Flame propagation in a $H_2/O_2/N_2$ mixture with a concentration gradient

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1. Introduction

The investigation of flame propagation accompanying the explosions of unconfined gaseous reactive clouds which are diluted in atmosphere ambient is a fundamental interest in the analysis of industrial risk assessment. It is now recognized that the release and subsequent explosion of a cloud of inflammable vapor constitutes a credible accident.

Much of the work performed with non-uniform mixtures deals with the propagation of flames in directions normal to the gradient (Philipps 1965 , Hirano et al. 1977, Girard et al. 1978, Badr and Karin 1984, Karin and Lam 1986, Whitehouse et al. 1996). Most of this work are performed in closed apparatus, expected the analysis of Girard et al. which has been conducted in ambient air. In the last case, the gradient were obtained with concentric soap bubble containing fuel and oxidizer.

2. Experiments

Tests were performed with a stoichiometric H_2/O_2 mixture initially confined in a hemispherical soap bubble (0.07m of radius). When the bubble is broken, the gaseous mixture diffuses into surrounding air. The gradient of reactivity is formed. The ignition source (electrical spark) can be located at different positions (Ri, Zi) from the center of the initial hemisphere. Pressure transducers allow to follow the wave pressure propagation following up the explosion. We use an optical system to measure the flame velocity. It contains an interferential filter at 750 nm with a bandwidth of 10 nm corresponding to a OH band, and support a focusing lens. This system allows to determine a fast signal (1~µs) at a precise point of the dispersion of the H_2/air mixture.

3. Experimental results

The burning velocity D can be calculated by two ways : a direct and an indirect methods. The direct method consists to use the optical transducer. The burning velocity is then simply give by d/t ratio where d is the optical tranducer-ignition distance and t the arrival time of flame front to the optical tranducer (fig.1).

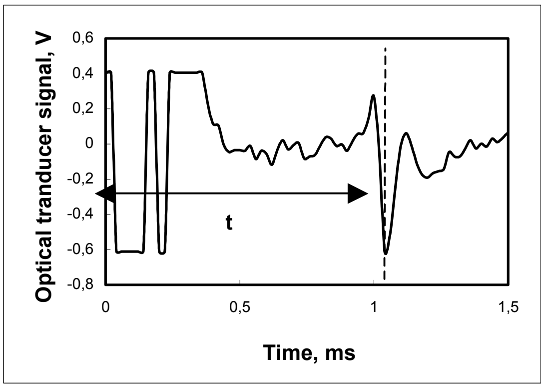

Figure 1 : Optical tranducer signal versus time

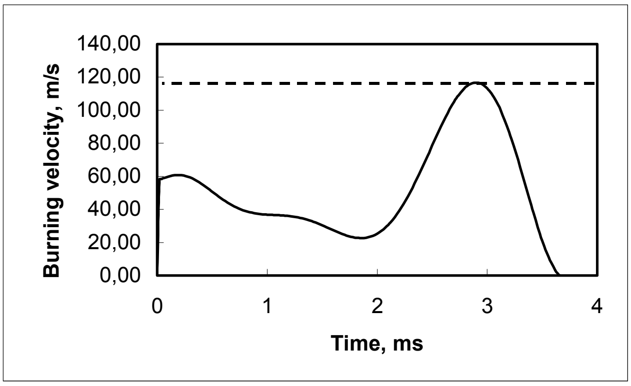

Figure 2 : Burning velocity calculated from pressure record (at 0.692 m)
$2\ H_2+O_2$ - 1 atm - 298 K

The indirect method is based on the analogy of piston proposed by Deshaies [7]. This model consists to divide the flow field of a deflagration in two zones : incompressible and acoustic. The solution gives the pressure P at the radius R and time t as a function of flame propagation $R_F(t)$, the expansion celerity of flame front and its acceleration. By two successive integrations of the pressure signal, the history of flame is deduced. The burning velocity is then defined by the ratio of the expansion celerity of flame front over the expansion ratio (fig.2). Actually, the real limitations of this model are not known, a priori. However, this model is based on the uniform gaseous cloud. For that, we use it only for uniform H_2/O_2 mixture (i.e. with no diffusion time delay).

4. Modelling

The modelling is realized with fluent software.

