac{+\tilde{u} \cdot \tilde{u} + \beta \varepsilon_k c}{c} \right) \partial \rho_k \\
\partial W^3 &= \frac{1}{\rho} \tilde{t}_1 \cdot \partial \tilde{u} - \sum_k \frac{1}{\rho} \tilde{t}_k \cdot \partial \rho_k \\
\partial W^4 &= \frac{1}{\rho} \tilde{t}_2 \cdot \partial \tilde{u} - \sum_k \frac{1}{\rho} \tilde{t}_k \cdot \partial \rho_k \\
\partial W^{4+k} &= \frac{Y_k}{c^2} \tilde{u} \cdot \tilde{n} \partial \rho - \frac{Y_k}{c^2} \partial \mathcal{E} + \partial \rho_k - \frac{Y_k}{c^2} \sum_j (\beta \varepsilon_j + \chi_j) \partial \rho_j \\
\lambda^1 &= \tilde{u} \cdot \tilde{u} + c \\
\lambda^2 &= \tilde{u} \cdot \tilde{u} - c \\
\lambda^3 &= \tilde{u} \cdot \tilde{u} \\
\lambda^4 &= \tilde{u} \cdot \tilde{u} \\
\lambda^{4+k} &= \tilde{u} \cdot \tilde{u} 
\end{align*}
\]

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 \(\tilde{u} \cdot \tilde{u}\) and thus this pseudo-wave is also convected at the speed \(\tilde{u} \cdot \tilde{u}\).

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

We also have the following inverse relations:

\[
\begin{align*}
\partial(\tilde{u} \cdot \tilde{u}) &= \frac{1}{2} (\partial W^1 - \partial W^2) \\
\partial(\tilde{u} \cdot \tilde{u}_1) &= \partial W^3 \\
\partial(\tilde{u} \cdot \tilde{u}_2) &= \partial W^4 \\
\partial u &= \frac{1}{2} n_x (\partial W^1 - \partial W^2) + t_{1x} \partial W^3 + t_{2x} \partial W^4 \\
\partial v &= \frac{1}{2} n_y (\partial W^1 - \partial W^2) + t_{1y} \partial W^3 + t_{2y} \partial W^4 \\
\partial w &= \frac{1}{2} n_z (\partial W^1 - \partial W^2) + t_{1z} \partial W^3 + t_{2z} \partial W^4 \\
\partial P &= \frac{1}{2} \rho c^2 (\partial W^1 + \partial W^2) \\
\partial \rho_k &= \frac{d}{c} (\partial W^1 + \partial W^2) + \partial W^{4+k} \\
\partial \rho &= \frac{d}{c} (\partial W^1 + \partial W^2) + \partial W^S \\
\partial Y_k &= \frac{1}{c} \left(\partial W^{4+k} - Y_k \partial W^S\right) \\
\partial \sigma &= \frac{1}{c} \left(\sum_k r_k \partial W^{4+k} - \tau \partial W^S\right) \\
\partial T &= \frac{\beta T}{2c} (\partial W^1 + \partial W^2) - \sum_j r_j \frac{T}{\rho} \partial W^{4+j} \\
\partial \rho u &= \frac{\rho(u + \rho c^2)}{2c} \partial W^1 + \frac{\rho(u + \rho c^2)}{2c} \partial W^2 + \rho t_{1x} \partial W^3 + \rho t_{2x} \partial W^4 + u \partial W^S \\
\partial \rho v &= \frac{\rho(v + \rho c^2)}{2c} \partial W^1 + \frac{\rho(v + \rho c^2)}{2c} \partial W^2 + \rho t_{1y} \partial W^3 + \rho t_{2y} \partial W^4 + v \partial W^S \\
\partial \rho w &= \frac{\rho(w + \rho c^2)}{2c} \partial W^1 + \frac{\rho(w + \rho c^2)}{2c} \partial W^2 + \rho t_{1z} \partial W^3 + \rho t_{2z} \partial W^4 + w \partial W^S
\end{align*}
\]
B.3 LODI relations

This section presents some theory about the NSCBC method. As said in section 5.2.2, following the development of Poinsot, we can introduce the \( \mathcal{L} \) notation for wave amplitude variations:

\[
\mathcal{L} = \lambda \frac{\partial W}{\partial n}
\]  

(B.59)

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

<table>
<thead>
<tr>
<th>Inflow boundary</th>
<th>Type</th>
<th>Way</th>
<th>NSCBC MS [119]</th>
<th>AVBP V5.X</th>
<th>Annex B</th>
</tr>
</thead>
<tbody>
<tr>
<td>acoustic wave</td>
<td>out</td>
<td>-( \mathcal{L}_- \Delta t )</td>
<td>strength(5)</td>
<td>( \partial W^2 )</td>
<td></td>
</tr>
<tr>
<td>entropy wave</td>
<td>in</td>
<td>-( \mathcal{L}_s \Delta t )</td>
<td>strength(1)</td>
<td>( \partial W^s )</td>
<td></td>
</tr>
<tr>
<td>transverse shear</td>
<td>in</td>
<td>-( \mathcal{L}_{t1} \Delta t )</td>
<td>strength(2)</td>
<td>( \partial W^3 )</td>
<td></td>
</tr>
<tr>
<td>transverse shear</td>
<td>in</td>
<td>-( \mathcal{L}_{t2} \Delta t )</td>
<td>strength(3)</td>
<td>( \partial W^4 )</td>
<td></td>
</tr>
<tr>
<td>acoustic wave</td>
<td>in</td>
<td>-( \mathcal{L}_+ \Delta t )</td>
<td>strength(4)</td>
<td>( \partial W^1 )</td>
<td></td>
</tr>
<tr>
<td>species waves</td>
<td>in</td>
<td>-( \mathcal{L}_k \Delta t )</td>
<td>strength(5+k)</td>
<td>( \partial W^{4+k} )</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Outflow boundary</th>
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<td>strength(1)</td>
<td>( \partial W^s )</td>
<td></td>
</tr>
<tr>
<td>transverse shear</td>
<td>out</td>
<td>-( \mathcal{L}_{t1} \Delta t )</td>
<td>strength(2)</td>
<td>( \partial W^3 )</td>
<td></td>
</tr>
<tr>
<td>transverse shear</td>
<td>out</td>
<td>-( \mathcal{L}_{t2} \Delta t )</td>
<td>strength(3)</td>
<td>( \partial W^4 )</td>
<td></td>
</tr>
<tr>
<td>acoustic wave</td>
<td>out</td>
<td>-( \mathcal{L}_+ \Delta t )</td>
<td>strength(5)</td>
<td>( \partial W^1 )</td>
<td></td>
</tr>
<tr>
<td>species waves</td>
<td>out</td>
<td>-( \mathcal{L}_k \Delta t )</td>
<td>strength(5+k)</td>
<td>( \partial W^{4+k} )</td>
<td></td>
</tr>
</tbody>
</table>

