SIMULATION OF EXPLOSION IN BUILDINGS
BY LARGE EDDY SIMULATION

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DATE: April - September, 2010
LOCATION: CERFACS

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Abstract

This report is concerned with the important issue of safety aspects in buildings. The propagation of a premixed flame in a confined configuration in presence of obstacles has been investigated numerically by Large Eddy Simulation (LES).

The aim of this study is twofold: the first objective is to assess the capability of the Computational Fluid Dynamics (CFD) code AVBP to predict the critical parameters related to building safety. The second objective is to build the basis of our future work on explosion in the framework of a PhD thesis funded by TOTAL.

Different chemistry mechanisms for a propane/air combustion have been tested in a first time. Then, laminar propagation of spherical flames have been simulated in two dimensions and compared to the theory. Finally, LES simulations in three dimensions have been carried out for a stagnant stoichiometric propane/air mixture, ignited from rest in a small scale chamber.

Results have shown on the one hand the ability of AVBP to reproduce the flame structures observed in the experiments, and on the other hand the capacity to capture the critical physical quantities linked to building safety issues. The sensitivity of the results to several numerical parameters are also highlighted.
Abstract

Ce rapport s’intéresse au sujet important des risques liés aux bâtiments. La propagation d’une flamme prémélangee en milieu semi confiné et en présence d’obstacles a été étudiée par Simulation aux Grandes Echelles (SGE).

Le but de cette étude est double. Le premier est de confirmer que le code de calcul de Mécanique des Fluides Numérique (MFN) AVBP est capable de prédire les grandeurs critiques liées à la sécurité dans les bâtiments. Le second est de mettre en place les bases de notre futur travail sur les explosions dans le cadre d’une thèse financée par TOTAL.

Plusieurs mécanismes chimiques d’une combustion propane/air ont été testés dans un premier temps. Des simulations de propagation laminaire de flamme sphériques ont ensuite été réalisées en deux dimensions et comparées à la théorie. Finalement, des calculs SGE en trois dimensions ont été menés pour un mélange au repos propane/air en conditions stoechiométriques, allumé dans une chambre à échelle réduite.

Les résultats montrent la capacité d’AVBP à reproduire les structures de flamme présentes dans les résultats expérimentaux d’une part, et à capturer les grandeurs physiques critiques liés aux problèmes de sécurité dans les bâtiments d’autre part. La sensibilité des résultats à différents paramètres numériques est également mise en évidence.
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Introduction

Development of the industry connected with burnable gases causes growing interest to safety aspects of design and operation condition in this kind of buildings (Hysafe commission working on H$_2$ safety [18], the Buncefield Major Incident Investigation Board (BMIIB) working to enlighten the conditions of the Buncefield oil depot accident [3]).

Today TOTAL[49] is highly interested in these issues and wants to be able to locate the critical areas in buildings, especially oil platforms, in order to design it as safe as possible. With the growing computational means, Computational Fluid Dynamics (CFD) appears as an interesting alternative to experiments which are expensive, and may be dangerous in such a kind of studies. A code is already used by TOTAL teams, based on a RANS (Reynolds Averaged Navier Stokes) approach named FLACS[2] [27]. In the aim to improve this tool, and to develop more accurate techniques, a thesis study is about to be funded by TOTAL in close collaboration with CERFACS[9]. The present internship has been realized in this context.

Flame propagation in a confined configuration (a building for example) is a topic highly related to these safety issues and present many analogies with the flame propagation in piston engines or gas turbines. For these configurations, the Large Eddy Simulation (LES) on massively parallel computers has considerably improved the ability to precisely simulate fully unsteady flows in complex geometries, using machines with tens of thousand processors (Schmitt et al. [45], Gourdain et al. [21], Boileau et al. [4]). The aim of the present study is to use the LES code AVBP[10] to compute a configuration related to flame propagation in a confined area.

This work is consequently focused on the simulation of turbulent propagating flames in a semi-confined explosion chamber. The combustion chamber built at the University of Sydney [32] is studied. The low dimensions of the chamber (25 cm x 5 cm x 5 cm) make this configuration particularly suitable for LES. Moreover, a lot of published experimental and numerical data are available for this configuration (Kent et al.[32], Gubba et al. [24] [25] [23], Hall et al. [26], Ibrahim et al. [29]). The calculations presented in this report have been carried out to enlighten the various difficulties to capture the specific phenomena of flame propagation in confined environment with the objective to estimate the right overpressure peak in the chamber, which is the critical parameter in safety related studies.

The global problem of the simulation of explosions in a building can be split in three parts:

- Ignition of the first kernel: as shown by Champion et al. [11], a minimum energy is needed to ignite any combustible mixture. Determining this ignition energy is critical for safety since it can be used to design electrical systems for example to minimize accidental discharge in electrical systems. This question was not addressed at all in this work: we always assumed that the spark was powerful enough to initiate combustion.

- First development of the kernel: the first instants where a spark transforms a gas into a spherical flame are very complex. A plasma phase is formed, a strongly curved flame grows and later transitions to a standard deflagration. In this work, we looked at the modeling of this phase, neglecting the plasma phase and adding energy locally to a premixed gas. We show that this phase is difficult to predict, even though it is laminar, because the flame is strongly curved and kinetic and transport effects combine to strongly modify the flame speed.
Finally, the flame propagates and interacts with walls and obstacles, becoming turbulent. This phase was computed here for the Sydney experiment. The most important information at this point is the overpressure value because this is what can destroy the building. We will show that LES provides a precise evaluation of this phase and investigate which parameters (chemistry, mesh) influence this result.
1 Large Eddy Simulation and Combustion

1.1 Large Eddy Simulation

Most of flows studied in industry have a large scope of characteristic eddies. It is ranging from large eddies, which are dependant on the flow geometry, to the smaller, related to viscous energy dissipation.

In the flow, the largest structures, which are more energetic, transfer a part of this energy to smaller structures, which transfer themselves a part of the energy they received to even smaller structures and so on, up to Kolmogorov scale which represents the smallest scale of the turbulence (viscous energy dissipation). This concept comes from Richardson’s view of the energy cascade [44] and the Kolmogorov’s hypothesis [33]. Focusing on these scales, most of them shows complex dynamics with an inhomogeneous and anisotropic behavior. However, smallest eddies dissipate the energy and have an isotropic and homogeneous behavior, slightly dependant on geometry (Kolmogorov hypothesis). The Large Eddy Simulation principle starts from this observation: on one hand, large eddies must be solved, and on the other hand, the universality of smaller eddies enable modelization, thus permitting to reduce the number of degrees of freedom necessary to the calculation. LES is thus a tridimensional method of computation giving an unsteady description of turbulent flows by numerical calculation of filtered Navier Stokes equations.

![Figure 1 – Turbulent energetic spectrum in function of wave number.](image)

LES filtering principle is shown in Fig. 1. It is compared to RANS where all turbulent scales are modelled, and Direct Numerical Simulation (DNS) where all scales are solved. This filtering may be either explicit or implicit as Pope [42] explains. AVBP uses an implicit filtering: the cut-off length is the cell size.

1.2 Combustion

One difficulty in LES is to simulate the combustion correctly. Indeed, the flame thickness is usually much smaller than the resolution used. Consequently, the flame cannot be directly resolved. Many methods have been developed to overcome this issue:

- Flame Surface Density model (FSD) [28]
- G-Equation [40]
Thickened Flame model (TF) [14]

In AVBP, the Thickened Flame approach is used (Appendix C.5). It consists in thickening the flame from its laminar thickness $\delta_L^0$ to $F\delta_L^0$ using the thickening factor $F$ while the laminar flame speed is the same as the non-thickened flame. $F$ can thus be adapted to be able to resolve the flame front over many grid points.

