LARGE EDDY SIMULATION OF TURBULENT PREMIXED FLAMES PROPAGATION IN A SMALL SCALE VENTING CHAMBER: INFLUENCE OF CHEMISTRY AND TRANSPORT MODELLING

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Abstract

Flame propagation in a semi-confined chamber with obstacles constitutes a representative configuration of gas explosion phenomena occurring in buildings like power plants or refineries. In order to understand them, the small-scale combustion chamber built at the University of Sydney [1] is studied by Large Eddy Simulation (LES). Four configurations which differ by the number of turbulence generating grids along the flame path are considered.

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 one is to investigate the influence of the chemistry modelling on the results, in the context of reduced schemes.

Results show the ability of AVBP to reproduce accurately the over-pressure generated in the explosion chamber in terms of timing and magnitude for the four configurations. The analysis reveals that a correct description of the initial laminar propagation phase, which occurs between the ignition of the mixture and the interaction with the obstacles, is essential in the prediction of the over-pressure: (1) the burnt gas temperature must be accurately predicted by the reduced chemical scheme to obtain the right expansion ratio, (2) the use of realistic species Lewis numbers is mandatory to capture the flame response to curvature. Only the combination of these two ingredients allows a good prediction of the laminar phase, which largely influences the whole combustion process and the resulting over-pressure history.

Introduction

Accidents due to gas explosions have generated a growing interest in safety aspects of design and operation condition in industrial buildings. A major concern for oil and chemical industries is to be able to locate precisely the hazardous areas in buildings, typically offshore oil and gas producing platforms, in order to design them as safe as possible. Thanks to the growing computational power, Computational Fluid Dynamics (CFD) appears as an interesting alternative to experiments which are expensive, and may be also dangerous. Nowadays codes based on a URANS (Unsteady Reynolds Averaged Navier Stokes) approach are classically used to simulate gas explosion configurations at industrial scales [2, 3]. The emergence of the Large Eddy Simulation (LES) approach opens a new perspective on this field of application. This technique has already shown its ability to give more reliable predictions than URANS in unsteady complex configurations, especially in gas explosion related studies [4, 5], even if this statement is most of the time restricted in practice to laboratory-scale experiments.

The experimental setup of Sydney [1] is a typical example of these small-scale experiments built to study the mechanisms of gas explosions in semi-confined environments. It consists in a vented explosion chamber where a premixed flame propagates first as a laminar spherical front, gets wrinkled by obstacles and becomes a turbulent flame propagating at very high speeds.

The interaction of the flame with the obstacles is known to largely control the over-pressure in the chamber, which is certainly the critical parameter in industrial safety. This configuration is particularly attractive to study gas explosion phenomena by LES: the dimensions of the chamber are low (0.625 litre) and a lot of published experimental and numerical data are available [1, 5, 6].
The main objective of this work is to assess the capability of the LES solver AVBP to capture the specific phenomena controlling flame propagation in semi-confined environment and to correctly predict the parameters of critical relevance for safety related study, in particular the over-pressure peak in the chamber. A second objective is to highlight the influence of chemistry modelling in this kind of applications. The flame propagation in a stagnant flow is an academic problem mixing laminar phases (controlled by chemistry and thermodiffusive effects), and turbulent phases (where the influence of the flow structures will dominate). Constructing an LES which can handle both phases is a new problem, which has been almost untouched up to now. The impact of the number of steps used to describe chemistry when reduced schemes are used is studied. The importance of the unity Lewis assumption, often used in the context of reduced schemes, is also investigated using existing theories and Direct Numerical Simulations (DNS) of academic configurations.

The test case
The configuration studied in this work was set up at the University of Sydney [1]. It consists in a square cross section premixed combustion chamber (25cm x 5cm x 5cm) with solid obstacles. The obstacles consist in three removable turbulence generating gris and one fixed central obstacle, as shown in Fig. 1 (left). The bottom end of the chamber is closed and the top end is opened out to the atmosphere. The vessel is initially filled with a stoichiometric mixture of air and LPG (88% propane by volume) at atmospheric pressure and temperature. The mixture is then ignited by laser and the flame propagates past the obstacles. Additional details may be found in Kent *et al*. [1].