1. Diffusion

The modelling of the dispersion of the H_2/O_2 cloud is based on the Fick law and considers a compressible flow coupled with the buoyancy effect.

2. Combustion

Combustion modelling is essentially based on eddy-dissipation model, a turbulence-chemistry interaction model based on the work of Magnussen and Hjertager (1976) .An extension of this one, eddy-dissipation-concept model, which includes detailed chemical mechanism in turbulent flows was used. It assumes that reaction occurs in small turbulent structures, called the fine scales. Combustion at this fine scales is assumed to occur as a constant pressure reactor, with initial conditions taken as the current species and temperature in the cell. A global Arrhenius rate for a one step overall reaction was used for chemical kinetic related to the model (Marinov et al.).

5. Numerical results

1. Uniform mixture

We present the evolution of the combustion process of the uniform H_2/O_2 cloud (fig.3a) in terms of mass fraction of burned gas for three times at t = 40, 80 and 120 µs (fig.3b-3c-3d). Hence, the expansion of gas can be followed.

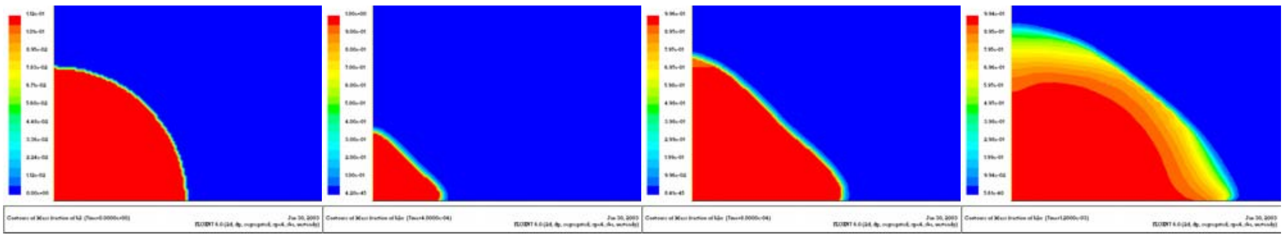

Figure 3a **Figure 3b** **Figure 3c** **Figure 3d**

2. Non uniform mixture

We consider in this section, a diffusion time delay (215 ms) for which the concentration distribution takes a mushroom shape (fig.4a). The mixture is then ignited at (0,4).The expansion of burned gas is represented for three times after the ignition, at t = 100, 160 and 200 µs (fig.4b-4c-4d) .

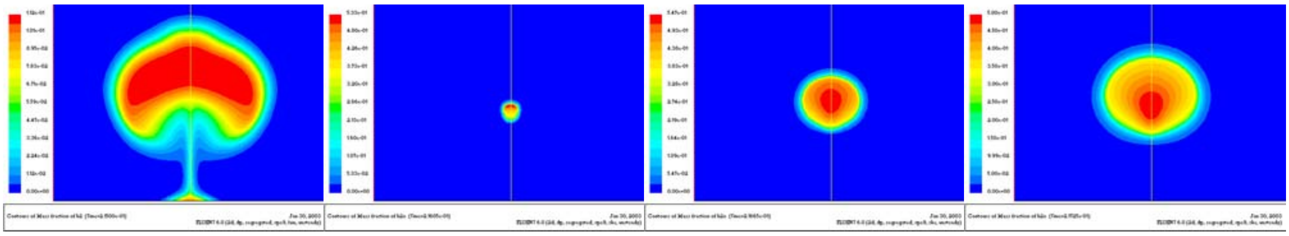

Figure 4a **Figure 4b** **Figure 4c** **Figure 4d**

6. Conclusion

The correlation obtained for a uniform gaseous cloud between experiments and numerical results are in a good agreement. Hence, the burning velocity is equal to 94.68 m/s by using the optical transducer, is 116.69 m/s by applying the piston model (Deshaies 1981), and is 96.2 m/s with the modelling.

In case of the non uniform gaseous cloud, the results obtained by the numerical case are in a good agreement according to the concentration of $H_2/O_2/N_2$. The experimental values are in average three times higher than the numerical results. This disagreement is explained by assumptions used in the diffusion part of the modelling : the physical boundary of the initial gaseous charge and the electrodes are not represented. A better modelling is today in course.

7. References

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