In turbulent flows, the interaction between chemistry and turbulence is altered by the thickening of the flame front: eddies smaller than $F\delta_L^0$ do not interact with the flame any longer. The thickening of the flame thus reduces the ability of the smallest vortices to wrinkle the flame front: as the flame surface is reduced, the reaction rate is underestimated. In order to correct this effect, an efficiency function $E$ is introduced to reproduce the subgrid wrinkling [14].

1.3 Chemistry

The description of combustion processes leads very often to reaction mechanisms with above hundred chemical species which react within more than a thousand of elementary reactions. In the context of LES of complex configurations, the integration of detailed kinetics is impossible due to their prohibitive computational cost. Various techniques have been developed to overcome this issue.

Tabulation methods for example have already shown their potential to accurately account for chemistry in premixed and non-premixed flame configurations [36]. Another alternative method is the use of a reduced chemical scheme [19]. In this method, the number of species and reactions is reduced to the main ones in order to model the combustion process without solving hundreds of partial differential equations. In this study, this method has been used.
2 The test case

The configuration consists in a premixed combustion chamber with a solid obstacle. A flame propagating in a square cross section tube is considered, as shown in Fig. 2. One end of the channel is closed. The mixture is centrally ignited at this closed end. In the early stage of propagation the flame is laminar and develops with a hemispherical shape, then it transitions to a "finger" shape [7] when it reaches the walls. Finally, the flame front hits the obstacle, generating strong turbulence which self accelerates the flame.

![Series of experimental video images of flame propagation in a channel with obstacle respectively at 6.0, 12.0, 12.5, 13.0, 13.5, 14.0, 14.5, 15.0, 15.5 ms after ignition (Gubba et al.[23]).](image)

The chamber has a square cross-section of 50 mm and an overall length of 250 mm. It has a total volume of 0.625 L. The square obstacle of 12 mm is placed at 94 mm from the ignition end running throughout the chamber cross-section and causes significant disruption to the flow. Three turbulence generating grids can be placed at 20 mm, 50 mm, and 80 mm downstream of the ignition point. Geometric features are summed up in Fig. 3.

Before starting three dimensional computations, more basic configurations must be studied.
First, the chemistry must be checked through 1D flame propagation to ensure the good thermodynamics and kinetics behaviors. In addition, a semi-confined configuration of 1D flame will be used to bring out expansion effects.
Then, a two-dimensional configuration of a laminar spherical flame will be used to mimic the first times after ignition. This simplified configuration will be compared with theoretical results to check the pertinence of the numerical setup. A special attention will be paid to the curvature effects.
Finally, the three dimensional configuration of the Sydney chamber will be simulated to evaluate the influence of several numerical parameters over the results. None of the turbulence generating grids has been placed in the chamber for the calculations presented. Only the square obstacle disrupts the flow.
Figure 3 – Schematic of the experimental rig used for explosion of deflagrating flame [24]. All dimensions are in mm.
3 Chemistry

A Liquified Petroleum Gas (LPG) and air mixture with an equivalence ratio of 1 has been used to run experiments in Sydney. LPG is composed of many gases (88% $C_3H_8$, 10% $C_3H_6$, and 2% $C_4H_{10}$) but in the present study, propane $C_3H_8$ is used as fuel since it represents the main part of LPG. The laminar flame speed and adiabatic temperature should not be affected by this simplification which is necessary for AVBP calculations. Two reduced mechanisms of propane/air combustion have been tested in a 1D premixed flame configuration:

- a one-step mechanism proposed by Thobois [48] (1S\_LU);
- a one-step mechanism with Lewis numbers equal to 1 for all species designed with CANTERA[20] (1S\_Le1).

Calculations are done with AVBP on a refined mesh with the constraint of a front flame fully resolved over forty nodes using DNS (cell size of $10^{-5}$ m). Fresh mixture and theoretical burnt gas properties obtained with an equilibrium calculation are listed in Appendix A.1. The resulting flame temperature is 2275K.

3.1 1D flame

3.1.1 One-step mechanism - 1S\_LU

Only the propane oxidation reaction is taken into account with no reverse reaction. The parameters of this one-step mechanism are presented in Appendix A.2 and the resulting flame and burnt gas characteristics in Appendix A.4. Note that the laminar flame speed $S_0^L$ is 36.5 cm/s at $\Phi = 1$ which is within the range of the different values found in the literature (Metghalchi and Keck [39], Peters et al. [31], Vagelopoulos and Egolfopoulos [50], Jomaas et al. [30], GRI-Mech 3.0 [47]).

Laminar flame speed variation in function of the fuel/air (F/A) equivalence ratio $\Phi$ is shown in Fig. 4. The scheme provides good estimations of $S_0^L$ in poor mixture and until $\Phi = 1.2$ where the laminar flame speed starts to be overestimated.

Figure 5 shows the burnt gases temperature variation in function of the F/A equivalence ratio. The temperature is maximum around $\Phi = 1$ and decreases for $\Phi > 1$ and $\Phi < 1$. This one-step mechanism overestimates the burnt gases temperature with regard to Peters et al. [31].

3.1.2 One-step mechanism with Lewis number 1 - 1S\_Le1

In this part, a new chemical scheme has been built from the 1S\_LU scheme but setting all species Lewis number to 1 (Table 1) and adjusting the pre-exponential factor to obtain the same laminar flame speed as 1S\_LU scheme.

Le is defined as:

\[
Le = \frac{Sc}{Pr} = \frac{\alpha_T}{D}
\]  

where Sc and Pr are the Schmidt and Prandtl numbers and $\alpha_T$ and D are the thermal and mass diffusivities.
Figure 4 – Laminar flame speed in function of $\Phi$ for the two one-step schemes. Comparison with different experimental and detailed schemes results.

Figure 5 – Burnt gases temperature in function of $\Phi$ for the two one-step schemes. Comparison with Peters et al. results [31].

This mechanism has been established in order to avoid preferential diffusion in our calculation and check its influence over results of Sydney set-up. The properties of this mechanism and the characteristics of the resulting flame are respectively displayed in Appendix A.3 and A.4. Note that the burnt gases temperature and the laminar flame speed at $\Phi=1$ are equal to the 1S_LU mechanism (Fig. 4 and 5).

Equidiffusion behavior is shown in Fig.6 on which the fuel and oxidant mass fractions are normalized by their fresh gas value. As one can see in Fig. 6 b), with the 1S_Le mechanism, there is no preferential diffusion and the two species profiles are coincident whereas on the 1S_LU
scheme results in Fig. 6 a), $O_2$ has been more diffused than $C_3H_8$ since its Schmidt number is smaller.

<table>
<thead>
<tr>
<th>Lewis Number</th>
<th>$C_3H_8$</th>
<th>$H_2O$</th>
<th>$CO_2$</th>
<th>$O_2$</th>
<th>$N_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1S_LU</td>
<td>1.655</td>
<td>0.716</td>
<td>1.255</td>
<td>0.971</td>
<td>0.920</td>
</tr>
<tr>
<td>1S_Le1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 1 – Reduced one-step chemistries - species Lewis numbers.

3.2 Semi confined 1D flame

A one dimensional flame configuration is set up with a closed end at one side as in Fig. 7. Burnt gases are trapped against the wall and the speed of the flame front toward the fresh mixture is studied.

\[
S = \frac{\rho_f}{\rho_b}S_L^0
\]

where $\rho_f$ and $\rho_b$ are respectively the fresh and burnt gas densities, and $S_L^0$ is the laminar flame speed.