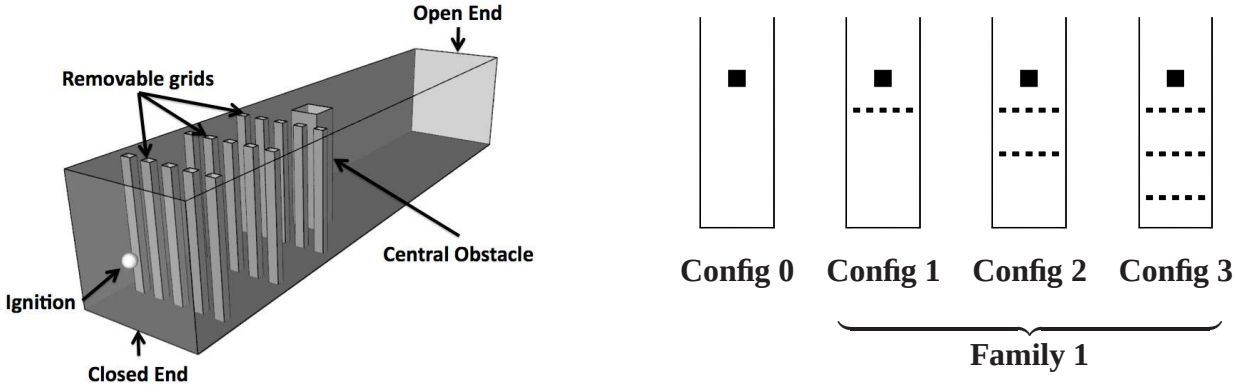

Figure 1. Left: Explosion chamber configuration of Kent *et al*. [1]. The vessel is orientated vertically in the experiment : the bottom end of the vessel is on the left of the figure and the top end on the right. Right: Classification of the studied configurations.

This experimental explosion chamber has already been investigated using LES [5, 6, 7]. Family 1 is studied, where the number of grids is progressively increased from one to three, located farthest from the ignition point (configurations 1, 2, and 3). Illustrations of the investigated configurations can be found in Fig. 1 (right).

Numerical Modelling

The LES solver used in this study is the AVBP code [8, 9]. In AVBP, the unsteady compressible Navier-Stokes equations are solved on unstructured grids. The present simulations are performed with a second order Lax-Wendroff centered scheme. The WALE model [10] is used as subgrid scale model. Navier-Stokes Characteristic Boundary Conditions (NSCBC) [11] are used at the outlet of the plenum which is located at the open end of the chamber in order to mimic the atmosphere. The solid walls that represent the obstacles and the explosion chamber are adiabatic non-slip walls. Combustion is described by the TFLES method [12] in order to resolve the flame front on the LES grid. Ignition is modelled by an energy deposition in the energy equation as explained by Lacaze *et al*. [13].

A special interest is brought to chemistry modelling in this paper. Chemistry is modelled by reduced schemes [14] due to the prohibitive computational cost of detailed kinetics. Several one-step and two-step reduced schemes have been developed for this work. Their impact on the results are pointed out and investigated in section ”Reduced Scheme Influence”.

Results

The primary objective of this section is to simulate flame propagation past repeated obstacles and capture the critical physical quantities related to explosions in semi-confined areas. Simulations are performed on meshes of 15 millions tetrahedra with a typical cell size of 0.4 mm in the chamber.

Figure 2 shows typical LES results for the configuration 1. In the early stage of propagation, the flame is laminar and develops with a hemispherical shape, then it transitions to a ”finger” shape when it reaches the walls. Finally, the flame front hits the obstacles, generating strong turbulence which accelerates the flame.

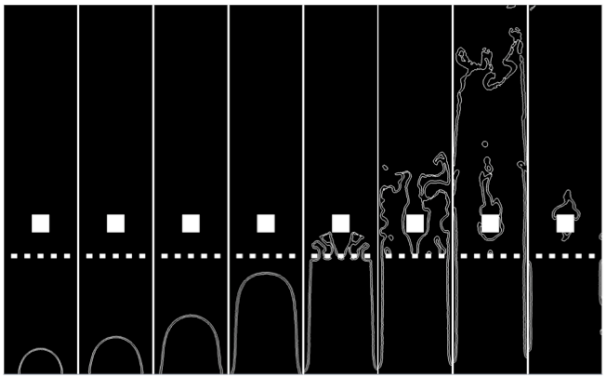

Figure 2. Heat release contours at 3, 5, 7, 9, 10, 11, 12, and 13 ms from AVBP results .

