Numerical Study of Detonation Cells under Non-Monotonous Heat Release

Vianney Guilly, Boris Khasainov, Henri-Noel Presles, Daniel Desbordes, Pierre Vidal
Laboratoire de Combustion et de Détonique, UPR 9028 CNRS, ENSMA, BP 40109,
86961 Futuroscope, France

Corresponding author, Vianney Guilly: guilly@lcd.ensma.fr

Introduction

Presles et al. (1996) observed a double detonation structure in pure nitromethane and nitromethane-oxygen mixtures. Joubert et al. (2003) observed a similar structure in gaseous mixtures where NO_2/N_2O_4 was the oxidizer, the fuel being hydrogen, methane or ethane. Indeed, Fig. 1 shows two sets of detonation cells**.** The characteristic size of the larger cells is a few orders of magnitude greater than that of the smaller ones. Lamoureux et al. (2001) numerically studied the detonation reaction zone in these mixtures in the frame of the ZND model using a detailed scheme for the chemical kinetics of decomposition and oxidation of the considered explosive mixtures (Djebali et al. 1997). They have shown that the chemical energy is mainly released in two distinct exothermic steps. The first step is very fast (its characteristic time is of the order of 10 ns) while the second step is much slower (a few microseconds). The ratio of the two characteristic reaction times strongly depends on the mixture composition (its richness). Experimental studies confirm that this ratio controls the difference in sizes of fine and coarse detonation cells.

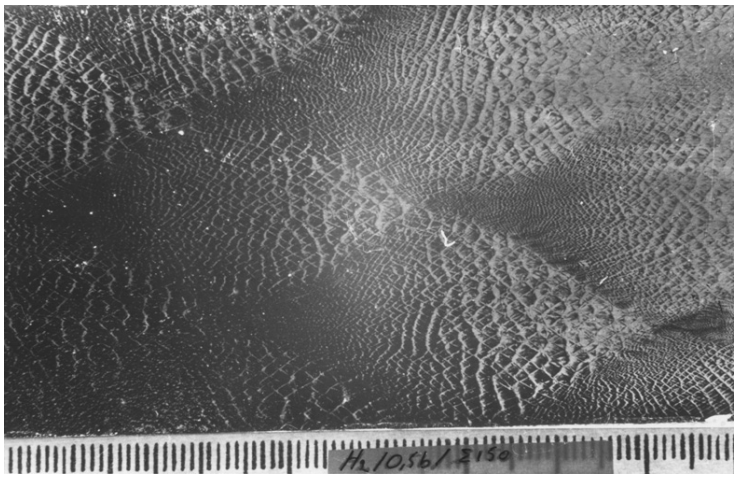

Figure 1. An example of soot traces record of detonation in the mixture H_2 + $0.25\{NO_2/N_2O_4\}$. Detonation propagates from left to right.

Moreover, Desbordes et al. (2004) have observed low velocity detonation regimes in lean H_2-NO_2/N_2O_4 mixtures. Neither two-level detonation cell structure nor low velocity regimes in these mixtures were studied numerically. Apparently, from numerical point of view, the simulation of so complicated structures as shown in Fig. 1 presents important difficulties due to the multi-scale character of detonation structure.

Nevertheless, Gamezo et al. (2000) have succeeded in showing numerically the existence of three levels of detonation cells of very different sizes in type Ia SUPERNOVAE using two-dimensional simulations that take into account multiple thermonuclear reactions. Nevertheless, their simulations neglected interactions between cellular structures and did not permit their simultaneous observations. Here, we present preliminary results of numerical modelling of detonation cell structure one could observe when chemical reaction proceeds in two exothermic steps due to a simple model of non-monotonous heat release caused by two successive exothermic reactions. The resulting numerical flow pattern qualitatively reproduces the aforementioned experimental observation.

Numerical Study

Two-dimensional numerical simulations of detonation propagating in a plane channel were performed solving the Euler equations thanks to the Flux Corrected Transport (FCT) technique developed by Oran and Boris (1987) and the adaptation procedure described by Khasainov et al. (2003). Minimal size of numerical meshes in the well resolved zone at the detonation front is 0.05 mm. Wall losses are ignored.

Here it was assumed that chemical reaction comprises two successive steps: $A \rightarrow B$ and $B \rightarrow C$. Both steps are exothermic and modeled according to Arrhenius laws : $K_i=Z_{i.}\rho ni.\exp(Ea_i/RT),i=1,2$; where Z_i is the pre-exponential factor, n_i the reaction order and Ea_i the activation energy of reaction i .

Figure 2 displays calculated traces of maximum pressure for the case when the second reaction is very fast. In this condition, the products of the first reaction are immediatly consumed by the second reaction. The heat release then proceeds the same way as in the classical monotonous case and the correponding detonation cell pattern comprises one single set of cells. The detonation velocity is close to the ideal CJ value.