Figure 6 – Normalized reactant mass fraction for the two one-step schemes.

Figure 7 – Schematic of the 1D semi-confined configuration.
Calculations are made using a coarser mesh than for the 1D flame configuration and a thickening factor is applied in order to resolve the flame front over five points. The cell size has been chosen equal to the typical cell size of the 3D mesh corresponding to the Kent et al. configuration [32] ($\Delta_x = 1.3\,mm$). The resulting flame front speed using the 1S$_L$U scheme is presented in Table 2 and compared to the speed obtained with Eq. 2 using $S_0^L = 0.38\,m/s$ (Metgalchi and Keck), and the density of fresh (resp. burnt) gases at 300K (resp. 2275K). This mechanism slightly underestimates the front speed. Nevertheless expansion effects are taken in account, correctly increasing this front speed with regard to the open configuration.

<table>
<thead>
<tr>
<th>mechanism</th>
<th>Front speed</th>
<th>$\frac{\partial S^L}{\partial \rho}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1S$_L$U</td>
<td>2.86 m/s</td>
<td>2.99 m/s</td>
</tr>
</tbody>
</table>

Table 2 – Flame front speed in 1D semi-confined flame configuration.
4 Spherical Propagation - Curvature Effects Investigation

As it has been mentioned earlier, right after ignition, the flame is laminar and propagates hemispherically. At this time, the front flame curvature is high ($\sim \frac{1}{r}$) and its effects on the flame speed are not negligible. This study has been realized in two dimensions to limit the grid size of DNS computations.

This part is focused on the investigation of the effects of the curvature and the preferential diffusion on the consumption speed and the temperature profile with a particular interest in the thickening and Lewis number influence.

4.1 Configuration

The one-step chemistry 1S$_1$LU has been chosen to run these simulations and Fig. 8 shows the mesh used. Using symmetry boundary conditions, only a quarter circle is needed to simulate a spherical propagation. The mesh is refined within a radius $r$ of 30 mm from the circle centre with a specific cell size of 0.03 mm in order that the flame front can be fully resolved over most than 10 points using DNS (assuming a flame thickness $\delta_0 = 0.36$mm, cf. section 3.1.1). Then, the cell size is progressively increased from 0.03 at $r=30$mm to 2 mm at $r=60$ mm. A non-reflecting boundary condition is used at the outlet to avoid reflected waves in the domain (Granet et al. [22]).

A propane and air mixture has been used with an equivalence ratio equal to 1 as initial condition. The gas is then ignited by an energy deposition (Lacaze et al. [34]) at the centre of the circle (left bottom corner of the mesh). Table 3 shows the parameters used to ignite the premixed gases.

The one-step chemistry with Lewis numbers set to one 1S$_1$Le has been used to be compared with the results of 1S$_1$LU and check the influence of the Lewis number.

The study has been focused on two types of results:
- the consumption speed $S_c$;
- the burnt gases temperature $T_b$.

![Figure 8 – 2d spherical mesh.](image-url)
4.2 Consumption speed investigation

4.2.1 Theoretical flame propagation

The consumption speed is defined in Eq. (3) from the integral of the burning rate across the flame front:

\[ S_c = \frac{1}{\rho_f Y_F^f} \int_{-\infty}^{\infty} \dot{\omega}_F dx \]

(3)

where \( \rho_f \) is the fresh mixture density, \( Y_F^f \) is the fuel mass fraction in fresh gas, and \( \dot{\omega}_F = W_F q \) is the fuel burning rate with \( q \) the reaction rate.

For spherical flames and neglecting the thickness of the flame, it can be derived (Poinsot [41]) that the consumption speed \( S_c \) is equal to the laminar flame speed \( S_{0L} \). Nevertheless, at the beginning of spherical propagation, \( S_c \) is limited by stretching effect and depends on the curvature \( \kappa \):

\[ \kappa = \frac{1}{S} \frac{dS}{dt} \]

(4)

with \( S \) the flame surface area. In the case of two dimensional spherical flames, \( \kappa \) becomes:

\[ \kappa = \frac{1}{2\pi r} \frac{d(2\pi r)}{dt} = \frac{1}{r} \frac{dr}{dt} \]

(5)

where \( r \) is the radius of the spherical flame. Using Eq. 2 for \( \frac{dr}{dt} \) which is the front flame speed, Eq. 5 can be written as:

\[ \kappa = \frac{1}{r} \frac{\rho_f}{\rho_b} \frac{S_{0L}}{S_{0L}} \]

(6)

where \( \rho_b \) and \( \rho_f \) are respectively burnt and fresh gas densities.

In the limit of small curvature terms, it has been shown (Buckmaster and Ludford [5], Bush and Fendell [6], Clavin [12]) that the expression of the corrected consumption speed can be written in function of \( \kappa \) as:

\[ \frac{S_c}{S_{0L}} = 1 - L_{0a}^c \frac{\kappa}{S_{0L}} \]

(7)

where \( L_{0a}^c \) is the Markstein length[37]. Using Markstein number \( M_{0a}^c = L_{0a}^c / \delta \), Eq. 7 can be recast as:

\[ \frac{S_c}{S_{0L}} = 1 - M_{0a}^c \frac{\kappa \delta}{S_{0L}} \]

(8)

with \( \delta \) a characteristic flame thickness:

\[ \delta = \frac{D_f}{S_{0L}} \]

(9)
where \( D_{th} \) is the thermal diffusivity of the fresh gas.

Eq. 8 can be rearranged using Eq. 6:

\[
\frac{S}{S_L} = 1 - M_c \frac{\delta}{r} \rho_f
\]  

(10)

Many expressions of \( M_c \) can be found in the literature. The Clavin and Joulin [13] formulation of the Markstein number has been used to evaluate the correction on \( S_c \):

\[
M_c = \frac{L}{\delta} = \frac{1}{2} \beta (Le_F - 1) \frac{T_f}{T_b - T_f} \int_{T_b - T_f}^{T_b - T_f} \frac{\ln(1 + x)}{x} \, dx
\]  

(11)

where \( T_b \) and \( T_f \) are respectively the burnt and fresh gas temperatures. \( Le_F \) is the fuel Lewis number. The parameter \( \beta \) measures the activation energy:

\[
\beta = \frac{(T_b - T_f)T_a}{T_b^2}
\]  

(12)

with \( T_a \) the activation temperature.

Three conclusions can be drawn from these formulations:

- First of all, Eq. 10 shows that the consumption speed \( S_c \) varies in \(-\frac{1}{r}\) and tends towards the laminar flame speed when \( r \) tends towards the infinity.

- Secondly, the second term of the right hand side of Eq. 10, which limits the consumption speed, depends on the flame thickness. Consequently, when the flame is thickened by a factor \( F \) in LES computations, this term is multiplied by this same thickening factor \( F \), thus artificially increasing the curvature effect.

- Finally, it can be noticed from Eq. 11 that, if the fuel Lewis number \( Le_F \) equals 1, the consumption speed is not affected by curvature effects since the resulting Markstein number is zero. This is why it has been interesting to create the chemical scheme \( 1S_{Le1} \) described in section 3.1.2.

### 4.2.2 Simulations of spherical propagation

The sphere radius \( r \) is calculated from the mean \( CO_2 \) mass fraction \( Y_{CO_2} \) using Eq. 13:

\[
\frac{\pi}{4} Y_{CO_2} = \frac{V_{mesh}}{V_{CO_2}} \rightarrow r = \left( \frac{Y_{CO_2} R_{mesh}^2}{V_{CO_2}} \right)^{1/2}
\]  

(13)

where \( Y_{CO_2}^b \) is the \( CO_2 \) mass fraction in the burnt gases, \( V_{mesh} \) is the total volume of the mesh, and \( R_{mesh} \) is the radius of the mesh.