Values for the amplitude variations in the spatial form are:

\[
\begin{pmatrix}
\mathcal{L}_+ \\
\mathcal{L}_- \\
\mathcal{L}_{t1} \\
\mathcal{L}_{t2} \\
\mathcal{L}_k
\end{pmatrix} = \begin{pmatrix}
(u_n + c) \left( \frac{\partial u_n}{\partial n} + \frac{1}{\rho c} \frac{\partial P}{\partial n} \right) \\
(u_n - c) \left( -\frac{\partial u_n}{\partial n} + \frac{1}{\rho c} \frac{\partial P}{\partial n} \right) \\
u_n \frac{\partial u_{m1}}{\partial n} \\
u_n \frac{\partial u_{m2}}{\partial n} - \frac{\partial y \partial P}{\partial n} \\
u_n \frac{\partial y}{\partial n} - \frac{\partial y \partial P}{\partial n}
\end{pmatrix}
\]  

(B.60)
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.61)

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.62)

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 [145]. 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 [145]. These LODI relations are obtained by assuming the flow as 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.63)

where

\[
N \frac{\partial V_n}{\partial n} = 
\begin{pmatrix}
u_n \frac{\partial u_n}{\partial n} + \frac{1}{\rho} \frac{\partial P}{\partial n} \\
u_n \frac{\partial u_{t1}}{\partial n} \\
u_n \frac{\partial u_{t2}}{\partial n} \\
u_n \frac{\partial P}{\partial n} + \rho c^2 \frac{\partial u_k}{\partial n} \\
u_n \frac{\partial \rho}{\partial n} + \rho_k \frac{\partial u_k}{\partial n}
\end{pmatrix}
= 
\begin{pmatrix}
\frac{1}{2}(\mathcal{L}_+ - \mathcal{L}_-) \\
\mathcal{L}_{t1} \\
\mathcal{L}_{t2} \\
\frac{\rho c}{2\gamma} (\mathcal{L}_+ + \mathcal{L}_-) \\
\frac{\rho_k}{2c} (\mathcal{L}_+ + \mathcal{L}_-) + \mathcal{L}_k
\end{pmatrix}
\]  
(B.64)

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 \( \beta = \gamma - 1 \)):
**Characteristic wave decomposition**

\[
\begin{align*}
\frac{\partial P}{\partial t} + \frac{\rho c}{2} (L_+ + L_-) &= 0 \\
\frac{\partial u}{\partial t} + \frac{1}{2} (L_+ - L_-) &= 0 \\
\frac{\partial H}{\partial t} + L_1 &= 0 \\
\frac{\partial H}{\partial t} + L_2 &= 0 \\
\frac{\partial P}{\partial t} + \frac{\rho c}{2} (L_+ + L_-) + L_k &= 0 \\
\frac{\partial H}{\partial t} + \frac{L}{2} (L_+ + L_-) + L_S &= 0 \\
\frac{\partial H}{\partial t} + \frac{1}{\rho} (L_k - Y_k L_S) &= 0 \\
\frac{\partial T}{\partial t} + \frac{1}{\rho} (-T L_S + \sum r_k L_k) &= 0 \\
\frac{\partial H_m}{\partial t} + L_+ \left( \frac{\rho}{2} (\gamma M_n + 1) \right) + L_- \left( \frac{\rho}{2} (\gamma M_n - 1) \right) + \frac{\rho c M_n}{T} \frac{\partial T}{\partial t} &= 0 \\
\frac{\partial H_m}{\partial t} + L_+ \left( \frac{\rho}{2} (M_n + 1) \right) + L_- \left( \frac{\rho}{2} (M_n - 1) \right) + c M_n L_S &= 0
\end{align*}
\]

(B.65)

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, eq. B.65 suggests that the incoming wave \( L_+ \) must be equal to \( L_- \).
Annexe C

Article soumis au 31\textsuperscript{st} Symposium International on Combustion
Large Eddy Simulation of piloting effects on turbulent swirling flames

Sengissen A. X.⋆, Giauque A. S.⋆, Staffelbach G. S.⋆, Porta M.⋆, Krebs W.†, Kaufmann P.† and Poinset T. J.‡

⋆ CERFACS, 42 Avenue G. Coriolis, 31057 Toulouse cedex, France
† Siemens PG, 45466 Mülheim an der Ruhr, Germany
‡ Institut de Mécanique des Fluides de Toulouse, Avenue C. Soula, 31400 Toulouse, France

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 favor robust stabilisation is to use small pilot flames in these regions, usually by adding pure fuel injection. A drawback of this approach
is that the stoichiometric zones created by these pilot fuel injections lead to increased NO\textsubscript{X} levels and therefore a compromise between stabilisation and pollution levels must be sought. Identifying this compromise is not straightforward because predicting stabilisation in real gas turbines is a difficult task: basic mechanisms controlling flame stabilization in a piloted swirled zone are not well understood and cannot be investigated in simpler cases (e.g. jet flames). The experience gained on simple flames (see for example the TNF workshop at www.ca.sandia.gov/TNF) is often not sufficient to predict how intense a pilot fuel injection must be in a gas turbine to provide proper stabilization while minimizing NO\textsubscript{X} emission. The influence of these small additional fuel injections is recognized and even used experimentally in active control devices for gas turbines 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]. But very few methods are available to predict this influence in the absence of experimental tests. Moreover the exact links between stabilization (the mechanisms which control the flame location) and stability (the possible oscillations of the flame position and therefore the noise and the unsteady activity generated by these movements) are often unknown.

Large Eddy Simulation (LES) is becoming a standard tool to study the dynamics of turbulent flames [16–18]. LES has been used successfully for many academic flames but still very rarely for complex realistic chambers which raise specific difficulties in terms of mesh quality, Reynolds numbers, complex fuel characteristics or sophisticated geometries so that many codes used for LES of academic flames cannot be used for real chambers anymore [17]. For example, unstructured grids are required as well as high parallel efficiency; in many cases, sophisticated and expensive subgrid-scale models cannot be used in such large codes. Beginning to compute complex cases is therefore needed today to evaluate the challenges which LES users will face in the future and which have not been identified yet on simpler cases. The objective of this paper is to use LES (section 2) in a complex burner using pilot fuel injections to compare two different cases of piloting: either 2 or 6 percent of the total methane used in the burner is injected additionally through pilot fuel lines, leading to drastic flow changes. The burner is described in section 3. Experimentally, 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, the first objectives here are to verify whether LES can be performed for such a geometry, whether the details of pilot fuel injection can be included in the computation and whether LES can bring a relevant answer for the effects of fuel injection changes by predicting the transition which is seen experimentally when going from 2 to 6% of pilot fuel injection.