The over-pressure generated by the flame propagation is extracted from the pressure trace recorded at the closed end of the chamber both in experiments and LES. Its maximum value and its corresponding time of occurrence are reported in Fig. 3 for the three configurations of Family 1 and compared to experimental results from Kent *et al*. [1] and LES results from Gubba *et al*. [5]. The results provided by AVBP for the over-pressure generated in the chamber are in correct agreement with experiments in terms of trend and magnitude. The differences with regard to experimental results for the peak value are similar to the ones observed by Gubba *et al*. [5] (approximatively 5%). These discrepancies have to be put into perspective because the experimental results are averaged over fifty realizations whereas the LES results are only single realizations. The increase of the peak over-pressure when increasing the number

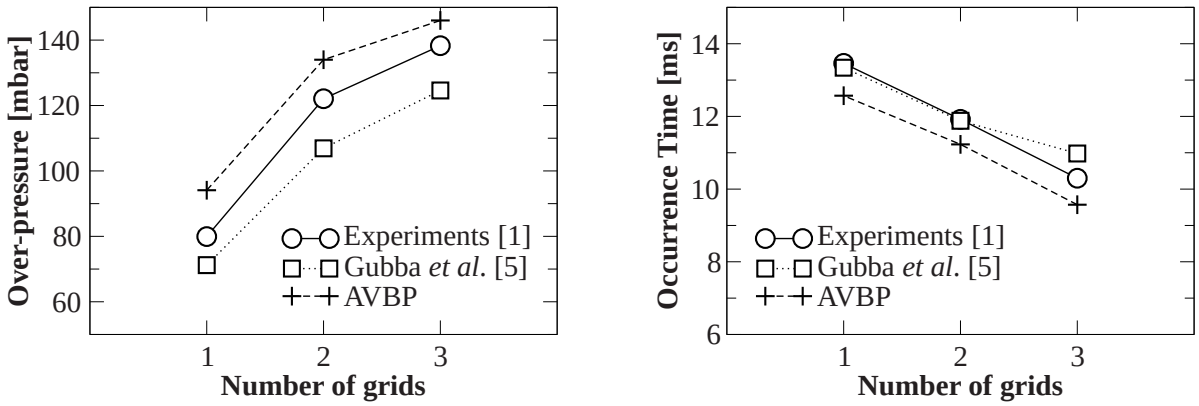

Figure 3. Maximum over-pressure (left) and corresponding time of occurrence (right) for the three configurations of Family 1.

of grids is also correctly predicted. The main phenomena driving the pressure variations seem consequently well reproduced by the computations. The time shifting of the peak over-pressure obtained with AVBP can be explained by the crude ignition model used in this work, which does not account for the early times after ignition. Note that, as explained by Hall *et al*. [15] for a similar configuration, pressure traces of the experimental realizations may be offset in time up to 2ms and have been shifted such that the locations of the peak pressure overlap.

Chemistry Modelling

In the context of LES, the integration of detailed kinetics is impossible due to their high computational cost. For propane-air combustion, typical schemes include 50 species and 350 reactions. Tabulated chemistry methods [16] have demonstrated their potential to replace detailed kinetics [17]. However, this method can become difficult to handle when dealing with complex industrial configurations [14] and curvature and strain effects (important in the laminar phase) can not be included easily. Another alternative solution is to use reduced chemical schemes [14, 18]. In this method, the number of species and reactions is reduced to the main ones. Reduced mechanisms are employed here for all calculations presented in this paper. A common simplification used for reduced schemes is also to set the Lewis numbers equal to one for all species. In the following, the choice of the reduced scheme (including the unity Lewis number assumption) is investigated to estimate its impact on the results of the semi-confined explosion configurations.

Reduced Scheme Influence

The first stage when building a reduced chemical scheme is to choose the number of steps. A first solution is to take into account the fuel oxidation reaction only, with no reverse reaction. In all calculations presented, LPG is replaced by propane C_3H_8, which is its main component (88%) and should not induce drastic modification of the flame properties (the same assumption is made in Gubba *et al*. [5]). Table 1 presents the main characteristics of this one-step scheme C3H8-PQ1.

Coefficients are related to the Arrhenius formulation of the reaction rate:

$$q = Ae^{\frac{-E_a}{RT}} \prod \left(\frac{\rho Y_k}{W_k}\right)^{n_k} \tag{1}$$

Table 1. Reduced one-step chemical scheme C3H8-PQ1.

n	Reaction	A $[\mathbf{cm^3/mole.sec}]$	Ea **[cal/mole]**
1	$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$	3.07E+012	3.347E+004
	Forward : ${n_{C_3H_8}}^F = 0.569$ and ${n_{O_2}}^F = 1.097$		

where E_a is the activation energy of the reaction,W_k and n_k are respectively the molecular mass and reaction exponent for species k.