Then, the consumption speed \( S_c \) is derived from Eq. 3:

\[
S_c = -\frac{1}{\rho_f Y_F^f} \frac{W_F \overline{V}_{mesh}}{2\pi r/4}
\]  

(14)
where \( \bar{q} \) is the mean reaction rate in the domain and \( r \) is the flame radius given by Eq. 13.

Figures 9 (resp. Fig. 10) shows the results relative to the consumption speed normalized by the laminar flame speed (resp. the product of the Markstein number by the thickening factor). This product is derived from Eq. 10, assuming that \( \delta = F\delta_L^0 \):

\[
M_c F = (1 - \frac{S_c}{S_L^0}) r \frac{\rho_b}{\rho_f} \frac{1}{\delta_L^0}
\]

where \( F \) is the thickening factor and \( \delta_L^0 \) is the laminar flame thickness.

**Le \( \neq 1 \)**
The first comment over these results is that, from Fig. 9, the more the flame is thickened, the more the flame consumption speed is affected by the curvature. Indeed, focusing on Le\( \neq 1 \) curves for example (solid line), at a flame radius of 5mm, the consumption speed for \( F = 1, 4, \) and 8 is respectively at 93%, 77%, and 55% of \( S_L^0 \). The flame thickening has consequently a strong influence during the early stage of spherical propagation. In order to quantify this effect and check whether or not this influence is consistent with the theory, Fig. 10 shows the product of \( M_c F \) by \( F \) using Eq. 15. These results do not permit to confirm that the limitation of \( S_c \) is directly proportional to the thickening factor. This may be explained by the fact that the mixture used is in stoichiometric proportions whereas the theory assumes that the mixture is poor. The problem is thus more complex since the two species are deficient. Nevertheless, the amplification of the curvature effect by the flame thickening has been confirmed, even with a stoichiometric mixture.

**Le = 1**
The second point investigated is the dependance on the fuel Lewis number. Results relative to computations using a Lewis number of 1 for all species (instead of 1.655 for the fuel Lewis number \( Le_F \) used with the 1S\_LU scheme) are as well displayed in Fig. 9 and 10 in dashed line. In this case, for the same reasons as above, results do not match the theory since curvature should not have any effect on flame propagation (from Eq. 11 \( M_c^L = 0 \)). Here, the correction term on \( S_c \) varying in \( \frac{1}{r} \) is still present and the thickening effects are still effective. Nevertheless, it can be noticed that these effects are stronger in the case of non-equidiffusive mixture (\( Le \neq 1 \)).

To sum up these results, the following conclusions have been brought out:

The flame thickening considerably slows down the flame propagation because of a wrong estimation of curvature effects.

Since the consumption speed is less affected by the thickening in the case of \( Le = 1 \), this scheme could be a solution in order to avoid a numerical slowing down of combustion.

In the future, other calculations will be carried out using a poor mixture to confirm the ability of LES to accurately predict the spherical propagation of a laminar flame.
4.3 Burnt gases temperature investigation

After the investigation of the curvature effects on the consumption speed, attention has been paid to the burnt gases temperature. Tests have been carried out to evaluate and clarify the links between the Lewis number and the temperature field in the burnt gases.
4.3.1 Theoretical curvature and preferential diffusion effects over burnt gases temperature

Besides the consumption speed limitation, curved flames are subject to modifications of the burnt gases temperature with regard to the adiabatic temperature $T_{ad}$. C.K. Law[35] gives a conceptual demonstration of the effects of curvature in the presence of preferential diffusion for an expanding spherical flame.

$\Phi \neq 1$

Consider a spherical outwardly propagating flame (Fig. 11). In this demonstration, it is assumed that the mixture is not in stoichiometric proportions, and sufficiently diluted in one of the reactant such that the deficient reactant controls the reaction rate.

On the one hand, the burnt gases volume loses thermal energy (solid array) due to the concave nature of the flame which defocuses the heat out of the flame thus decreasing the temperature.

On the other hand, mass diffusion focuses the deficient reactant concentration in the reaction zone (dashed array), which brings more chemical energy to the burnt gases and raises the burnt gases temperature.

Consequently, this two phenomena are in competition and the temperature tendency depends on the mixture Lewis number $Le$ based on the deficient reactant ($Le = \frac{\alpha_T}{D_i}$ with $\alpha_T$ the thermal diffusion coefficient and $D_i$ the mass diffusion coefficient of the deficient species). If $Le > 1$, heat loss exceeds the gain in concentration and $T_b < T_{ad}$. On the opposite, $T_b > T_{ad}$ if $Le < 1$. If the heat and mass diffusion rates are equal ($Le=1$), then the two effects compensate each other and $T_b = T_{ad}$ is expected.

![Figure 11 – Schematic of the outwardly propagating flame showing thermal and reactant diffusion.](image)

$\Phi = 1$

In the above demonstration, the mixture has been assumed to be rich or poor but in the configuration studied, the mixture is in stoichiometric proportions so the behavior might be different from the one described above:

This is obvious that the temperature diffusion still induces thermal energy losses in this case.

But the mass diffusion effects at $\Phi = 1$ are not the same as for $\Phi < 1$ or $\Phi > 1$. Indeed, the diffusion coefficient of the $O_2$ and the fuel are not equal. Consequently, due to the curvature and
the fact that the two species are deficient, preferential diffusion becomes preponderant. Hence, the combustion will be incomplete, thus decreasing the chemical energy brought to the burnt gases with regard to the 1D flame configuration. The two effects cannot compensate each other and the temperature should be decreased in the burnt gases.

If $Le = 1$, the two reactants diffuse in the same way and in the same way as the temperature as well. Hence, since $Le = 1$, the two phenomena should compensate each other and the temperature should not be affected.

**Asymptotic behavior**

In all cases, rich, poor or stoichiometric, when the flame expands, the curvature intensity steadily decreases as $1/r$ and the diffusion due the the concave nature of the flame tends toward zero. The asymptotic behavior of the flame is the same as the planar flame, which means that $T_b$ tends toward $T_{ad}$. The laplacian expression in polar coordinates (Eq. 16), representative of diffusive effects in the energy and species equations confirm this behavior when $r \rightarrow \infty$. It gives, after simplification due to cylindrical symmetry:

$$\Delta f = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r} \frac{\partial f}{\partial r}$$

(16)

When, $r$ tends toward the infinity, the term varying in $1/r$ tends toward zero, thus remaining to the planar expression in cartesian coordinates where $\Delta f = \frac{\partial^2 f}{\partial x^2}$.

To conclude this demonstration, the following behaviors are expected :

As a result, the temperature obtained with the 1S LU scheme should be reduced from the burnt gases temperature obtained for the 1D flame.

As the flame propagates, this reduction should become lower until the burnt gases temperature reaches $T_{ad}$ when $r$ tends toward the infinity.

When the unity chemical scheme 1S $Le1$ is used, due to a compensation between mass and thermal diffusions, the burnt gases temperature is expected to be equal to $T_{ad}$ even for small flame radii.

Finally, since the temperature variations depends on diffusive effects, these phenomenon should be enhanced when the flame is thickened.

**4.3.2 Numerical investigation**

In this part, the dependance on the Lewis number is investigated through the temperature profiles in the burnt gases along the radial direction.