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] using genetic algorithms. The objective of the algorithm 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 $\phi = 1.2$. Fig. 1 shows that the reduced two-step scheme obtained by the genetic algorithm matches the GRI mechanism quite well in this range of equivalence ratios.

![Fig. 1: Comparison of reduced two-step chemical scheme used for LES with GRI V3 mechanism for methane air flames.](image)

The flame / turbulence interaction is modeled by the Dynamic Thickened Flame (DTF) model [22] which accounts for both mixing and combustion taking place in partially premixed flames. The DTF model is an extension of the TF model developed initially for perfectly premixed flames [23, 24]. It has demonstrated its ability to handle partially premixed combustion [25, 26] and will not be detailed further in this paper. 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 [27], for which the acoustic impedance is controlled to minimise the acoustic reflections at boundaries [28]. The adiabatic walls are handled using a logarithmic law-of-the-wall formulation which is known to perform well with the classical Smagorinsky model [29]. Typical runs are performed on a grid composed of 1.4 million tetrahedra on parallel archi-
3. Target configuration

The test geometry is an axisymmetric combustion chamber (Fig. 2-a), with a 3MW full scale burner inlet (Fig. 2-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. 2-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.

Fig. 2: a) Global view of the test geometry and b) zoom on the burner (pilot and premix passages) inner parts.

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. 3).

4. Results and discussion

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 4 and 6 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. 3. 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. 4-b): burnt gases are found along the axis from $x = 0$ to $x = 2R$. Flame lift-off appears in the 2% case (Fig. 4-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. 4-a). A clearer understanding of the differences between the two cases can be gained by plotting isosurfaces of temperature and stoichiometric equivalence ratio (Fig. 5). For the 6% case, the hot zone ($T = 2/3 \cdot T_{ref}$) is directly connected to the pilot passage hub (Fig. 5-b). For the 2% case, the flame is stabilised on a ‘finger’ of burnt gases which is rotating around the x-axis (Fig. 5-a), thereby inducing the large RMS fluctuations of temperature seen in Fig. 4-a.

The axial velocity fields (Fig. 6) 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. 6-b). This zone contains the hot gases (Fig. 4-b) which provide stabilisation. The 2% case (Fig. 6-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. 4-a) which experience intense fluctuations. Even when the temperature increases (downstream of $x = 3R$), the velocity RMS values (Fig. 6-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. 7). 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 vigorously, these zones provide the robust stabilisation observed in Fig 5-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. 8. 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 ($\phi < 0.4$),
Fig. 6: Profiles of mean velocity (thick line), RMS of velocity (error bars) and $U = 0$ reference line (dashed line) for a) 2% case and b) 6% case.

Fig. 7: Scatter plot of instantaneous heat release versus mixture fraction for a) 2% case and b) 6% case.

which rotates around the x-axis.

The near stoichiometric zone of Fig. 8-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. 8-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 8 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. 6) 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. 6 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 9 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. 9-a), and are well correlated with the cold (Fig. 9-b) and lean (Fig. 9-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 [33].

The flame then features a cold non-reacting “finger-like” rotating structure protruding within the stabilisation zone (illustrated by Fig. 5-a and sketched on Fig. 10). 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. 9-a’), less cold gas reaches the plane at $x = 3R$ (Fig. 9-b’) and lean gases are not found around the axis (Fig. 9-c’).

The mechanism leading to the PVC formation in the 2% case is purely due to hydrodynamic and combustion effects but not to flame / acoustics 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). Using the mean temperature field provided by the LES a Helmholtz solver [25] was used to compute the acoustic modes of the chamber: the fundamental transverse eigenmode is 575 Hz and significantly differs from the frequency of the PVC (408 Hz). Moreover the non-reflecting inlet/outlet treatment [28] is built to damp all the longitudinal modes and the 575 Hz mode is strongly damped. Even though PVC’s and acoustic modes are known to sometimes interact, this is not the case here.
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 and cannot be addressed in simpler geometries: 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.

Acknowledgments

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References

Annexe D

Article soumis à *Combustion and Flame*
Response of a swirled non-premixed burner to fuel flow rate modulation

Sengissen A. X. a,*, Van Kampen J. F. b, Huls R. A. b, Stoffels G. G. M. b, Kok J. B. W. b and Poinsot T. J. a,c

aCERFACS, 42 Avenue G. Coriolis, 31057 Toulouse cedex, France
bUniversity of Twente, Faculty of Engineering, 7500 AE Enschede, The Netherlands
cInstitut de Mécanique des Fluides de Toulouse, Avenue C. Soula, 31400 Toulouse, France

Abstract

Studies of combustion instabilities require determination of the combustion chamber response. In non-premixed devices, combustion processes are influenced by oscillations of the air flow rate but may also be sensitive to fluctuations of the fuel flow rate entering the chamber. This paper describes a joint experimental and numerical study of the mechanisms controlling the response of a swirled, non-premixed combustor burning natural gas and air. The flow is first characterized without combustion and LDV results are compared to Large Eddy Simulation (LES) data. The non-pulsated reacting regime is then studied and characterized in terms of heat release field. Finally the combustor fuel flow rate is pulsed at several amplitudes and the response of the chamber is analyzed using phase-locked averaging and acoustic analysis.

Key words: Flame transfer functions, non premixed, swirled, Large Eddy Simulations

1 Introduction

The ability to predict the stability of a given burner is the center of many present research programs. These efforts can be experimental [1–10] or numerical [11–15].

* Corresponding author. Tel: +33-5-61-19-3131; fax: +33-5-61-19-3030.
Email address: sengis@cerfacs.fr (Sengissen A. X.).
A common specification of modern gas turbines is to operate in very lean regimes to satisfy emission regulations. The resulting flames can be sensitive to combustion oscillations, but the exact phenomena leading to instability are still a matter of discussion. A central question for modeling approaches is to know what induces an unsteady reaction rate (necessary to sustain the oscillations) when an acoustic wave enters the combustion chamber. This unsteady combustion process described in Fig. 1 may be due to (at least) two effects:

1. The formation of vortices in the combustion chamber (Fig. 1-a): These vortices are usually triggered by strong acoustic waves propagating in the air passages. These structures capture large pockets of fresh gases which burn only later in a violent process leading to small scale turbulence and high reaction rates [16, 17].

2. The modification of the fuel and oxidizer flow rates when the acoustic wave propagates into the fuel and air feeding lines (Fig. 1-b). This can lead to local changes of the equivalence ratio and therefore to a modification of the burning rate when these pockets enter the chamber. If the burner operates in a very lean mode, this effect may be important since variations of inlet equivalence ratio may trigger localized extinction and strong combustion oscillations [18].