A common and major drawback of one-step schemes is their inability to correctly predict the adiabatic flame temperature for near stoichiometric and rich mixtures. Then, the mechanism can be improved by adding a second reaction, the CO-CO2 equilibrium, to better reproduce the adiabatic flame temperature on a wider range of equivalence ratio.

Table 2. Reduced two-step chemical scheme C3H8-PQ2.

n	Reaction	A $[\mathbf{cm^3/mole.sec}]$	Ea **[cal/mole]**
1	$C_3H_8 + 3.5O_2 \rightarrow 3CO + 4H_2O$	1.1E+012	4.15E+004
	Forward : ${n_{C_3H_8}}^F = 0.55$ and ${n_{O_2}}^F = 0.9$		
2	$CO + 0.5O_2 \leftrightarrow CO_2$	4.5E+010	2.0E+004
	Forward : ${n_{CO}}^F = 1.0$ and ${n_{O_2}}^F = 0.5$		
	Reverse : ${n_{CO_2}}^F = 1.0$		

This two-step scheme C3H8-PQ2 is described in Table. 2. Both schemes have been built to give a laminar flame speed S_L^0 equal to 38,4 cm/s at $\Phi = 1$ which is within the range of the values found in the literature [19, 20].

Both schemes also use realistic Schmidt numbers for all species. Table 3 shows the corresponding Lewis numbers for each species. All the results presented in the first part of the paper are obtained with C3H8-PQ2.

Table 3. Species Lewis numbers for reduced schemes C3H8-PQ1 and C3H8-PQ2.

C_3H_8	H_2O	CO_2	O_2	N_2	CO
1.655	0.716	1.255	0.971	0.920	0,998

The burnt gases temperature of one-dimensional premixed laminar flames are plotted against equivalence ratio in Fig. 4 for the two mechanisms C3H8-PQ1 and C3H8-PQ2. Results are compared to CANTERA [21] computations made with the GRI-Mech 3.0 [20] mechanism and to the results of an equilibrium computation. The burnt gases temperature is better predicted with C3H8-PQ2 compared to C3H8-PQ1 when the equivalence ratio is larger than 0.9.

Both schemes have been tested using LES on configuration 0, described in Fig. 1, in order to estimate the influence of the kinetic mechanism. Configuration 0 has been chosen because the turbulence generated is moderate (no grids) with regards to the other setups. Consequently, it enables to investigate easily the effects of the chemistry reducing the impact of the turbulence

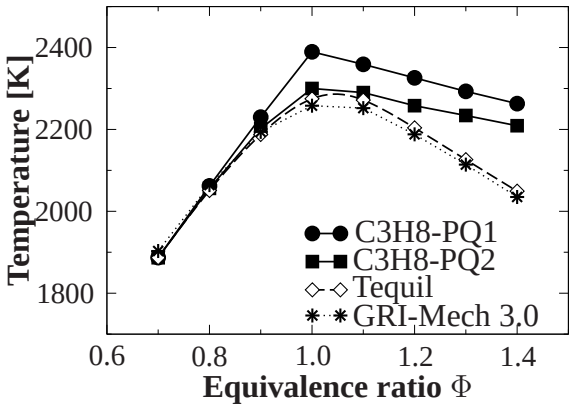

Figure 4. Burnt gases temperature in function of the equivalence ratio Φ.

model for example. Results are presented in Fig. 5. As for the three configurations of Family 1, the peak pressure is correctly reproduced by C3H8-PQ2 in terms of magnitude and timing for configuration 0. On the other hand, with the one-step scheme C3H8-PQ1, the pressure increase is too fast and largely over-estimated (about 110% higher than the two-step prediction and experiments). This result is a direct consequence of the over-estimation of the burnt gases temperature by C3H8-PQ1 : expansion effects, which are due to the unburnt over burnt gas density ratio, are over-estimated, the flame is accelerated too strongly (Fig. 5 right), inducing a higher over-pressure in the chamber.