**Lewis number influence**

Figure 12 a) shows the $O_2$ mass fraction for $Le \neq 1$ and $Le=1$ (respectively 1S LU and 1S $Le1$).
As expected, when the lewis numbers are different from one, due to an higher diffusion of oxygen ($Sc_{O_2} < 1 < Sc_F$), there is unburned $O_2$ in the burnt gases. This result highlights the preferential diffusion of the 1S\_LU scheme and the fact that the combustion is incomplete.

![Graphs](image.png)

**Figure 12** – Radial profiles of $O_2$ mass fraction and temperature with and without preferential diffusion for $F=1$.

Figure 12 b) shows that for Lewis numbers non equal to one, there is a temperature drop inside the burnt gas area which is not present on unity Lewis calculations ($T_b = 2220K$ for 1S\_LU instead of 2389). This is consistent with the demonstration of the previous part (section 4.3.1). For the 1S\_LU scheme, the thermal diffusion induces the decrease of the temperature with regard to the 1D planar flame configuration.

For $Le=1$, thermal diffusion and species diffusion compensate each other and the temperature remains constant to the 1D flame burnt gases temperature. The bump at the beginning of the curve correspond to the transitory part of energy deposition where the temperature in the calculations reach temporary 4000K (simulations using an other type of ignition confirm this assumption).

**curvature influence**

It has been seen that when the flame propagates, diffusion effects become weaker since the curvature varies in 1/r. When r tends toward the infinity, the spherical flame can be likened to a planar flame for which the burnt gas temperature is the adiabatic temperature. Figure 13 shows the evolution of the burnt gases temperature as the flame expands. The temperature of the burnt gases increases when the flame radius increases which is good agreement with the fact that when the curvature decreases, the thermal energy losses are reduced. The temperature seems to tend toward the 1D flame burnt gases temperature (2391K), which is relevant with the theory derived earlier.

**Thickening influence**

As expected, when the flame is thickened, diffusive effects increase and the thermal loss is higher. The results for two different thickening factors are displayed in Fig. 14 for the 1S\_LU scheme.
Figure 13 – Radial profiles of temperature for $Le \neq 1$ at different times and for $F=1$.

The temperature in the burnt gases is lower for $F=4$ (dotted line) than for $F=1$ (solid line).

Figure 14 – Radial profiles of temperature for $Le \neq 1$ for different thickening factors $F$.

Like for the consumption speed investigation, in the future, complementary calculations will be made in non-stoichiometric conditions to confirm the behavior predicted by C.K. Law. Nevertheless, the simulations are in good agreement with the assumptions made from the C.K. Law conceptual demonstration of the effects of curvature on the flame temperature and some conclusions can be drawn from these results:

The temperature obtained with the 1$S_L$U scheme is lower than for the 1D flame due to
curvature.

When the flame propagates, this reduction becomes lower and the burnt gases temperature tends toward $T_{ad}$ when $r$ tends toward the infinity.

For the 1S$_{Le1}$ scheme, the burnt gases temperature remains equal to $T_{ad}$. This scheme is not able to predict the temperature decrease $T_b < T_{ad}$.

Finally, since the temperature variations depends on diffusive effects, these phenomenon are enhanced when the flame is thickened.

4.4 Conclusion

In this section, it has been showed that, mainly due to the thickening of the flame, the effects of the curvature over the flame speed and temperature can be altered. Some effects slow down the flame whereas others accelerate it. Table 4 recaps the action of the different phenomena over the flame front speed when the flame is thickened.

<table>
<thead>
<tr>
<th>Curvature alteration</th>
<th>Le$\neq$1 : 1S$_{LU}$</th>
<th>Le=1 : 1S$_{Le1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>of consumption speed</td>
<td>(\nearrow)</td>
<td>(\nearrow)</td>
</tr>
<tr>
<td>on burnt gases temperature</td>
<td>(\nearrow)</td>
<td>(\nabla)</td>
</tr>
</tbody>
</table>

Table 4 – Action of different phenomena over flame propagation (\(\nearrow\) : speed up, \(\nabla\) : slow down, \(\nabla\)\(\nabla\) : high slow down).

1D flame propagation simulations (section 3) shows that both chemical schemes overestimate the burnt gases temperature (Fig. 5) which induces an overestimation of the flame front speed. This difference of temperature (\(~200K\)) is not negligible with regard with the others phenomena and considerably affects the results. In the future, the use of a two-step mechanism with a CO-CO$_2$ equilibrium which allows to correctly predict the adiabatic flame temperature might be a solution to this issue.

For both schemes, the consumption speed is affected by the flame curvature. The flame propagation is slowed down and this effect is amplified by the thickening of the flame. The 1S$_{Le}$ scheme is less altered than the 1S/LU scheme.

Finally, the burnt gases temperature behavior depends substantially from the two schemes. The 1S$_{LU}$ mechanism slows down the flame since the thickening amplifies the thermal losses for high curvature. On the opposite, the thermal losses are compensated for the 1S$_{Le}$ mechanism and the flame is consequently propagating too quickly.
5 Investigation of the Sydney Explosion Chamber

In the previous section, the two dimensional configuration allowed to bring out the phenomena which govern the flame motion of a laminar spherical flame. This configuration corresponded to the early stage of the flame propagation of the Sydney set-up. As it has been said earlier, this first stage of propagation is determinant for the overpressure generated in which we are interested. Some tests have been carried out for the three dimensional configuration of the explosion chamber developed in Sydney (section 2).

Besides the qualitative estimation of the validity of the calculations, two criteria are used to compare the various results:

- Front flame position: defined as the distance of the furthest point of the flame front from the closed end of the channel.
- Overpressure in the chamber. In experiments the pressure is measured at the closed end of the chamber and is uniform. In experiment, pressure probes are located on the closed end of the chamber as well.

5.1 Numerical Set-up

5.1.1 Meshes

The geometry presented is section 2 has been meshed using CENTAURSOFT\[8\] for the tetrahedral meshes and ICEMCFD\[1\] for the hexahedral meshes.

A plenum is placed at the open end of the chamber in order to avoid numerically reflected waves at its outlet. This is thus representative of the experimental conditions where the chamber is open in a wide space.

Three meshes have been used during this study. Two meshes with tetrahedral elements (one coarse and one fine) and one mesh with hexahedral elements with a typical cell size equivalent to the fine tetrahedra mesh.

Appendix B gives an overview of the three meshes. More specific information can be found in Table 5.

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Cell number (x10^6)</th>
<th>Node number (x10^6)</th>
<th>Smallest cell [m^3]</th>
<th>Cell size in zone [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tetra-Coarse</td>
<td>1</td>
<td>0.2</td>
<td>6.5e^-12</td>
<td>1.3 3 3→150</td>
</tr>
<tr>
<td>Tetra-Fine</td>
<td>7.7</td>
<td>1.4</td>
<td>3.1e^-12</td>
<td>0.4 1.3 2.6→150</td>
</tr>
<tr>
<td>Hexa</td>
<td>5.7</td>
<td>5.8</td>
<td>4.8e^-11</td>
<td>0.4 2.4 5→300</td>
</tr>
</tbody>
</table>

Table 5 – Mesh parameters (zone1 : spherical propagation area; zone2 : chamber; zone3 : plenum).

5.1.2 Numerical parameters

For all computations, the following parameters have been used (detailed information about these parameters can be found in Appendix C): 
- Numerical scheme: Lax-Wendroff (finite volume explicit second order)
- Subgrid scale model: Smagorinsky (Appendix C.4)
– Artificial viscosity model: Colin sensor with a species mass fraction sensor (Appendix C.3)
– Wall boundary condition: Adiabatic condition with a logarithmic law-of-the-wall formulation for the velocity.

