Parametric Study of Double Cellular Detonation Structure

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1 Abstract

A parametric numerical study of detonation cellular structure is performed with a model gaseous explosive mixture whose decomposition occurs in two successive exothermic steps with markedly different characteristic times. Kinetic and energetic parameters of both reactions are varied in a wide range. Results present one-dimensional solutions for steady detonation and unsteady two-dimensional solutions of Euler equations. The range of governing parameters of both exothermic steps within which the double cellular structure is observed is identified for the considered model example. Since it is quite difficult to use detailed chemical kinetics in unsteady 2D case, our results should help to identify the mixtures and the domain of their equivalence ratio where double detonation structure could be observed.

2 Introduction

In some gaseous explosives containing NO_2 groups, i.e. in gaseous nitromethane with O_2 [1] or in mixtures of H_2, CH_4 and C_2H_6 with NO_2-N_2O_4 as an oxidizer [2,3,4], the so called "double cellular detonation structure" is observed when large detonation cells are completely filled by much smaller ones. Analysis of the structure of steady plane detonations in these mixtures based on the detailed chemical kinetics with 365 elementary reactions and 67 chemical species [4] shows that the heat release occurs in two exothermic steps with markedly different characteristic times. The first very fast step is mainly due to a reaction $NO_2 + H \rightarrow NO + OH$, its induction time is of the order of 0.1 μs. Depending on the composition of the mixture, the induction period of the second exothermic step can vary from O(1 μs) to O(100 μs). The two-level detonation structure exists however only in some domain of mixture equivalence ratio. Indeed, the detonation of gaseous NM, pure or mixed with oxygen, manifests a double cellular structure in the range of equivalence ratio Φ=1.3-1.75 [1]. In mixtures of gaseous nitromethane and tetranitromethane the two-level structure was observed at Φ=0.45 and Φ=0.84 but it does not exist in the intermediate domain of Φ [4] that shows that existence of two maxima of heat release rate inside the detonation zone is not sufficient to ensure the appearance of double detonation structure.

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In this work we study numerically a model mixture undergoing a two-step exothermic reaction (A➔B, B➔C). Varying its governing kinetic and energetic parameters we display both 1D steady solution and corresponding cellular structure for quasi-steady 2D detonation.

The examples demonstrate the change of the quality of the double-level structure, from "sharp" (as in [1-3,5]) to "weak" (as in [6]) up to its complete disappearance. Thus, these results should be useful to identify the mixtures and their equivalence ratio where the double detonation structure could be observed more or less easily.

3 Structure of Steady 1D Plane Detonations

The model mixture studied here is the same as we considered before [7], namely, for simplicity we assume that its molecular mass μ=0.0303 kg/mole, γ=1.25 and heat capacity c_v=1097.7 J/(kg·K) do not change in the course of the two-step chemical reaction A==>B and then B==>C. The total heat effect of both steps is Q=4.40286 MJ/kg and at first it is assumed that the fraction of heat released by the first step is q_1=0.5, i.e. in the "base line" set of governing parameters both reaction steps have the same heat effect $Q_1 = Q_2 = q_1 Q$ =2.20143 MJ/kg. Thus, at the initial pressure of P_o=0.05 bar and T_o=298K and in the case of complete reaction the detonation should propagate at the CJ detonation velocity D_{CJ}=2270.6 m/s with the CJ pressure P_{CJ}=1.423 bar and temperature T_{CJ}=4787 K. The shock front pressure and temperature are P_{ZND}=2.8 bar and T_{ZND}=2146 K (these two extreme temperatures correspond to the final and shocked states of the mixture in Figure 1a). However, if the second reaction step is so slow that it does not contribute at all to the detonation propagation, then it would propagate as the "low-velocity detonation" (LVD) with $D_{CJ\text{-}LVD}$ = 1636.2 m/s, $P_{CJ\text{-}LVD}$ =0.75 bar and $T_{CJ\text{-}LVD}$=2558 K, $P_{ZND\text{-}LVD}$=1.45 bar and $T_{ZND\text{-}LVD}$=1253 K.

The reaction rate constants of both steps are expressed as $K_i = Z_i \rho \exp(-E_i / RT)$ where i=1,2 and $Z_1^* = 2.08 \cdot 10^{11}$ m^3/(s·kg), $Z_2^* = 3 \cdot 10^8$ m^3/(s·kg), $E_1^* = E_2^* = 59808.6$ cal/mole (the standard values belonging to the base line case are marked with an asterisk). Thus, the reduced activation energy of the first step in the case of complete reaction is quite high, i.e. $\beta_1 = E_1 / RT_{ZND} = 14$.

Figure 1 shows profiles of temperature behind a shock front of steady detonation propagating at D_{CJ} in the base line case and their transformations when Z_i or q_1 are changed. The shape of temperature profiles in the considered model case is similar to that obtained with detailed chemical kinetics for the mixtures studied in [1-4]. Note that spatial coordinate is shown in a logarithmic scale. Hence, the induction length of the second step L_2 measured at the point where maximum value of temperature gradient is reached (Figure 1b) is nearly 20 times larger than L_1 of the first step. Decreasing (increasing) Z_1 by a factor of 2 makes the first step longer (shorter) by the same factor but does not change the second stage of the reaction. The induction period of the second step is also inversely proportional to Z_2. The smaller is the fraction of heat q_1 released in the first stage of the reaction, the longer is the first induction period and the smaller is the temperature at the beginning of the second reaction step, i.e. the more irregular should be the detonation structure corresponding to the slowest reaction step. Let us look now how these changes modify the detonation cellular structure.