Figure 3 shows an opposite case when the second reaction rate is very slow. In this condition, the detonation has to propagate on a quite long distance for all the energy to be released. The detonation transits from a low-velocity detonation regime where only the energy contained in the first reaction supports the detonation, to the Chapman-Jouguet regime where all the energy has been released. In Fig.3 , an important part of the second reaction chemical energy has not been released yet and the detonation is almost only supported by the heat released by the first reaction. This explains why the detonation velocity is significantly (20%) lower than in Fig. 2 (like in observations by Desbordes et al., 2004). Consequently, mean pressure is also smaller than in previous case and so Fig. 3 seems darker than Fig.2 (the same pressure scale was used for Fig.2-Fig.4). The detonation cell pattern comprises quite large cells with a thickness of nearly 40 mm, which are partially filled with much smaller ones. This fine cell structure is most likely not a consequence of non-monotonous heat release. Indeed such structures are frequently observed in combustible-O_2 (Gamezo et al. 1999) mixtures whith reduced activation energy that satisfies the Manzhalei criterion (Manzhalei 1977), i.e. $E/RT_{shock}>6$. Thus, the model with two successive exothermic reactions can be helpful in interpreting the observations of low velocity gaseous detonations.

Finally, Fig. 4 shows an intermediate case. One can clearly see that there are two distinct detonation cell structures: larger cells have a size of about 80 mm and smaller ones of a few mm. In contrast to Fig.3, here finer cells fill completely the larger cell. The ratio of the calculated characteristic sizes of both structures is smaller than in experiments. However, the

numerical resolution was insufficient to capture very fine cells at the beginning of the greater detonation cells where pressure is larger. Nevertheless, these calculations show unambiguously that a stabilized two-level detonation structure can be reproduced numerically under non-motonous heat release produced by two-successive exothermic reactions.

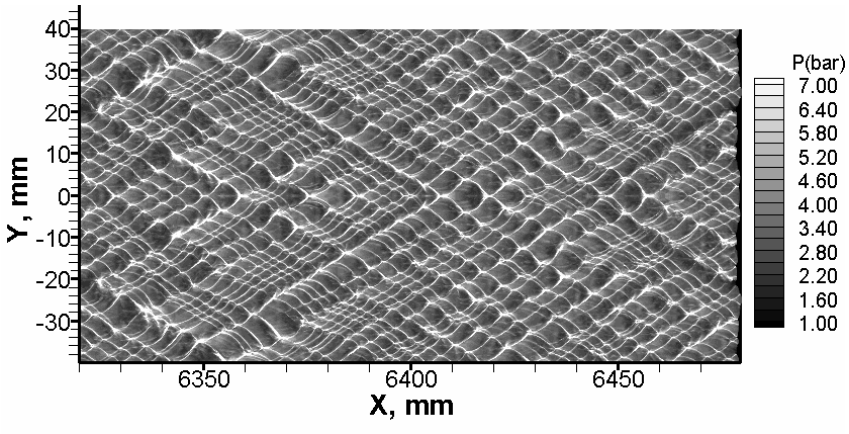

Figure 2. Traces of maximum pressure for the case of a very fast second reaction.

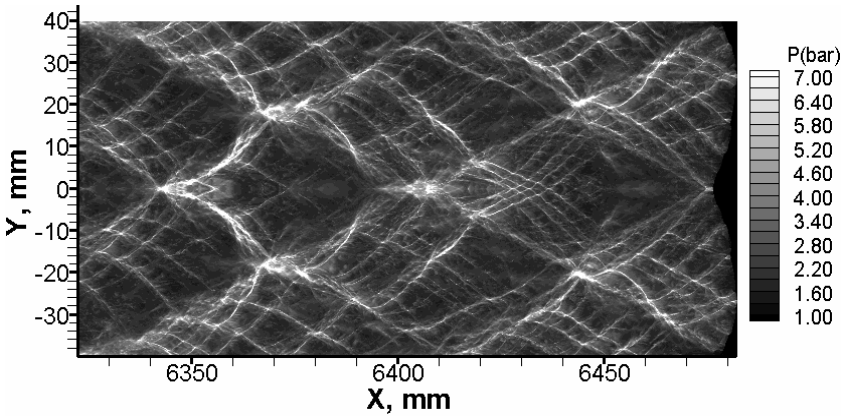

Figure 3. Traces of maximum pressure for the case of a very slow second reaction.

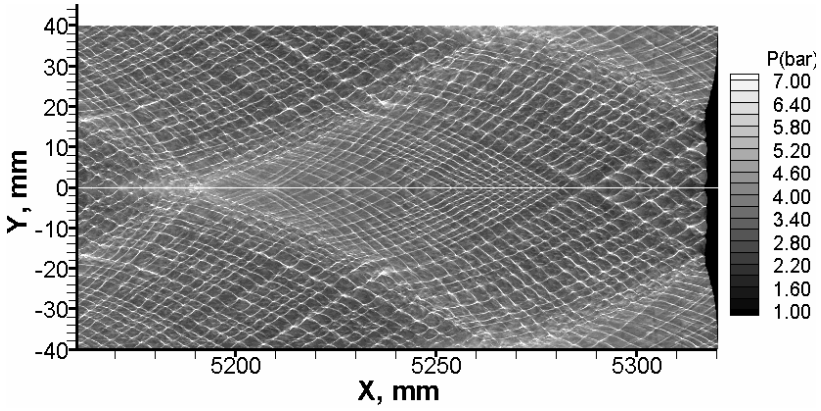

Figure 4. Traces of maximum pressure in intermediate case.

Conclusions

A stabilized two-level detonation structure was numerically reproduced for the case of two successive exothermic reactions. However, further studies are needed with an improved resolution. The work is ongoing to complete the study of the effect of governing parameters on the characteristics of two-level detonation structures arising under non-monotonous heat release.

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