5.2 Results

In the calculations presented, the flow is initialized by a gas-out procedure: a small sphere of burnt gases is located around the spark location. It allows to avoid the transitory part of ignition and focus on the phenomenon discussed in the previous part. Consequently, the timing of the pressure peak occurrence is not aimed to be right since the ignition phase is not simulated.

5.2.1 Flame propagation

Figure 15 shows the flame propagation in the chamber from a calculation on the Tetra-Coarse mesh and from experiments. The propagation of the flame of the numerical results meets the experimental behavior presented in section 2.

![Flame propagation images](image)

(a) Experimental video images at 6.0, 12.0, 12.5, 13.0, 13.5, 14.0, 14.5, 15.0, 15.5 ms after ignition (Gubba et al.[23]).

(b) Simulation images of reaction rate field at 6.0, 12.0, 12.5, 13.0, 13.5, 14.0, 14.5, 15.0, 15.5, 16.0, 16.5 ms.

Figure 15 – Flame propagation.

Figure 16 shows the overpressure evolution. The pressure peak occurs when the two flames meet after the obstacle as described by Di Sarli et al. [15]. For the numerical results, the oscillations with a period of approximatively 3ms located before the peak are caused by a quarter wavelength wave in the chamber. This is due to the velocity node at the closed end of the chamber and the pressure node at the outlet:

\[ T = \frac{4L}{c} = \frac{4}{340} = 2.9 \text{ms} \]  

(17)

whith T the oscillation period, L the chamber length, and c the sound velocity.

Besides, Fig. 16 shows that the pressure peak (the most important data for safety since it controls the building structure survival) obtained during the explosion is very well captured by LES and confirms the capacity of this method to address this issue.

5.2.2 Chemical scheme comparison

In this part, the Tetra-Coarse mesh has been used to compare the two chemical schemes used earlier and check the influence of the phenomenon which have been studied in two dimensions, over the three dimensional configuration.
Figure 16 – Overpressure evolution.

Figure 17 shows the flame front position and the overpressure evolution for the two mechanisms, compared to experimental values published by Gubba et al. [23].

As it can be seen in Fig. 17 a), the flame front moves faster when the 1S_{Le1} scheme is used. This agrees with the remarks made in the two dimensional spherical propagation part. The curvature effects over the consumption speed are lower when Le=1 and the burnt gases temperature is higher than for Le\neq 1. This two phenomena induce a higher propagation speed for the 1S_{Le1} scheme than for the 1S_{LU} scheme. This first result shows that the chemical scheme is preponderant: for one scheme the flame is slowed down with regard to experiments, and speeded up for the other scheme.

The overpressure induced by the flame is plotted in Fig. 17 b). The 1S_{LU} scheme provides a good estimation of the overpressure peak whereas it is highly over-estimated by the 1S_{Le1}
scheme. This confirms the fact that the early stage of propagation, when the flame is spherical, is critical for the whole behavior of the flame and more particularly for the overpressure.

### 5.2.3 Mesh resolution comparison

The mesh resolution is another parameter which is expected to have a strong effect over the results. Results relative to calculations on the Tetra-Coarse and Tetra-Fine meshes using the $1S_{Le1}$ scheme are compared in Fig. 18. As expected, the flame propagation is accelerated when the mesh is refined. Curvature effects are less important since the thickening factor is decreased. Consequently, the consumption speed is closer to the laminar flame speed (cf part 4.2) and the burnt gases temperature is higher (cf part 4.3), the flame is thus speeded up. This acceleration is directly transferred on the pressure which is higher when the mesh is refined.

![Graphs showing mesh comparison](image)

**Figure 18 – Mesh comparison.**

### 5.3 Conclusion

First of all, the results of these three-dimensional simulations are in agreement with the laminar propagation phase investigation. One the one hand this validates the tendencies brought out in the spherical propagation investigation section. On the other hand, this confirms that the early stage of propagation is determinant for the overpressure generated.

Consequently, the following numerical parameters have been found to have a particular influence over the results:

- As it has been seen, the use of the $1S_{Le1}$ chemical scheme induces a higher overpressure than the $1S_{LU}$ scheme.

- Then, a refined mesh causes a higher overpressure prediction with regard to a coarser mesh, due to the reduced flame thickening factor.
Nevertheless, the results relative to the 1S_LU calculations on the coarse mesh shows the ability of LES to solve problems related to semi confined explosions in spite of a sensitivity to numerical parameters.
General Conclusion

The objective of our numerical investigation is to validate the capacity of LES to correctly predict critical parameters related to building safety issues. The study shows that AVBP is able to reproduce aspects observed in experiments and capture the overpressure generated in this configuration of semi-confined explosion chamber.

Nevertheless, it is observed that the results are sensitive to the numerical parameters and particularly to the thickening factor. Consequently, the parameters have to be tuned in order to compensate the different numerical parameters effects, and reduce as much as possible the alteration of the flame propagation.

Although the simulations related to the curvature influence do not exactly match the theory, various tendencies have been brought out in two dimensions and confirmed in the three dimensions real case. In the future, further calculations will be carried out to check the ability of AVBP to accurately predict the laminar propagation phenomena of curved flames.

Within the framework of the thesis study funded by TOTAL, the Sydney setup investigation will be continued with extra obstacles in the chamber. Then, the semi-confined tube configuration studied by Renou et al. [43] will be used since it constitutes a midway case between the two dimensional spherical propagation configuration and the full three dimensional Sydney explosion chamber. This set-up will allow to focus on ignition issues, which have not been investigated in the present report.

To globally conclude about this work, the numerical study with the bibliography researches made have established the basis of our work on explosion in semi-confined areas. Besides, it constitutes a first approach of this subject with AVBP which allowed to bring out some difficulties linked to this kind of simulations.
Références


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A Chemistry

A.1 Theoretical flame properties

Table 6 lists the Fresh mixture and theoretical burnt gas properties obtained with equilibrium calculations.

<table>
<thead>
<tr>
<th></th>
<th>Fresh gases</th>
<th>Burnt gases</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature $T$</td>
<td>300 K</td>
<td>2275 K ($T_{\text{eqil}}$)</td>
</tr>
<tr>
<td>Pressure $P$</td>
<td>1.013E+005 Pa</td>
<td>1.013E+005 Pa</td>
</tr>
<tr>
<td>Equivalence ratio $\phi$</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$Y_{C_3H_8}$</td>
<td>6.024E-002</td>
<td>0.</td>
</tr>
<tr>
<td>$Y_{H_2O}$</td>
<td>9.860E-002</td>
<td>0.</td>
</tr>
<tr>
<td>$Y_{CO_2}$</td>
<td>1.807E-001</td>
<td>0.</td>
</tr>
<tr>
<td>$Y_{O_2}$</td>
<td>2.1906E-001</td>
<td>0.</td>
</tr>
<tr>
<td>$Y_{N_2}$</td>
<td>7.207E-001</td>
<td>7.207E-001</td>
</tr>
<tr>
<td>Density $\rho$</td>
<td>1.197 kg/m$^3$</td>
<td>1.520E-001 kg/m$^3$</td>
</tr>
</tbody>
</table>

**Table 6** – Fresh mixture and burnt gases properties.

A.2 One-step mechanism - 1S_{LU}

The characteristics of the one-step mechanism 1S_{LU} are presented in Table 7. Only the propane oxydation reaction is taken into account with no reverse reaction.

$$q = A e^{-\frac{E_a}{RT}} [\text{fuel}]^{n_{\text{fuel}}} [\text{O}_2]^{n_{\text{O}_2}}$$  \hspace{1cm} (18)

where $E_a$ is the activation energy of the reaction and $n_k$ is the reaction exponent for species $k$.

