Flame front perturbations induced by concentration gradients

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1 Introduction

Explosion modelling tools improved significantly during the last thirty years. They become steadily more and more predictive but often important simplifications are made such as assuming a homogeneous combustible cloud. In real situations, heterogeneities exist. For instance, turbulent jets, induced by massive leaks, are characterised by a much larger concentration near the breach than further downstream. As explosion effects are linked to the history of the flame through the cloud, a reactivity gradient may modify significantly the pressure evolution, maximum levels reached and impulse [1] .The purpose of this work is to evaluate the influence of a reactivity gradient of combustible cloud upon the subsequent perturbations of explosion effects.

2 The likely incidences of a gradient of reactivity upon the explosion effects of unconfined cloud

A semi quantitative examination seems to be possible for unconfined explosions since a rather precise model may be applied. Provided the pressure induced by the explosion is not too large, the flow resulting from an isotropic flame propagation can be modelled by considering the flame as a spherical acoustic source for which exact analytical solutions exist [2] :

$$\boxed{\Delta p(r,t) = \rho_0 \frac{(1-\alpha^{-1})}{4\pi r}\frac{d^2V_f}{dt^2}}, \quad \boxed{\frac{\partial^2 V_f}{\partial t^2} = \frac{\partial}{\partial t}(A_f \times S_f)}, \quad \boxed{A_f = 4\pi r_f^2} \text{ with}$$

- r : distance to ignition source
- t : time elapse since ignition
- $\Delta p(r,t)$: Pressure level at t and r
- ρ_0 : density of the atmosphere
- α : expansion rate of the burnt gases
- V_f : flame ball volume
- A_f : flame area
- S_f : spatial flame speed
- r_f = flame ball radius at t

We propose to use this tool to investigate the intrinsic flame dynamics and to try to implement the incidence of an heterogeneous repartition of reactivity.
First of all, we try to put in relief the real flame behaviour on the basis of the deflagration of a 130 m^3 H2/Air mixture (60 %) contained in a stratospheric balloon [3]. The use of a stratospheric balloon allows being the closest of the conditions of validity to apply the Leyer model (the flame develops freely in the open atmosphere with very few pressure reflections)

A sharp analysis of the results makes appear clearly that the flame speed increases continuously from the standard laminar flame expansion speed $\alpha.Su$ = 2.1 x 5 = 10.5 m/s (Su = laminar flame speed) to twice this value. In the present situation, with a flame developing freely in the open atmosphere with very few pressure reflections, able to trigger the Taylor instability [4] and with a mixture unlikely to favour the thermo-diffusive it seems that the remaining phenomena capable of accelerating the flame would be the hydrodynamic instability [5].
One of the consequences of the hydrodynamic instability is that such a flame is covered with "large bubbles" sometimes with several tens of centimetres in diameter and responsible for a large increase of the flame area and so increase of flame speed. To take into account this phenomena, we combine to the acoustic model a model of flame acceleration [4] due to bubbles appearance :

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$$\boxed{S_f = \alpha.Su + \delta_{LD}.\, r_f} \quad \text{with} \quad \boxed{\delta_{LD} = \frac{(\sqrt{\alpha}-1).Su.2\pi}{\Lambda}}$$

t : time elapse since ignition
ρ_0 : density of the atmosphere
α : expansion ratio of the burnt gases
S_f : spatial flame speed
r_f : flame ball radius at t
Su : fundamental flame speed
δ_{LD} : growth rate of "bubbles"
Λ : wave number

This model is quite rough but may nevertheless be sufficient for simulating the flame and explosion dynamics in a cloud with a gradient of reactivity. As an illustration, we imagine that the envelop of the balloon in the experiment has been removed for some time before ignition so that some diffusion with the outside atmosphere is allowed. The concentration of the cloud before the beginning of the diffusion process has been selected so that, at the ignition time, the cloud diameter and total quantity of hydrogen inside the explosive boundary is the same than in the experiment.

Explosion simulations are shown on figure 1 by considering the following cases :

- The basic situation of the corresponding homogeneous cloud (60% H_2/Air) with a laminar stable flame propagating steadily through the cloud (no instabilities) ;
- The incidence of the gradient of reactivity upon the laminar flame expansion velocity neglecting the hydrodynamic instability ;
- The incidence of the gradient of reactivity upon the laminar flame expansion velocity taking into account of the hydrodynamic instability