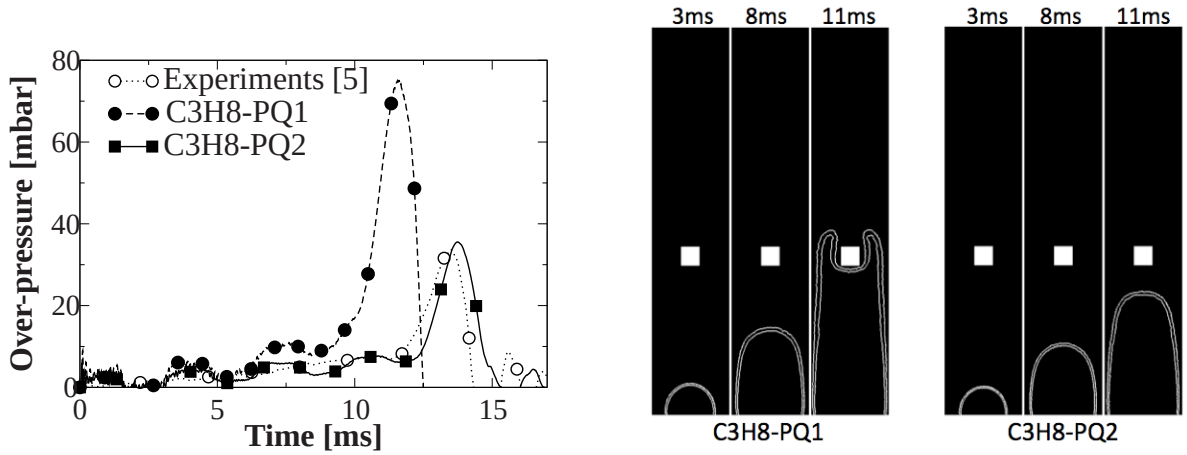

Figure 5. Reduced scheme influence - Left: Over-pressure time traces. Right: Heat release contours at 3, 8, and 11ms - Configuration 0.

The same conclusions may be drawn for configurations 1-2-3. These results illustrate the high sensibility of semi-confined explosion LES to thermochemistry models. In the context of reduced schemes, the use of a two-step mechanism is therefore a minimum prerequisite.

Lewis number Influence

A common simplification when using reduced schemes is to set Lewis numbers Le_k to one for all species. Le_k characterizes the thermal to mass diffusion ratio of species k: $Le_k = \alpha_T / D_k$

where α_T and Dk are the thermal and mass diffusivities.

For simplicity, the investigation of Lewis number influence is performed with one-step mechanisms. Another mechanism, referenced as C3H8-PQ1-Le1, has thus been developed adjusting all Le_k to one. Both C3H8-PQ1 and C3H8-PQ1-Le1 have the same laminar flame speed S_L^0 and adiabatic burnt gases temperature T_{ad}. The first effect of this simplification is that mass and thermal diffusion compensate each other for each species. The second one is that for C3H8-PQ1-Le1, all species diffuse in the same way, consequently avoiding preferential diffusion [22]. Comparison of the two schemes C3H8-PQ1 and C3H8-PQ1-Le1 on configuration 0 using LES is shown in Fig. 6. The peak over-pressure predicted using C3H8-PQ1-Le1 is 220% higher than the experimental value instead of 110% with C3H8-PQ1: the $Le_k = 1$ simplification has a strong impact on this semi-confined configuration. This underlines again the high sensitivity to the way chemistry and transport are modelled and demonstrates that, even though the turbulent phase is the most spectacular in Fig. 2 for example, the quantity of interest (the over-pressure) is strongly controlled by the initial laminar phase. In other words, a critical question is to be able to compute the initial laminar spherical flame using a model built first for turbulent flames and a grid adapted to turbulent flames brush and not to the resolution of transport and chemistry effects in laminar fronts.