**Table 7** – One-step reduced chemistry characteristics (1S_{LU}).

A.3 One-step mechanism - 1S_{Le1}

The characteristics of the one-step mechanism with Lewis numbers equal to one are presented in Table 8.

A.4 1S_{LU} and 1S_{Le1} flame and burnt gas characteristics

The resulting flame and burnt gas characteristics of the 1S_{LU} and 1S_{Le1} schemes are listed in Table 9.
\[ \text{Table 8} - \text{One-step with Le=1 reduced chemistry characteristics (1S\_Le1).} \]

<table>
<thead>
<tr>
<th>( n )</th>
<th>Reaction</th>
<th>( A ) ( [\text{cm}^3/\text{mole}\cdot\text{sec}] )</th>
<th>( \beta )</th>
<th>( \text{Ea} ) ( [\text{cal/mole}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} )</td>
<td>3.28E+012</td>
<td>0.000</td>
<td>3.347E+004</td>
</tr>
<tr>
<td></td>
<td>Direct: ( n_{\text{C}_3\text{H}<em>8} = 0.569 ) and ( n</em>{\text{O}_2} = 1.097 )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( n )</th>
<th>Reaction</th>
<th>( A ) ( [\text{cm}^3/\text{mole}\cdot\text{sec}] )</th>
<th>( \beta )</th>
<th>( \text{Ea} ) ( [\text{cal/mole}] )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O} )</td>
<td>3.28E+012</td>
<td>0.000</td>
<td>3.347E+004</td>
</tr>
<tr>
<td></td>
<td>Direct: ( n_{\text{C}_3\text{H}<em>8} = 0.569 ) and ( n</em>{\text{O}_2} = 1.097 )</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \text{Laminar flame speed} \ S_{L}^f )</th>
<th>1S_LU</th>
<th>1S_Le1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{Flame thickness} \ d_{f}^L )</td>
<td>3.65E-004</td>
<td>3.65E-004</td>
</tr>
<tr>
<td>( \text{Thickening sensor} \ \Omega_0 )</td>
<td>5.78E-005</td>
<td>4.97E-005</td>
</tr>
<tr>
<td>( \text{Burnt gas Temperature} )</td>
<td>2389.5 K</td>
<td>2389.5 K</td>
</tr>
<tr>
<td>( \text{Burnt gas Density} )</td>
<td>0.144 kg/m(^3)</td>
<td>0.144 kg/m(^3)</td>
</tr>
<tr>
<td>( \text{max Heat Release} \ (J/K^{-1}.m^{-3}.s^{-1}) )</td>
<td>5.73E+009 units</td>
<td>5.79E+009 units</td>
</tr>
<tr>
<td>( \text{max reaction rate} \ q_{1f} \ (mol.m^{-3}.s^{-1}) )</td>
<td>2.79E+003</td>
<td>2.82E+003</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( \text{Mass Fraction} )</th>
<th>1S_LU</th>
<th>1S_Le1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Y_{\text{C}_3\text{H}_8} )</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>( Y_{\text{H}_2\text{O}} )</td>
<td>9.86E-002</td>
<td>9.86E-002</td>
</tr>
<tr>
<td>( Y_{\text{CO}_2} )</td>
<td>1.80E-001</td>
<td>1.80E-001</td>
</tr>
<tr>
<td>( Y_{\text{O}_2} )</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>( Y_{\text{N}_2} )</td>
<td>7.20E-001</td>
<td>7.20E-001</td>
</tr>
</tbody>
</table>

\text{Table 9} - \text{Flame and burnt gas properties for the two reduced mechanisms 1S\_LU and 1S\_Le1.}
B Meshes

B.1 Coarse-Tetra

Figure 19 – Coarse tetrahedral mesh.
B.2 Fine-Tetra

Figure 20 – Fine tetrahedral mesh.

(a) Full geometry.

(b) Chamber close-up.
B.3 Hexa

Figure 21 – Hexahedral mesh.

(a) Full geometry.

(b) Chamber close-up.
C AVBP CFD code [10][21]

AVBP[10] is a parallel CFD code that solves the three-dimensional compressible Navier-Stokes equations on unstructured and hybrid grids. The prediction of unsteady turbulent flows is based on the Large Eddy Simulation (LES) approach that has emerged as a prospective technique for problems associated with time dependent phenomena and coherent eddy structures. An Arrhenius law reduced chemistry model allows to investigate combustion for complex configurations.

C.1 Equations

Filtered quantities \( \bar{f} \) are resolved whereas sub grid quantities \( f' = f - \bar{f} \) result from unresolved flow motion. LES equations are obtained filtering instantaneous equations:

\[
\frac{\partial \bar{\rho} \bar{u}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{u}_i \bar{u}_j}{\partial x_j} = - \frac{\partial}{\partial x_j} \left[ \bar{P} \delta_{ij} - \bar{\tau}_{ij} - \bar{\tau}_{ij}^l \right] \tag{19}
\]

\[
\frac{\partial \bar{\rho} \bar{E}}{\partial t} + \bar{\rho} \bar{E} \bar{u}_j \frac{\partial}{\partial x_j} = - \frac{\partial}{\partial x_j} \left[ \bar{u}_i (P \delta_{ij} - \bar{\tau}_{ij}) + \bar{q}_j + \bar{q}_j^l \right] + \bar{\omega}_T + \bar{Q}_r \tag{20}
\]

\[
\frac{\partial \bar{\rho} \bar{Y}_K}{\partial t} + \bar{\rho} \bar{Y}_K \bar{u}_j \frac{\partial}{\partial x_j} = - \frac{\partial}{\partial x_j} \left[ J_{J,k} + J_{J,k}^l \right] + \bar{\omega}_K \tag{21}
\]

C.2 Numerical schemes

Three numerical schemes can be used:

- Lax-Wendroff:
  FV explicit second order scheme.

- TTG4A:
  FE explicit third order scheme

- TTGC [16]:
  FE explicit third order scheme

C.3 Artificial Viscosity

The numerical discretization methods in AVBP are spatially centered. These types of schemes are known to be naturally subject to small-scale oscillations in the vicinity of steep solution variations. This is why it is common practice to add a so-called artificial viscosity (AV) term to the discrete equations, to avoid these spurious modes (also known as wiggles) and in order to smooth very strong gradients. Different AV methods are used in AVBP. These AV models are characterized by the linear preserving property which leaves unmodified a linear solution on any type of element. The models are based on a combination of a shock capturing term (called 2nd order AV) and a background dissipation term (called 4th order AV). In AVBP, adding AV is done in two steps:

- first a sensor detects if AV is necessary, as a function of the flow characteristics
then a certain amount of 2nd and 4th AV is applied, depending on the sensor value and on user-defined parameters.

Sensors
A sensor $\zeta_{\Omega_j}$ is a scaled parameter which is defined for every cell $\Omega_j$ of the domain that takes values from zero to one. $\zeta_{\Omega_j} = 0$ means that the solution is well resolved and that no AV should be applied while $\zeta_{\Omega_j} = 1$ signifies that the solution has strong local variations and that AV must be applied.

Operators
There are two AV operators in AVBP: a 2nd order operator (acting locally) and a 4th order operator (acting globally). All AV models in AVBP are a blend of these two operators. These operators have the following properties:

- **2nd order operator (smu2)**: it acts just like a classical viscosity. It smoothes gradients, and introduces artificial dissipation. It is thus associated to a sensor which determines where it must be applied. Doing this, the numerical scheme keeps its order of convergence in the zones where the sensor is inactive, while ensuring stability and robustness in the critical regions. Historically, it was used to control shocks, but it can actually smooth any physical gradient.