![Diagram of flame response to velocity and equivalence ratio perturbations](image-url)

**Fig. 1.** Flame response to a) velocity perturbations and b) equivalence ratio perturbations.

In non-premixed combustors, the second mechanism has been identified as a key element controlling combustor stability [6, 18]. According to Lieuwen [6], the mechanism is the following: even away from Lean or Rich Blow Off (LBO or RBO), equivalence ratio fluctuations produce heat-release oscillations which trigger combustion instabilities through pressure oscillations feedback. A direct proof of the importance of fuel injection on stability is that the location of fuel injectors often alters the stability of the system. The crucial role of fuel modulation can also be
readily identified by considering active control examples in which a small modulation of the fuel lines feeding a combustor can be sufficient to alter the stability of the combustor [19–22].

Even though the general idea of the mechanism proposed by Lieuwen [6] is fairly clear, the details of the coupling phenomenon are still unknown. For instance, real instability mechanisms are often a mixture of mechanisms 1 and 2 and not of only one of them. A possible method to gain more insights into this instability mechanism is to pulsate the fuel flow rate in a non-premixed combustor. Multiple studies have examined the behaviour of combustors submitted to a pulsation of the air stream to measure their transfer function [23,16,24]. Less data is available for fuel pulsation in non-premixed devices [25].

The objective of this paper is to analyze the response of a swirled non-premixed combustor to a pulsation of the fuel flow rate. The corresponding experimental setup is a 125 kW burner installed at University of Twente (The Netherlands) and described in Section 2. The work is performed using Large Eddy Simulation (section 3) [7,12], 3D Helmholtz solver (section 4) [26,27] and several experimental methods (section 5) [28,29]. The experiment was specifically developed to allow a full LES computation from inlet to chimney, thereby suppressing uncertainties related to boundary conditions.

LES and experimental results are first compared for the non-reacting flow (section 6). Reacting unforced results are detailed in section 7 before presenting results with fuel flow rate pulsation (section 8).

2 Investigated configuration

2.1 Geometry

The test rig is a 125 kW lab-scale burner developed by University of Twente and Siemens PG in the European Community project DESIRE (Design and Demonstration of Highly Reliable Low Nox Combustion Systems for Gas Turbines).

Figure 2 presents the whole geometry and summarises the flow path. Figure 3 shows closer views of the various flow passages. The preheated air comes out of the compressor into the air supply chamber. Then it flows into the plenum through the acoustic decoupling system pipes (Fig. 3-b). After the swirler (Fig. 3-a), the air
mixes with natural gas which is injected at a normal angle into the air cross flow through four small holes to ensure sufficient mixing. The mixture then reaches the combustion chamber where the flame is stabilized and burnt gases leave the chamber through the outlet flange (Fig. 3-c). A cooling channel surrounds the combustion chamber in order to maintain wall temperatures below $T = 1200\, K$.

The LES computational domain (Fig. 2) includes all parts from the air supply chamber to the outlet flange. This is necessary to have the right acoustic impedance for the combustion chamber, to predict accurately the chamber acoustic modes and to minimize the uncertainties on boundary conditions. The cooling channel is not explicitely simulated but its thermal properties are taken into account in the wall treatment and detailed in section 7.2.
2.2 Operating and boundary conditions

The reference operating point investigated is the same for cold, reacting and pulsed flows. Table 1 summarizes the parameters of the LES runs.

- The air supply chamber feeds the chamber with 72.4 g/s of air, preheated at 573 K. This leads to a Reynolds number of 22000 (based on the bulk velocity at the burner mouth and its diameter) and a swirl number [30] of 0.7 (at the same location).

- The natural gas is injected at ambient temperature (298K) at a flow rate of 3.06 g/s. Note that the natural gas is replaced here by methane (76.7% in mass) and nitrogen (23.3% in mass), so that the global equivalence ratio of the setup is 0.55.

- The mean pressure of the test rig is 1.5 bar.

<table>
<thead>
<tr>
<th>CASE</th>
<th>AD_COLD</th>
<th>AD_STEADY</th>
<th>AD_FORCE05</th>
<th>AD_FORCE10</th>
<th>AD_FORCE15</th>
<th>AD_FORCE30</th>
<th>AD_FORCE50</th>
<th>AD_FORCE80</th>
<th>HL_FORCE15</th>
<th>HL_STEADY</th>
</tr>
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<tbody>
<tr>
<td>Wall law</td>
<td>Adiabatic</td>
<td>Heat loss</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m_A$</td>
<td>72.4 g/s at 573 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m_F$</td>
<td>N/A</td>
<td>3.06 g/s at 298 K</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$F$ (Hz)</td>
<td>N/A</td>
<td>N/A</td>
<td>300 Hz</td>
<td>N/A</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m_F'/m_F$</td>
<td>N/A</td>
<td>N/A</td>
<td>05%</td>
<td>10%</td>
<td>15%</td>
<td>30%</td>
<td>50%</td>
<td>80%</td>
<td>15%</td>
<td>N/A</td>
</tr>
</tbody>
</table>

Table 1
Cases simulated and corresponding operating parameters.

In the computation, the acoustic behaviour upstream of the combustion chamber is ensured by the fully reflecting acoustic decoupling system (Fig. 3-b) and downstream of the combustion chamber, the impedance at the outlet (Fig. 3-c) is controlled through the NSCBC linear relaxation method [31].
3 Large Eddy Simulations

The LES solver AVBP (see www.cerfacs.fr/cfd/CFDWeb.html) simulates the fully compressible multi-species (variable heat capacities) Navier-Stokes equations on hybrid grids. Subgrid stresses are described using the classical Smagorinsky [32] model. When wall functions are used, this model gives results comparable to the dynamic model [33]. A two-step chemical scheme is fitted for lean regimes on the GRI-Mech V3 reference [34]. 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 [15] for equivalence ratios ranging between $\phi = 0.4$ and $\phi = 1.2$. The flame / turbulence interaction is modelled by the Dynamic Thickened Flame (DTF) model [35] and allows to handle both mixing (which is crucial in partially premixed flames) and combustion. The numerical scheme uses third-order spatial and third-order explicit time accuracy [36].

The boundary condition treatment is based on a multi-species extension [37] of the NSCBC method [38], for which the acoustic impedance can be controlled [31]. The walls are handled using a logarithmic law-of-the-wall formulation for velocity and temperature: the thermal treatment can be either adiabatic or "realistic", in which case a wall heat resistance is imposed (see section 7.2). Typical runs are performed on grids between 600,000 and 2.7 millions tetrahedra on several massively parallel architectures (SGI origin 3800, Compaq alpha server, Cray XD1) with a very efficient speedup [39].