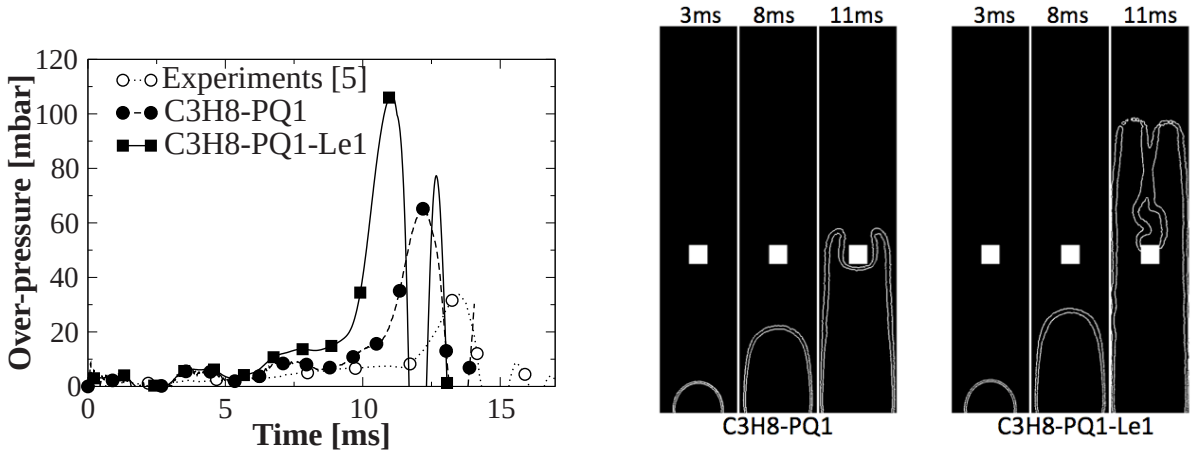

Figure 6. Lewis number influence - Left: Over-pressure time traces. Right: Heat release contours at 3, 8, and 11ms - Configuration 0.

To investigate this issue, a simplified DNS configuration was set up : the laminar premixed spherical flame. This case is indeed representative of the first times after ignition in the combustion chamber. In the next sections, the test case is first described and then the influence of the Lewis number on the consumption speed and the burnt gases temperature is highlighted.

Outwardly propagating flame - The configuration is sketched in Fig. 7. Computations are performed in two dimensions in order to reduce the CPU time. 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 so that the flame front can be fully resolved over more than 10 points using DNS (the flame thickness δ_l^0 is 0.4 mm). The TFLES model is consequently not used for these simulations. Non-reflecting boundary conditions are used at the outlet to avoid reflected waves in the domain [23]. A propane and air mixture is used at an equivalence ratio $\Phi = 0.7$ at atmospheric pressure and

temperature. This assumption enables to consider that the phenomena studied are governed by the deficient reactant Lewis number which is consequently the fuel C_3H_8 [22, 24]. Simulations performed at $\phi = 1$ showed the same trends for this configuration, which enables to extend the results of the following sections to the explosion chamber configuration. The gas is ignited at Point O by an energy deposition.

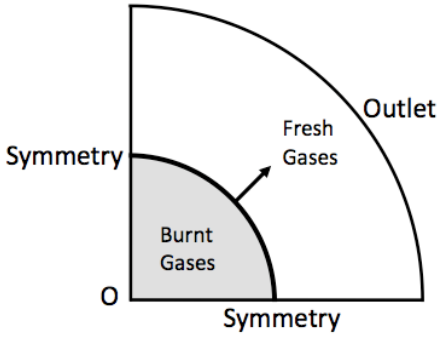

Figure 7. Two dimensional outwardly propagating flame configuration.

Consumption speed - The consumption speed S_c is defined in Eq. 2 from the integral of the fuel burning rate across the flame front:

$$S_c = -\frac{1}{\rho_f Y_F^f} \int_{-\infty}^{\infty} \dot{\omega}_F dx \tag{2}$$

where ρ_f is the fresh mixture density, Y_F^f is the fuel mass fraction in the fresh gases, and $\dot{\omega}_F = W_F q$ is the fuel burning rate with W_F the fuel molecular mass.

At the beginning of spherical propagation, S_c is limited by stretching effects. In the limit of small curvature terms, it has been shown that S_c can be written as [25, 26]:

$$\frac{S_c}{S_L^0} = 1 - L_a^c \frac{\kappa}{S_L^0} \tag{3}$$

where L_a^c is the Markstein length for the consumption speed and $\kappa = (1/S)dS/dt$ is the flame curvature with S the flame surface area.

This formulation is dependant on the Lewis number through L_a^c. Many expressions of L_a^c can be found in the literature. The Clavin and Joulin [27] formulation of the Markstein length has been used to evaluate the formulation of S_c for lean mixtures:

$$L_a^c = \delta \frac{1}{2} \beta (Le_F - 1) \frac{T_f}{T_b - T_f} \int_0^{\frac{T_b - T_f}{T_f}} \frac{ln(1+x)}{x} dx \tag{4}$$

where T_b and T_f are respectively the burnt and fresh gas temperatures, and δ is the unstretched flame thickness. The parameter $\beta = (T_b - T_f)T_a/T_b^2$ measures the activation energy, with T_a the activation temperature.

Eq. 3 and 4 show that the Lewis number has a direct influence on the consumption speed for high curvatures. The consumption speed of a fuel with $Le > 1$ should therefore be significantly reduced for high curvatures, as it is the case in the early times after ignition. On the other hand, assuming that $Le = 1$ should lead to a zero value for the Markstein length and a flame speed

independent of stretch to first order.