- **4th order operator (smu4)**: it is a less common operator. It acts as a bi-Laplacian and is mainly used to control spurious high-frequency wiggles.

C.4 SubGrid Scale models

The filtered compressible Navier-Stokes equations exhibit sub-grid scale (SGS) tensors and vectors describing the interaction between the non-resolved and resolved motions. The influence of the SGS on the resolved motion is taken into account in AVBP by a SGS model based on the introduction of a turbulent viscosity, $\nu_t$. Such an approach assumes the effect of the SGS field on the resolved field to be purely dissipative. Several models exist in AVBP:

Smagorinsky model \[46\]

$$\nu_t = (C_S \Delta)^2 \sqrt{2 \bar{S}_{ij} \bar{S}_{ij}},$$

where $\Delta$ denotes the filter characteristic length (cube-root of the cell volume), $C_S$ is the model constant set to 0.18 but can vary between 0.1 and 0.18 depending on the flow configuration. This closure has the particularity of supplying the right amount of dissipation of kinetic energy in homogeneous isotropic turbulent flows. Locality is however lost and only global quantities are maintained. It is known as being "too dissipative" and transitioning flows are not suited for its use.

A dynamic Smagorinsky model \[38\] can be used where the constant $C_S$ is calculated spatially and temporally.

WALE (Wall Adapting Linear Eddy) model \[17\]

$$s_{ij}^2 = \frac{1}{2} (\bar{g}_{ij}^2 + \bar{g}_{ji}^2) - \frac{1}{3} \bar{g}_{kk}^2 \delta_{ij},$$
\[
\nu_t = (C_w \Delta)^2 \frac{(s_d^d s_d^d)^{3/2}}{(S_{ij} S_{ij})^{5/2} + (s_d^d s_d^d)^{5/4}},
\]

where \( \Delta \) denotes the filter characteristic length (cube-root of the cell volume), \( C_w = 0.4929 \) is the model constant and \( \tilde{g}_{ij} \) denotes the resolved velocity gradient. The WALE model was developed for wall bounded flows in an attempt to recover the scaling laws of the wall. Similarly to the Smagorinsky model locality is lost and only global quantities are to be trusted.

### C.5 Flame Front Thickening

It consists in thickening the flame from its laminar thickness \( \delta^0_L \) to \( F \delta^0_L \) using the thickening factor \( F \).

It can be shown that the laminar flame speed \( S^0_L \) and the laminar flame thickness \( \delta^0_L \) are controlled by the diffusive and source terms as:

\[
S^0_L \propto \sqrt{D_{th} A}
\]

\[
\delta^0_L \propto \frac{D_{th}}{S^0_L} = \sqrt{\frac{D_{th}}{A}}
\]

where \( A \) is the pre-exponential factor of the Arrhenius formulation of the reaction rate.

\[
q = Ae^{-\frac{E_a}{RT}} [fuel]^{n_{fuel}} [O_2]^{n_{O_2}}
\]

where \( E_a \) is the activation energy of the reaction and \( n_k \) is the reaction exponent for species \( k \).

In the governing equations, in order to thicken the flame, the thermal and molecular diffusivities, \( D_{th} \) and \( D_k \) are replaced by \( F D_{th} \) and \( F D_k \) and the pre-exponential constant of the reaction rate \( A \) by \( \frac{A}{F} \).

Eq. 22 and 24 become:

\[
S^0_L \rightarrow \sqrt{F D_{th} A} = \sqrt{D_{th} A} = S^0_L
\]

\[
\delta^0_L \rightarrow \sqrt{F D_{th} A} = F \sqrt{\frac{D_{th}}{A}} = F \delta^0_L
\]

Consequently, the thickened laminar flame speed is the same as the non-thickened flame, while its thickness is multiplied by the factor \( F \). \( F \) can thus be adapted to be able to resolve the flame front over many grid points. A common way to set \( F \) is to compute it locally in function of the mesh size \( \Delta_x \) as \( F = n \Delta_x \), with \( n \approx 10 \), the number of points required in the flame front.
D CERFACS Presentation

CERFACS (Centre Européen de Recherche et Formation Avancées en Calcul Scientifique) is a research organization that aims to develop advanced methods for the numerical simulation and the algorithmic solution of large scientific and technological problems of interest for research as well as industry, and that requires access to the most powerful computers presently available. CERFACS is governed by a Conseil de Gérance with representatives from its shareholders, and benefits from the recommendations of its Scientific Council.

CERFACS has seven shareholders (CNES, the French Space Agency; EADS France, European Aeronautic and Defence Space Company; EDF, Electricité de France; Météo-France, the French meteorological service; ONERA, the French Aerospace Lab; SAFRAN, an international high-technology group, TOTAL, a multinational energy company).

CERFACS hosts interdisciplinary teams, both for research and advanced training that are comprised of: physicists, applied mathematicians, numerical analysts, and software engineers.

Approximately 115 people work at CERFACS, including more than 95 researchers and engineers, coming from 10 different countries. They work on specific projects in nine main research areas: parallel algorithms, code coupling, aerodynamics, gas turbines, combustion, climate, environmental impact, data assimilation, and electromagnetism.

Part of the research activity of CERFACS is associated with CNRS (Centre National de la Recherche Scientifique, www.cnrs.fr), as an "Unité de Recherche Associée" (SUC, URA 1875). CERFACS and INRIA (Institut National de Recherche en Informatique et Automatique (www.inria.fr) joined parts of their activities within a common laboratory. CERFACS participates in the TVE (Terre Vivante et Espace, www.omp.obs-mip.fr/tve) pole of laboratories. It is also a member of RTRA/STAE (Réseau Thématique de Recherche Avancée "Sciences et Technologies pour l’Aéronautique et l’Espace", www.fondation-stae.net/fr/, see also www.cerfacs.fr/RTRA-STAE.mpg) and participates in the activities of AESE (Pôle de Compétitivité "Aéronautique, Espace et Systèmes Embarqués", www.aerospace-valley.com).

Computational Fluid Dynamic group (CFD) The objective of the CFD group at CERFACS is to solve problems involving both CFD and High Performance Computing (HPC). Despite the recent progresses observed in CFD, the solution of many flows of interest is still beyond present capabilities and the challenge of HPC for CFD remains as open and difficult as it ever was. In most CFD problems, brute force approaches still fail and advances in this field rely on defining proper compromises between physics and numerics.

This is especially true in the fields of CFD chosen at CERFACS: aerodynamics, turbulence, combustion, unsteady flows, coupled phenomena between fluid mechanics and other mechanisms (fluid structure interaction, optimization, two-phase flows, radiation, etc).

In the last years, the requests of CERFACS partners as well as the general orientation of the CFD community have lead the CFD project to a deeper implication in Direct Numerical Simulation tools, especially for reacting flows or for flows in complex geometries as well as to the development of new aspects of CFD such as multiphysics or active control. This has been done through an increase of the CFD staff so that the classical expertise of the CFD team (aerodyna-
mics, turbulence modeling, optimization and parallelization, combustion) has been maintained or even reinforced. An important new field of application for CERFACS is Large Eddy Simulation (LES). The role of the CFD team and of its partners in the development of Large Eddy Simulation is now significant through multiple collaborations, contracts and dissemination of information and tools. The LES approach has emerged as a prospective technique for problems associated with time dependent phenomena and coherent eddy structures. This leading edge CFD technology can nowadays be applied to geometries of reasonable complexity (such as a combustion chambers in gas turbines but also in piston engines), which is the result of both constantly increasing computer capacities along with improved underlying numerical methods and grid techniques. In 2005, more than 50 scientists were working in the CFD project at CERFACS.