4 Acoustic analysis

The Helmholtz solver AVSP is a tool for acoustic analysis in 3 dimensional configurations [27,40–42]. Two kinds of results are provided by this code: eigen frequencies of the configuration and spatial structure of the corresponding eigenmodes via acoustic pressure and acoustic speed. The Helmholtz solver needs a description of the geometry, the sound speed at every point and the impedances at the boundaries. Here, the average sound speed field is provided by the average LES results. The impedances imposed at the inlet and outlet correspond to a velocity and a pressure node respectively. Since studies of low/mediumfrequency instabilities do not require refined meshes, eigenmodes of large configurations can be computed in a reasonable time because of the parallelism of AVSP.
5 Experimental diagnostics

5.1 Cold flow diagnostics

The LES velocity profiles are compared with measured profiles from a water tunnel experiment. The water tunnel is a geometrically copy of the combustion test rig. The fluid that is used is water instead of air. By equating the Reynolds numbers in the water tunnel and the isothermal flow simulations, both flows are similar.

The water tunnel is made out of perspex, allowing forward scattering Laser Doppler Velocimetry (LDV) to measure the velocity profiles downstream of the burner exit. The accuracy of the system is less than 0.1% of its full measurement scale, whereas the resolution depends on the size of the measurement volume. A 400 mm focal-length lens with a measurement volume of 6.5x0.22x0.22 mm is used. The measured velocity at a discrete point is the average velocity in the measurement volume. For all measured velocities, the axis of the measurement volume is aligned with the direction in which the velocity gradients are lowest, thereby increasing the resolution.

Data acquisition is done by a DIFA spectral analyser installed on a PC. The transient velocity signals from the photomultipliers are sampled at 800 Hz for 40.96 seconds. Subsequently, the mean value and the variance of the 32,768 samples are determined. The power spectral density (PSD) of the measured signal shows that the sampling frequency is high enough to catch most of the phenomena in the flow, i.e. the PSD at 400 Hz is more than two orders of magnitude lower than the velocity amplitudes at lower frequencies.

To compare simulation results (using air as a medium) with water tunnel results the mean velocities and the variances are non-dimensionalized by the bulk velocity at the burner mouth $U_B$ and by $(U_B)^2$, respectively [43].

5.2 Hot flow diagnostics

The combustion process can be observed optically through quartz glass windows that are mounted in the liner and pressure vessel on 3 sides of the combustion section (Fig. 4). The view port size is 120×150 mm, which is large enough to see the whole flame.
Chemiluminescence is the radiative emission given off by electronically excited radicals (indicated with a "*"). It is often assumed that $CH^*$ is linearly related to the heat release rate and is therefore a good indicator of flame position and intensity. $CH^*$ is only present in the reaction zone, in contrast to $OH$, which is formed due to splitting of water and therefore extends its zone with high concentration to the exhaust gas side of the flame zone. Since $OH$ has a steep increase in the reaction zone [28] not its concentration but its gradient is an indication for the flame front, which requires a better signal quality.

The radical $CH^*$ is measured by chemiluminescence with a high speed camera (Redlake) supplied with an intensifier (LaVision). A 430 nm band pass filter (bandwidth of 10 nm) is used to filter the $CH^*$ radiation at the $CH$ electronic band. The camera is gated for 100 $\mu$s and a movie of at least 100 images is recorded at 50 Hz. The images of the movie are corrected for background and non linear camera response and averaged.

A drawback of chemiluminescence is that no local flame behaviour can be studied since it is a line of sight technique, which means that the measured $CH^*$ concentration is the integral of all $CH^*$ in the line of sight of the camera. When the shape of the flame is known, special techniques can be applied to obtain a planar picture from line of sight measurements, e.g. Abel transformation (‘onion peeling’) for axi-symmetrical data [29]. Although the whole flow-field is not axi-symmetrical due to the square combustor, this assumption can be considered as valid for the flame itself. However, the reflections and cut off near the wall as well as the aberrations of
Abel transformation close to the axis yield non physical signal in these regions.

Moreover, in terms of thermo-acoustic measurements, the integrated $CH^*$ chemiluminescence measurements can be viewed as a direct measure for the volume-integrated heat release rate.

5.3 Acoustic diagnostics

To obtain the acoustic response of the system due to combustion, pressure measurements are made using Kulite pressure sensors. To decrease the thermal load on these sensors, they are placed in a sidetube (Fig. 4) ended by an anechoic tube. Furthermore, to allow high pressure measurements, the backside of the sensor is connected to the pressurised rig using a long thin tube, which damps out all dynamic pressure signal on the back side, only providing a static back pressure. The pressure sensor signal is amplified and subsequently acquired using a Siglab data acquisition system at a sample frequency of 2.56 kHz.

6 Cold flow

LES and LDV data are first compared using comparing one-dimensional velocity profiles on the central plane at several locations from the burner exit (Plane_A : 5mm, Plane_B : 15mm, Plane_C : 25mm, Plane_D : 45mm and Plane_E : 65mm). The numerical scheme is TTGC (Third order in space and time [36]) and the mesh contains 900,000 tetrahedral cells. The scale for all profiles in Fig. 5 is the same. Figure 5 shows the good agreement between experimental data and LES results in both shape and amplitude of the mean velocity components and even on its RMS fluctuations. The opening angle of the swirled jet, the intensity of central recirculation zone and the re-attachment of the top/bottom recirculation zones are predicted correctly.

Choosing a numerical scheme for LES is a far more difficult task than for steady RANS simulations. Special care must be taken about dissipation and dispersion properties. Results of Fig. 5 were obtained with a $3^{rd}$ order scheme (TTGC) and a fine mesh (900,000 elements). To evaluate both the influence of the mesh and the scheme accuracy, this subsection compares results obtained with a $2^{nd}$ order scheme (Lax-Wendroff) and the $3^{rd}$ order Taylor Galerkin scheme (TTGC). This investigation is performed on two different meshes : a coarse one (600,000 ele-
Fig. 5. Comparison of statistical profiles: a) axial, b) radial and c) swirling mean velocity; a') axial, b') radial and c') swirling RMS velocity; Symbols: Experiment; Solid line: LES; dashed line: zero line (case AD_COLD).
<table>
<thead>
<tr>
<th>TTGC (3rd order)</th>
<th>LW (2nd order)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fine Mesh</strong> : 0.9M cells</td>
<td><strong>Fine Mesh</strong> : 0.9M cells</td>
</tr>
<tr>
<td>Dimensionless mean axial velocity profiles</td>
<td>Dimensionless mean axial velocity profiles</td>
</tr>
<tr>
<td>Plane_A</td>
<td>Plane_B</td>
</tr>
<tr>
<td>Plane_C</td>
<td>Plane_D</td>
</tr>
<tr>
<td>Plane_E</td>
<td>Plane_E</td>
</tr>
</tbody>
</table>

**Coarse Mesh** : 0.6 M cells

![Graphs showing axial velocity profiles](image)

**Fig. 6.** Influence of the numerical scheme; Symbols : Experiment; Solid line : LES; dashed line : zero line (case AD_COLD).