The consumption speeds directly computed from the fuel burning rate are plotted on Fig. 8 against the flame radius (left) and against the flame curvature (right) for C3H8-PQ1 and C3H8-PQ1-Le1. As predicted by theory, the $Le = 1$ simplification induces non-negligible modification of the flame response to curvature. Even for strong curvature, the consumption speed obtained with C3H8-PQ1-Le1 remains almost constant and equal to the unstretched laminar flame speed. For C3H8-PQ1, the dependance to the flame curvature is correctly reproduced. The Markstein length relative to the consumption speed extracted from Fig. 8 for C3H8-PQ1 is 0.15mm, which is coherent with the order of magnitude found in the literature [28] (0.25 - 0.42mm) and Eq. 4 (0.46mm).

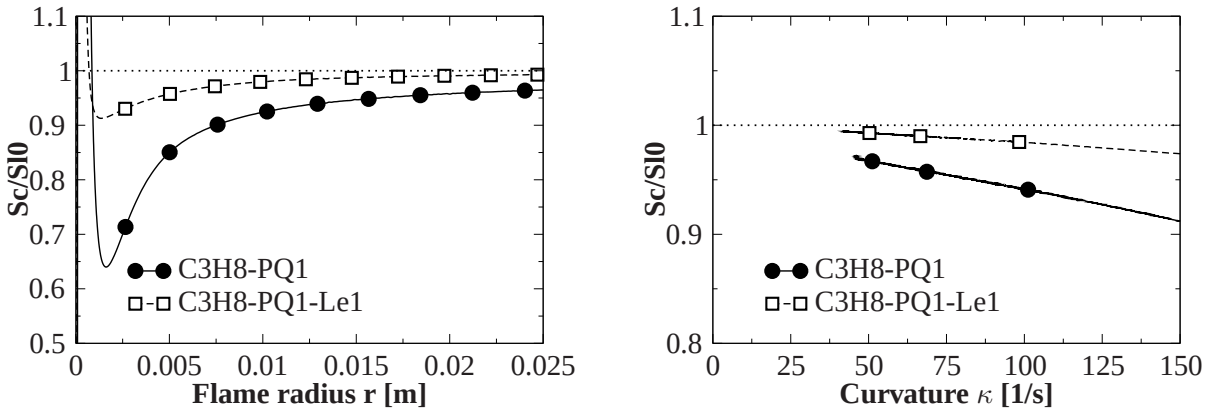

Figure 8. Normalized consumption speed in function of flame radius (left) and curvature (right).

Burnt gases temperature - Besides the consumption speed modification by stretch, curved flames are subject to modifications of the burnt gases temperature with regard to the adiabatic temperature T_{ad}. Law [24] gives a conceptual demonstration of the effects of curvature in the presence of preferential diffusion for an outwardly propagating flame. For $Le > 1$, heat losses due to the concave nature of the flame front exceed the gains in reactant concentration leading to a temperature in the burnt gases $T_b < T_{ad}$. On the opposite, $T_b > T_{ad}$ if $Le < 1$ and if the heat and mass diffusion rates are equal (Le=1), the two effects compensate each other and $T_b = T_{ad}$ is expected. When the flame expands, the curvature intensity steadily decreases as 1/r and the flame recovers the characteristics of a planar flame, which means that T_b tends toward T_{ad}.

It has been shown [29, 30] that the burnt gases modification by stretch in the limit of small curvature terms can be written:

$$\frac{(T_b - T_{ad})}{T_{ad}} = (\frac{1}{Le} - 1)\frac{D}{S_L^{0\,2}}\kappa \tag{5}$$

where D is a characteristic diffusivity.

Results of the outwardly propagating flame are shown in Fig. 9. As expected, C3H8-PQ1-Le1 is not able to predict the decrease in the burnt gases temperature for small radii. The temperature in the center of the spherical flame is always over-estimated with a difference reaching 150K in the first times compared to C3H8-PQ1. The over-estimation of the burnt gases temperature by C3H8-PQ1-Le1 induces an over-estimation of the fresh/burnt gases density ratio and

an acceleration of the flame absolute speed. With C3H8-PQ1, the burnt gases temperature is correctly estimated with regard to the prediction of Eq. 5 as shown in Fig. 10. The burnt gases temperature is reduced when the flame curvature is high (low radius) and tends towards T_{ad} for low curvature (high radius).