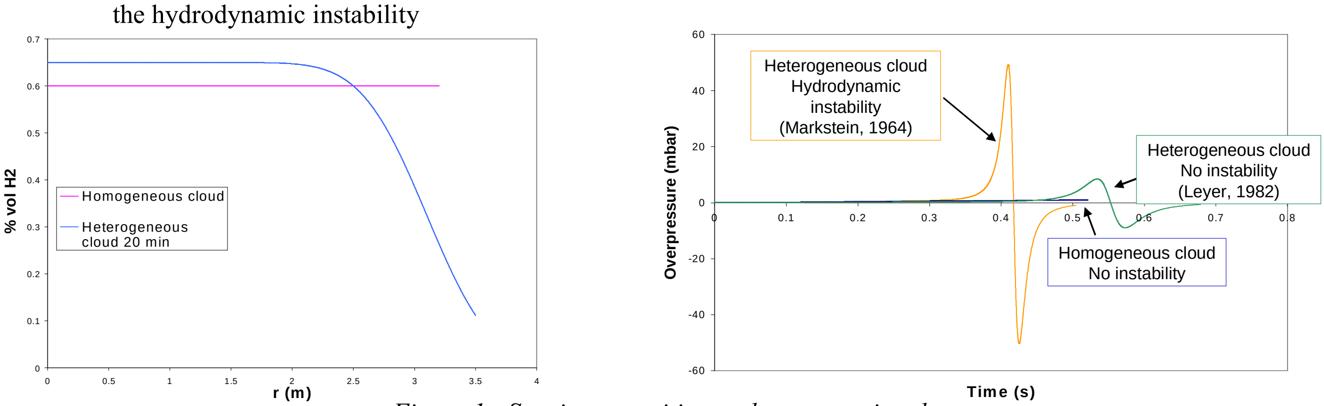


Figure 1 : Species repartition and pressure signal

It appears immediately that the traditional first situation, hardly visible on the graph, is one order of magnitude below the second one, the latter being also one order of magnitude below the third situation believed to be the most realistic.

It comes out that, not only, the acceleration or deceleration of the combustion due to the gradient of reactivity is important, but also, may be to an even larger extent, the excitation of the hydrodynamic instability of the flame. Because this kind of instability is extremely sensitive to any modification of the flow field, it is believed that its incidence should be greatly favoured in a confined situation.

3 An alternative numerical tool

Simulation of premixed flame propagation became one of the most challenging problem of the last thirty years. Simplest approaches (zero order physical models) like the acoustic one presented previously seem to be inadequate to tackle flame dynamics. Much more sophisticated approaches, based on direct numerical simulation require, at each time and space step, a simultaneous resolution of the chemical reactions and fluid dynamics equations. The stiffness and the non-linearity of chemical make the resolution a very difficult task [6]. Other codes, developed to treat industrial safety questions calculate over length scales of the order of metres to compute real scale industrial sites. The mesh size is however so large that the flame structure cannot be resolved and implemented. This the reason why **a**n alternative numerical method has been designed and tested, in which the essential aspects of hydrodynamically unstable flame are "naturally" featured.

This numerical approach is based on the first order well admitted assumption where the flame is considered as an interface, virtually without mass and thickness, turning cold unburned gas into hot burnt gas. The movement of this interface is tackled with an adaptation of the "Front Tracking Method" [7]. The interface is defined by a collection of points located on its surface. To move any point of the interface, the velocity field of the neighbouring fluid cells is interpolated to that particular point using a barycentric weighing function. But, this interface is not inert, flame has is own dynamic :

1- The flame propagates locally at the laminar burning velocity (Su) relative to the unburnt gases.

2- At each point of the interface (the flame front), the normal velocity component is expanded due to the thermal expansion whereas the tangential velocity component is unchanged

This dynamic is revealed in our algorithm by the fact that the interface separates two fluids of different densities which "communicate" across the flame only via interface relationships [8] :

$$\boxed{\frac{\delta u_1 - \delta u_0}{u_0} = (\alpha - 1)\frac{\delta S_u}{u_1} - \frac{\gamma - 1}{\gamma}(\alpha - 1)\frac{\delta p_0}{p_0}}$$

$$\boxed{\frac{\delta p_1}{p_1} = \frac{\delta p_0}{p_0}}$$

with

0, 1 = index respectively unburned and burnt gas
u = velocity of flow
p = pressure
α = expansion ratio
Su = laminar flame speed
δ = " an increment of "
γ = ratio of specific heats

As we are interested in the effect of concentration gradients, the same fluid flow solver is used for the prediction of the molecular diffusion question before ignition and for the calculation of the fluid motions during the propagation of the flame. A Predictor / Corrector Mac Cormack scheme is use, with a tiny time step (10^{-6} s) to reduce the effect of the necessary artificial viscosity.

We have tried to simulate a practical situation. A flame propagates through a vertical 1.5 m long tube (square section 10 x 10 cm) in a 6.3% vol. CH4 / Air mixture from the bottom open end to the top closed end. Ignition has been done near the open end so that the flame propagates freely. The initial number of interface points is 18 and the bi-dimensional computational domain is discrete by 10 x 75 mesh points. This "final" shape and flame speed are very close to the observation, the flow field is very realistic too.