Figure 6 shows the axial velocity profiles of Fig. 5-(a) for these two schemes (columns) and two meshes (rows) : the intensity of recirculations zones is clearly better computed with TTGC than with LW. High-speed zones are dissipated too rapidly with LW. Even TTGC on the coarse mesh performs better than LW on the fine mesh. However, in terms of cost efficiency, the conclusion differs slightly : LW on a fine mesh remains cheaper than TTGC on a coarse mesh. This explains why LW has been used for the reacting computations in the next sections.
Fig. 7. a) Instantaneous view of the flame (isosurface of temperature at 1200K) and of the methane jets (isosurface of fuel mass fraction at 0.1); b) Equivalence ratio distribution function of the same instantaneous solution (PDF of case AD STEADY).

7 Non-pulsated reacting flow

All reacting cases were computed on a 2.7 million cells mesh especially refined in the region where the flame is expected to be.

7.1 Adiabatic cases

The steady-state reacting flow and the cold flow dynamics are very similar. The only noticeable difference is the larger opening angle of the swirled jet. Figure 7-(a) exhibits the instantaneous three-dimensional flame structure, materialized by an isosurface of temperature at 1200K. Even though the flame is compact, it is strongly wrinkled by the turbulence.

The mixing is characterized on Fig. 7-(b) by the observed distribution function of local equivalence ratio $\phi$ (evaluated from the mixture fraction [44]), conditioned by a non negligible reaction rate. It assesses the quality of mixing, since very few points burn at equivalence ratio below 0.4 or above 0.7. The absence of stoichiometric reacting points also demonstrates that the flame never burn in pure diffusion regime.

Informations on the mean location of the flame are gathered on Fig. 8: heat release on a longitudinal cut in the central plane is first compared with an Abel transformation of chemiluminescence $CH^*$ intensity (Fig. 8-a). Then, an integration over a line of sight is performed to relate to the raw $CH^*$ intensity (Fig. 8-b). Both LES
and experiment yields a very compact flame, with a length ($\sim 80$ mm) shorter than twice the diameter of the burner outlet. However, despite the aberrations of Abel transformation close to the axis, the opening angle shown by chemiluminescence is slightly larger than predicted by LES case AD_STEADY. A possible way to improve LES results and especially the interaction between the flame and the outer recirculation zones may be to take into account heat losses. This issue will be discussed in section 7.2.

7.2 Non adiabatic cases

Heat losses are an important issue in combustion chambers since both the reaction rate and the acoustics of the chamber are strongly linked with temperature. Adiabatic walls can be a good assumption when the thermal barrier coating is efficient, e.g. when ceramic heat shield is employed on the chamber walls [15]. In the present test rig, the thin metallic liner surrounded by the cooling channel invalidates that assumption. Moreover, section 7.1 indicated that the simulated shape of the flame (e.g. opening angle) should be slightly improved to match perfectly the experiment (Fig. 8).

In the experiment, the heat loss to the cooling air can be calculated directly using the measured mass flow and temperatures at inlet and outlet. The total heat loss from the combustion chamber $Q_{Total}$ is the sum of the heat loss to the cooling air $Q_1$ and to the surroundings $Q_2$ (via the pressure vessel). Based on the adiabatic flame temperature and the measured temperature at the combustion chamber outlet, the total heat loss from the combustion gasses is estimated at approximately 28% of the burner total power, e.g. 35 kW. The heat transferred to the surroundings $Q_2$ is subsequently determined from the difference between the total heat loss and the
In the LES, heat losses are computed by taking into account two phenomena (Fig. 9):

- Turbulent convection to the chamber walls. Heat transfer to the chamber walls is modelled using a law-of-the-wall function [45]. A simple conjugate approach is used for conduction though the walls and convection through air in the cooling channel. A global heat resistance $R_w$ is used for these two mechanisms such that the heat flux $Q_w$ is:

$$Q_w = \frac{T_c - T_w}{R_w} \quad \text{with} \quad R_w = \frac{d_c}{\lambda_c \cdot Nu} + \frac{d_w}{\lambda_w}$$

where $T_w$, $d_w$ and $\lambda_w$ are respectively the temperature, thickness and conductivity of the wall, and $T_c$, $d_c$ and $\lambda_c$ are the temperature, the height and conductivity of the cooling channel air. The Nusselt number is given by a simple heat transfer correlation in the cooling channel:

$$Nu = 0.023 \cdot Re^{4/5} \cdot Pr^{1/3}$$

where $Re$ is the Reynolds number of the cooling flow $(Re = 5700)$.

- Radiation to the walls. Assuming that gases are optically thin, radiation can be modelled as a volumetric sink term calculated with a Stefan-Boltzman law [46]:

$$Q_r = 4\sigma (T^4 - T_s^4) \sum_{k=1}^{n} (Y_{kap,k})$$

where $\sigma$ is the Stefan-Boltzman constant.
where \( T_s \) is the adjustable temperature of the surroundings (here \( T_s = 1500 \text{K} \)), \( \sigma \) the Stefan-Boltzman constant, and \( Y_k \) and \( a_{\sigma,k} \) are the mass fraction and Planck mean absorption coefficient for species \( k \). These coefficients are obtained using the RADCAL programme [47] and curve-fits provided by Gore et al [48].

Table 2 summarizes the measured heat fluxes in the experiment and the values resulting from the LES case HL\_STEADY.

<table>
<thead>
<tr>
<th>Fluxes</th>
<th>Experiment</th>
<th>LES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cooling channel</td>
<td>Casing</td>
</tr>
<tr>
<td>( Q_1 )</td>
<td>27\text{kW}</td>
<td></td>
</tr>
<tr>
<td>( Q_2 )</td>
<td>7\text{kW}</td>
<td></td>
</tr>
<tr>
<td>( Q_{\text{Total}} )</td>
<td>34\text{kW}</td>
<td></td>
</tr>
<tr>
<td>( T_{\text{Outlet}} )</td>
<td>( \approx 1300\text{K} )</td>
<td>( \approx 1300\text{K} )</td>
</tr>
</tbody>
</table>

Table 2: Evaluation of the heat losses measured in the experiment and modelled in the LES.

As presented in section 7.1, Fig. 10 compares the field of heat release from LES case HL\_STEADY with chemiluminescence \( CH^* \). Effects of heat losses on the flame shape seem somehow limited. Its length and opening angle are very slightly increased, but the main effect of heat loss wall treatment is the modification of the acoustics of the chamber and will be introduced in the next sections.

Fig. 10. Comparison of measured \( CH^* \) intensity (Experimental result) with heat release (LES result of case HL\_STEADY). a) Cut in central plane. b) Integration over line of sight.

7.3 Acoustic analysis results using Helmholtz solver

Acoustic analysis is a powerful tool to understand the mechanisms leading to combustion instabilities [3,42]. The acoustic eigenmodes of the setup can be computed
using the 3D Helmholtz code AVSP [26,27,40,41] presented in section 4. The field
required for this analysis is the local mean speed of sound and is provided by a
time-averaged solution of the reactive LES (cases AD_STEADY and HL_STEADY).
Table 3 shows the lowest eigenfrequencies found numerically and compares them
to the values measured in the experiment.