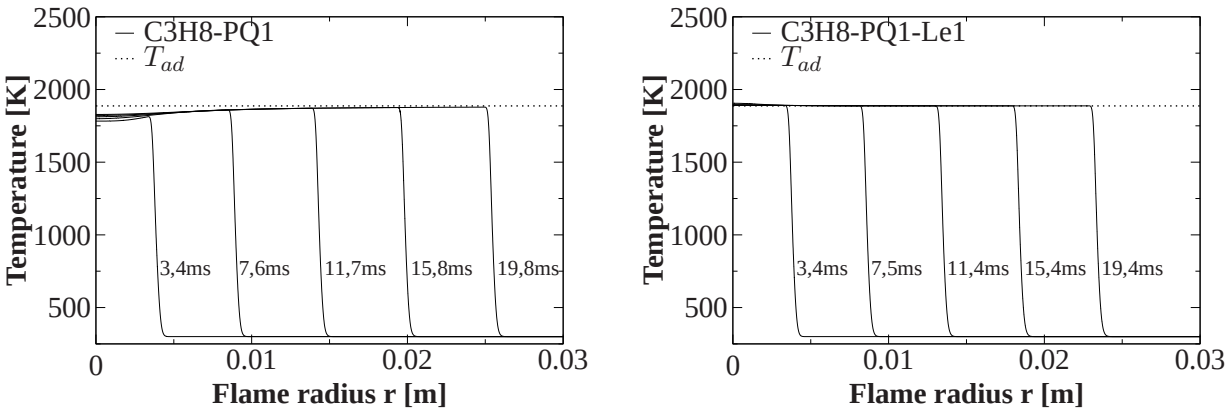

Figure 9. Temperature profiles along radial axis at different times for C3H8-PQ1 (left) and C3H8-PQ1-Le1 (right) schemes.

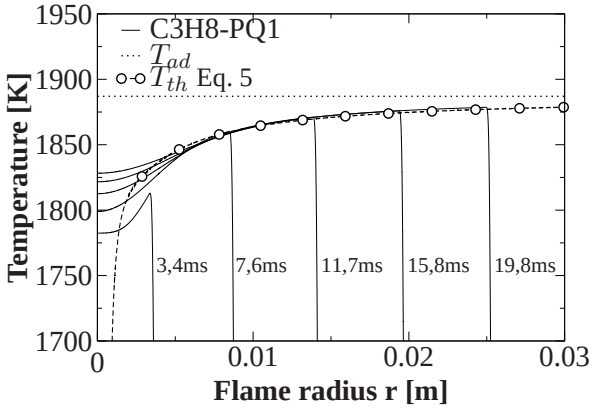

Figure 10. Close-up on the temperature profiles along radial axis at different times for C3H8-PQ1 compared to Eq. 5.

To conclude, assuming unity Lewis number as done for C3H8-PQ1-Le1 accelerates the flame because the effects of curvature on flame speed and temperature are not captured. This acceleration has a strong impact on the flame propagation, which raises significantly the peak over-pressure in the explosion chamber configuration, as it has been shown in Fig. 6.

Conclusion

The first objective of our numerical investigation was to use LES to predict critical parameters related to building safety issues. Results show that a compressible LES using the thickened flame model is able to correctly reproduce the flame propagation past the repeated obstacles

and capture the over-pressure for the four studied configurations, with or without turbulence generating grids.

However, results also show that the initial laminar flame propagation is essential to evaluate the pressure history. This laminar propagation phase is difficult to compute with classical turbulent combustion models, especially to capture curvature effects. Therefore, in a second part, the sensitivity of the results to models used for laminar transport chemistry has been highlighted. Errors observed rise up to 220% using a one-step reduced scheme with Lewis numbers set to one instead of 5% with a two-step scheme with realistic Lewis numbers.

The main conclusion of this work is that only the combination of: (1) a two-step scheme to obtain a satisfactory burnt gases temperature, (2) the use of realistic Lewis numbers to get the right flame response to curvature; allows a good prediction of this kind of configurations.

Due to the high sensitivity of over-pressure to calculation parameters such as the chemistry model, results relative to semi-confined explosion configuration should be put into perspective. Being able to fully predict critical parameters on this type on configuration appears to be a difficult task considering the dependance on the models used. A higher importance should be accorded to the trend of over-pressure when adding grids, which can correctly be predicted by LES, than directly to the magnitude or the timing of the peak pressure.

Acknowledgements
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