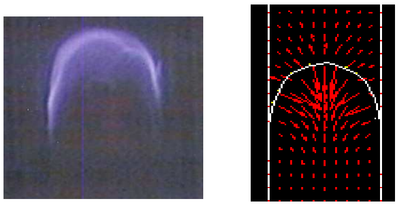


Figure 2 : Comparison between simulated and real 6.3% vol. CH4 flame propagating

4 Experimental Setup

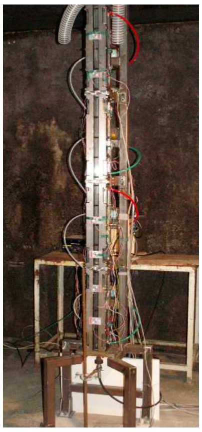
The small exercise presented section 2 put in relief that the interaction between a flame and aerodynamic conditions in front of it will be stressed in confined configuration. Therefore, we design a special setup

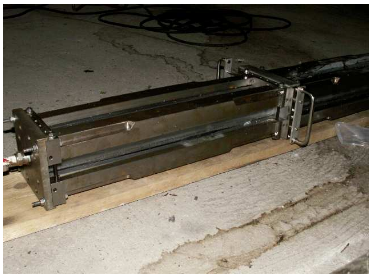
Since the flame may experience an exponential growth of disturbances, we need a very careful control of the initial conditions among which the repartition of the reactants. If any convection current would appear, erratic pockets of mixture may be produced. Because of this, the diameter of the tube needs to be kept small (a few centimetres) so that the formation of the gradients could result from molecular diffusion. It has further been estimated that a length of tube of the order of 1 m would permit to simulate the range of gradients of reactivity likely to be produced in practical situations (0.1 m to 1m).

The tested set-up is a 2 m long tube with a square section whose side is 0.03 m long. A gate valve separates the tube into equal parts. The composition of the gases is different on both sides of the valve. The opening of the valve permits the mixing of the gases by molecular diffusion.

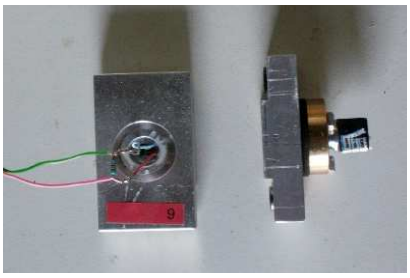
But the specificity of this setup is to be transparent and resistant in high pressure explosion (around 150 bars). It consists in three PMMA walls and one aluminium wall set in metallic skeleton. This skeleton gets back al the mechanical solicitations. The tightness is ensured only by silicone putty sticking (figure 3 (a.) and (b.)).

A specific effort had been made to develop instrumentation necessary to interpret conveniently the tests. A system of opacimeter (figure 3 (c.)) had been develop. It consists in laser diode and a photovoltaic cell fixed on two aluminium supports magnetized on metallic skeleton. Eight opacimeters are distributed along the tube. It function is double. It allows the detection of flame by a modification of laser luminous signal caught by the photovoltaic cell and, consequently, allows obtaining flame speed and trajectory. Moreover, it allows deducing the mixing ratio of gas from the measurement of opacification of luminous signal by nanoparticles of ammonium chloride swept along during molecular diffusion. A second optical technique had been developed to catch the flame area. It consists in illuminating a thin slab of the tube with an Argon / Ions Laser thanks to a rotating mirror (figure 3 (d.)) So, green light is diffused by the ammonium chloride particles. During its propagation, the flame dissociates the ammonium chloride particles without modifying the combustion. So the flame area can be detected via high speed video to the threshold between high and low contrast region. Pressure is captured by classical piezoresistive gauge.

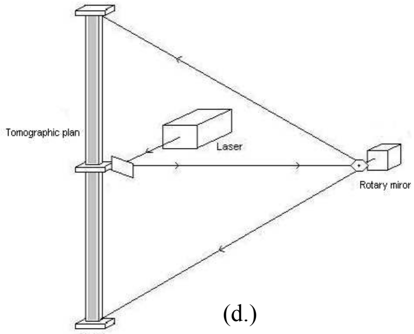




(b.)



(c.)



(d.)

Figure 3 : (a.) global sight of tube, (b.) one part and get valve, (c.) opacimeter, (d.) Illumination of laser thin slab

(a.)

First tests had been done for homogeneous an heterogeneous CH4 / Air mixture in the prototype of this tube. Although we notice the real influence of the reactivity gradients on the propagation at level of impulse, overpressure and flame speed, the phenomenon is compete with heat loss at the wall. This is the reason why we choose more reactive mixtures with H2 / O2 / N2. The first results we obtained are very promising.

5 Conclusion

Explosion modelling tools improved significantly during the last thirty years. They become steadily more and more predictive but often important simplifications are made such as assuming a homogeneous combustible cloud. In real situations, heterogeneities exist. The first exercise done in part 2 shows explosion effects are linked to the history of the flame through the cloud and a reactivity gradient modify significantly the pressure evolution, maximum levels reached and impulse.

As the classical numerical approach seemed not to be able to capture the hydrodynamic instability, we develop an alternative approach in which the flame is considered as an interface with its own dynamics, separating two fluids at different densities. Promising data have been obtained.

Since the hydrodynamic instability is extremely sensitive to any modification of the flow field, its incidence should be greatly favoured in a confined situation. So, a specific set-up a transparent tube (2m long , side of square section : 0.03 m) resistant to high pressure explosion to investigate this phenomena. An important effort had been made to develop an instrumentation necessary to interpret conveniently the tests.

This work is going on not only on the numerical aspects (with new fluid mechanics solvers), but also on the experimental side

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