Modes have been classified in three categories: the modes which correspond to
eigenfrequencies of the plenum (marked as "P" in the last line of Table 3), to
eigenfrequencies of the chamber (marked "C") and to eigenfrequencies coupling
the plenum and the chamber, thereby involving the full Setup (marked "S"). For
modes "P" and "C", this partial decoupling is possible because the inlet section of
the chamber acts essentially like a velocity node.

<table>
<thead>
<tr>
<th>Case</th>
<th>Eigenfrequencies (Hz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Helmholtz solver</td>
<td>Adiabatic 72 131 272 298 487 705 926 1093</td>
</tr>
<tr>
<td></td>
<td>Heat loss 64 128 250 294 443 642 844 1045</td>
</tr>
<tr>
<td>Experiment</td>
<td>Measured 62 171 270 433 625 820 1022</td>
</tr>
<tr>
<td>LES</td>
<td>Adiabatic X X X X 480 X 920 X</td>
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<tr>
<td></td>
<td>Heat loss X X X X 428 X X X</td>
</tr>
<tr>
<td>Mode description</td>
<td>1/4 3/4 5/4 7/4 5/4 7/4 9/4 1/2</td>
</tr>
<tr>
<td>related to</td>
<td>S S S S C^(a) C^(b) C^(c) P</td>
</tr>
</tbody>
</table>

Table 3
Eigenfrequencies computed by the Helmholtz code, measured in the experiment and in the
LES. S for "full Setup", P for "Plenum" and C for "Chamber". Superscripts (a), (b) & (c)
indicate that this mode is represented on Fig. 11-(a), (b) & (c) respectively.

The agreement between the predicted eigenmodes frequencies and the measured
results is reasonable. Note that it is greatly improved by using the mean temperature
field obtained from the LES case HL_STEADY instead of AD_STEADY which yields
lower and more realistic temperature and sound speeds. However, the 171 Hz mode
measured in the experiment is still difficult to link either with the 3 quarterwave or
with the 5 quarterwave mode of the setup.

7.4 Unsteady modes in the unforced case

All modes (listed in Table. 3) identified by the Helmholtz solver do not necessarily
occur in the LES or the experiment. In the experiment, a loud tonal noise appears
Fig. 11. Structure of the first eigenmodes of the combustion chamber given by Helmholtz solver: 487 Hz a), 705 Hz b), 926 Hz c). Acoustic pressure $|P'|$ in the central plane.

after a certain heating time of the setup at the frequency of 433 Hz. LES captures this instability too and Fig. 12 now demonstrates that the main peak at 433 Hz observed in the experiment is also predicted by LES in both cases AD_STEADY and HL_STEADY. Moreover, the Helmholtz analysis presented in section 7.3 reveals that this self-excited mode is an acoustic eigenmode. It corresponds to the $5/4$ wave mode of the chamber itself ($\lambda = 4/5L$ where $L$ is the combustion chamber length $L = 1.93$ m).

The frequency of this mode is 487 Hz for the Helmholtz solver and 480 Hz in the LES code using adiabatic walls and no radiation (case AD_STEADY). These values are too high because the temperature field is overpredicted. When heat-losses are accounted for (case HL_STEADY), the Helmholtz solver yields a frequency for the $5/4$ wave mode of 443 Hz while the LES gives 428 Hz. Both values match the experimental value (433 Hz) within 3% (see Table 3).

Figure 12 also exhibits that beyond the expected effect of heat losses on the prediction of self-excited mode frequency, the impact on the eigenmode amplitude is strong. Whereas the 480 Hz peak (Fig. 12, case AD_STEADY) is hardly distinguishable from the background noise (due to log scale), the corresponding 428 Hz peak (Fig. 12, case HL_STEADY) is much higher and closer to the measured level. In other words, by changing the mode frequency, the heat losses trigger a different flame response [49] and yield higher pressure fluctuations levels. This LES result demonstrates the impact of thermal boundary conditions on flame response.
8 Pulsated reacting flow

8.1 Forcing method and phenomenology

To study the flame transfer function, the reactants flow rate needs to be pulsed. Because of the acoustic decoupling system (Fig. 3-b), the air flow rate is difficult to force. Only the fuel line may be pulsed in the experiment.

In the LES, forcing the reacting flow is achieved by pulsating the fuel mass flow rate in the four fuel pipes (Fig. 3-a). Forcing is performed at 300 Hz for several amplitudes: 5, 10, 15, 30, 50, and 80 percent of the unforced mean mass flow rate. For all these amplitudes, the fuel pipes flows remain subsonic but the maximum Mach number can reach $M \approx 0.9$ in these pipes for case HL_FORCE80. The air flow rate provided by the "air supply room" remains constant, and is only affected by the flow modulations induced by acoustic waves propagation. Section 8.4 will show that these modulations are not negligible.
In the experiment, this fuel pulsator can have different forms. Some authors use a siren-like pulsator, i.e. with a rotating part [23,50,51]. An advantage of such a pulsator is its high maximum frequency of oscillation. The disadvantage is that the form of the excitation is fixed by the geometry of the siren, i.e. white noise excitation is not possible. Moreover, a sinus-like excitation would require a difficult form of the rotating disc.

Another option is to use a control valve [25,19]. This type of pulsator has a somewhat lower maximum frequency of oscillation but it can accept any excitation signal. Since the maximum frequency of excitation is still high enough for the experiments performed here, a D633-7320 MOOG control valve is used in this study. The maximum level of excitation by the MOOG valve depends on the frequency and the operating point [52]. At the operating point presented in section 2.2 and at the considered frequency of 300 Hz, the maximum forcing level is 12% of the mean fuel mass flow at the rim of the fuel pipes.

An overview of the different elements that play a role in the unsteady measurements is shown in Fig. 13. The MOOG valve is fed by an excitation signal $V'_{exc}$ leading to a displacement $\delta'$ of the MOOG’s piston. To obtain the fuel mass flow perturbation at the fuel nozzles, the transfer function $\frac{m'_{fuel}}{\delta'}$ has been determined in a separate experiment. Hence, the fuel mass flow perturbation can be determined from the measured piston displacement $\delta'$. The fuel mass flow perturbation will cause a heat release perturbation $Q'$, which can be detected by the optical measurements via the field of $CH^*$ radical.

![Fig. 13. Schematic layout of the method used in the unsteady measurements.](image-url)
8.2 Acoustic analysis

In forced cases as well, spectral analysis is required to highlight the link between acoustics and flame response. Figure 14 displays a typical pressure spectrum during forced operation at an excitation level of 15% at 300 Hz (cases AD_FORCE15 and HL_FORCE15).

The selfexcited mode at 433 Hz is still present and even increased by the forcing. As presented in section 7.4, taking into account wall heat losses improves the prediction of both frequency and amplitude of the 433 Hz eigenmode. Moreover, the forcing frequency (300 Hz) is also noticeable on these spectra. The response of the flame to this forcing is studied in sections 8.3 to 8.6.
Fig. 15. Phase locked heat release in the central plane and isosurface of equivalence ratio $\phi = 0.6$ for case AD_FORCE15.

8.3 Phase-locked averaged analysis

LES results can be phase-averaged (here on 7 cycles) to isolate the flame response at 300 Hz. Figures 15 and 16 display the shape and intensity of the flame at eight phases of the cycle for cases AD_FORCE15 and HL_FORCE15. They also show the evolution of rich pockets along this cycle, materialised by an isosurface of equivalence ratio at $\phi = 0.6$ (slightly richer than the mean $\overline{\phi} = 0.55$). After a certain time lag, these pockets reach the reacting zone. The flame does not move significantly when it is reached by these pockets but the local heat release oscillates and triggers the pressure fluctuations feeding the 433 Hz acoustic mode (as described in section 8.2).
Fig. 16. Phase locked heat release in the central plane and isosurface of equivalence ratio $\phi = 0.6$ for case HL_FORCE15.
8.4 Self amplification of excitation

A controversial question to understand excitation mechanisms when fuel flow rate is pulsated is the following: is the air flow rate remaining constant during fuel flow rate pulsation? This can be checked in the LES by evaluating the fuel and air mass flow rates at the mouth of the burner. The variation of the equivalence ratio at the chamber inlet can be split in two parts (Eq. 5): the contribution of instantaneous fuel flow rate to equivalence ratio fluctuations $\phi'_F$ and the contribution of instantaneous air flow rate to equivalence ratio fluctuations $\phi'_A$:

$$\phi' = \frac{\dot{m}_F'}{\bar{m}_F} - \frac{\dot{m}_A'}{\bar{m}_A}$$

Fuel contribution $\phi'_F$  Air contribution $\phi'_A$  

Figure 17 presents the two contributions $\phi'_F$ and $\phi'_A$ measured in the LES for two pulsation amplitudes: 15% and 30%. After a time delay of two cycles, the acoustic waves produced by the flame and partially reflected at the end of the chamber clearly perturb the air flow rate. In other words, the $X\%$ pulsation of the fuel line is seen by the flame as a $1.2 \cdot X\%$ equivalence ratio excitation. In the present situation and for a forcing frequency of 300 Hz, the air flow is also affected by the fuel flow modulation and amplifies its impact on the fluctuations of equivalence ratio at the burner inlet. This conclusion is not general (it depends on the air line impedance) but shows that this effect should be taken into account for modelling.

Fig. 17. Contribution of the fuel (thin line) and the air (thick line) fluctuations to equivalence ratio oscillations at the mouth of the burner for case AD_FORCE15 a) and case AD_FORCE30 b).
8.5 Linearity of the flame response

Recent experimental results in studies of forced flames [53,54] show that beyond a certain pulsation amplitude, a saturation effect is observed. LES can be a good tool to evaluate the response of the flame up to high amplitude excitations where measurements can be either dangerous or even not feasible due to the limitations of the MOOG valve. For this reason as well, LES case AD_FORCE15 will be compared to experimental results forced at 12%.

Figure 18 first compares the level of reaction rate fluctuations \( \frac{Q'}{\langle Q \rangle} \) observed in the LES (case AD_FORCE15) with the fluctuations of \( CH^* \) radical \( \frac{CH^*'}{\langle CH^* \rangle} \) along the cycle. Heat release \( (Q) \) and \( CH^* \) emission are probably not linearly related for such a partially premixed flame so that comparing \( \frac{Q'}{\langle Q \rangle} \) and \( \frac{CH^*'}{\langle CH^* \rangle} \) is a challenging test. However, results show that both amplitude and phase are in quite good agreement, despite the limited number of cycles used in the LES phase-averaging procedure.

![Fig. 18. Comparison of normalized global reaction rate fluctuations along the cycle (LES case AD_FORCE15 : solid line) with normalised chemiuminescence fluctuations (Experiment : circles).](image)

Figure 19 presents the reaction rate fluctuation level for several pulsation amplitudes (Fig. 19-a), up to 80%, and its evolution along the cycle (Fig. 19-b). The integrated \( CH^* \) fluctuations are also displayed on Fig. 19-a for low pulsation amplitudes. No saturation effect is noticed here : the flame behaves linearly within the range considered.

This major difference between the present results and [53,54] may be due to the way the equivalence ratio is pulsated : in Balachandran et al. [53,54], the fuel flow rate is constant (fuel line choked) and they pulsate the air flow. Therefore, both mechanisms (1) and (2) are involved (see section 1). Coherent structures (e.g. ring vortices) may wrinkle the flame and capture pockets of fresh gases [16]. In this study, since the momentum of the fuel jets is very small compared to the momen-
Fig. 19. Dependence of normalized global reaction rate fluctuations upon the forcing amplitude a) and its evolution along the cycle b).

8.6 Unsteady heat losses

In heavy duty gas turbines, the thermal load on the walls is an important issue: on one hand, the air used to cool down either the metallic liner or the tile-holders of ceramic heat-shield must be minimum to optimise the efficiency. On the other, even a temporary overheating may damage the structure and fluctuating heat load plays a crucial role in its long term fatigue. Therefore, the mean thermal balance is not sufficient to predict this. Unsteady heat losses must be investigated.

Figure 20 presents the temporal evolution of global heat losses in the LES for both forced (HL_FORCE15) and unforced (HL_STEADY) cases. The level of fluctuations of convective heat flux $Q_w$ (Fig. 20-a) as well as the radiative heat flux $Q_r$ (Fig. 20-b) are significantly increased by the forcing. The forcing frequency (300 Hz) is also clearly noticeable on these oscillations, which establishes the link between the
instability and the fluctuating heat load. In addition to the noise level inside the combustion chamber, this can constitute a fundamental input data for a structure code.

9 Conclusion

Computations of a partially premixed lab-scale burner are carried out using LES for both non-pulsated and pulsated cases. LES results are validated from velocity measurements performed at the University of Twente. The overall agreement with experiment is very good for both mean and RMS values. The mechanism leading to heat release oscillations is characterized using phase-locked analysis and a simple 3D Helmholtz solver. An amplification effect of the equivalence ratio excitations due to reflected acoustic waves perturbing the air flow rate is observed. No saturation effect is noticeable for the range of amplitudes considered, in contrast to that reported by Balachandran et al. [53,54]. A first evaluation of the impact of combustion instability on the heat load at the chamber walls is achieved. More generally, this study demonstrates that LES is able to capture the specific role of equivalence ratio fluctuations in phenomena leading to combustion instabilities and their consequences on the chamber structure.

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References