4 Detonation Cellular Structure

The detonation cellular structure was obtained numerically by solving Euler equations in 2D slab case using the FCT technique [8] and an adaptation technique along the longitudinal X-coordinate. Numerical $N_x \times N_y$ grid (2000×2000 meshes in the standard case) consists of two parts: a uniform one in the leading detonation zone with 1000×2000 cells with a mesh size Δx=Δy=75 μm and a nonuniform one with also 1000×2000 cells but with Δx slowly increasing from right to left, while Δy=75 μm in both parts (a channel width is 150 mm). The traces of maximum pressure shown below correspond to

detonation run distances of at least 50 tube diameters where detonation propagation becomes steady and autonomous.

Figure 2 displays the double detonation structure for the "base line" case described in the first line of Table 1. Indeed, one can see the large detonation cells completely filled by the smaller ones. Large cells have slightly irregular structure but fit well the given channel with a width of 15 cm. The natural size of large cells is however slightly below 15 cm since similar calculations with a 45-cm width channel result in 3.5 large cells across the channel height. Apparently, the small cells filling up the larger ones correspond to the first fast reaction step and the large cells are produced by the slow second reaction step. Cell width of smaller cells λ_1 which one can distinguish in the middle of the larger cells (with a size λ_2) is of about 5 mm, which equals to 67 mesh sizes. The cellular structure for the same case as in Figure 2 but with two times better resolution ($\Delta x=\Delta y=37.5$ μm) is shown in Figure 3. One can see that λ_1 (taken again in the middle of the large cell) is not changed while more details are distinguishable in the beginning of the large cell. Hence the principal resolution is sufficient for making the further analysis of sensitivity of the cellular structure to its governing parameters.

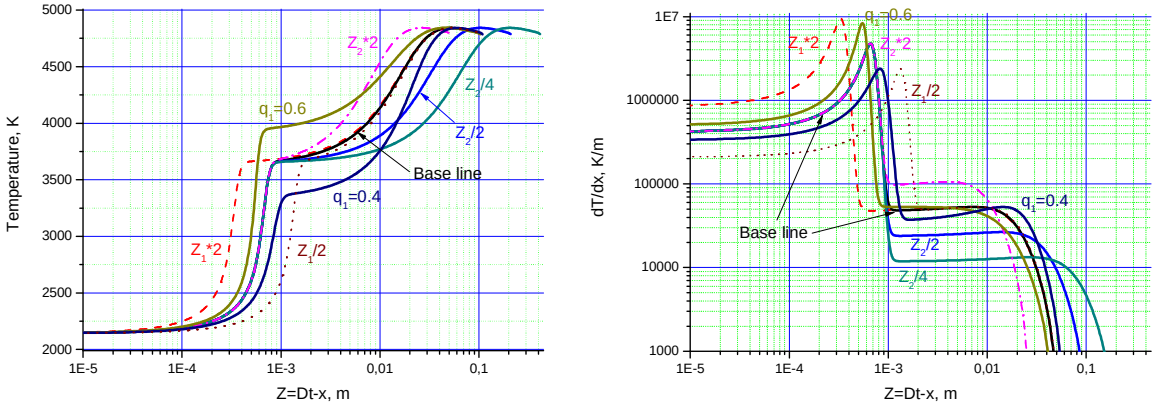

Figure 1. Effect of kinetic and energetic parameters on profiles of temperature (left) and its gradient (right) behind a steady plane detonation wave propagating at D_{CJ}=2270.6 m/s.

Figure 4 shows "extreme" detonation structures one could observe in the considered mixture when the second reaction step is either very slow or very fast. In the first case the second reaction step does not support the detonation wave which thus propagates at the LVD velocity close to 1636 m/s. The corresponding detonation structure reminds well that described by Manzhalei [9], when small cells are induced in the beginning of each "large" cells. The cell width corresponding to this "native" LVD detonation is of about 300 mm. However, in the case of double cellular structure in Figure 2 or 3 the same reaction prints much smaller cells since instantaneous detonation velocity at the beginning of large cells amounts to 3000 m/s and hence the detonation wave is strongly overdriven in respect to the LVD case. In another extreme case with very large Z_2 the total reaction heat is released just in one step and thus just a single regular detonation structure is observed (Figure 4b) with λ_1 of about 5 mm.

Table 1 lists the values of governing parameters of the model in different runs and briefly describes the corresponding detonation structures. Let us consider at first the effect of variation of Z_2. When the second reaction rate is made 2 times slower the double structure remains unchanged at first. Further decrease of Z_2 by 2 results in propagation of half-cell (Figure 5a) in the channel. Hence, as expected, the large detonation cells can adapt to the channel thickness After six-fold decrease of Z_2 the double structure becomes quite weak and it disappears completely after eight-fold decrease of Z_2 (even in two times larger channel) - see Figure 5b. Thus, for a given channel thickness a harmonization between the two cell networks disappears if the ratio of induction periods L_1/L_2 becomes too small. However, we have already seen above that the double structure cannot exist if this ratio becomes of

the order of 1 (Figure 4b). Indeed, only single structure is observed after a two-fold increase of Z_2, hence in the considered example the double structure exists when L_1/L_2 ranges from ≈0.01 to ≈0.1.

When the first reaction is made faster by a factor 2 and 4 due to an increase of Z_1 the double structure exists but one can hardly measure λ_1 due to a lack of numerical resolution. A decrease of Z_1 erases the difference between L_1 and L_2 and the double structure again rapidly disappears according to a former estimate of the range of ratio L_1/L_2.

A decrease of q_1 to 0.4 makes the double structure at first sharper than in the standard case, but at q_1=0.3 the double structure is replaced by a single one of Manzhalei kind (Figure 6a). An increase of this parameter (to q_1=0.6) makes the double cellular structure weaker but more regular (Figure 6b).

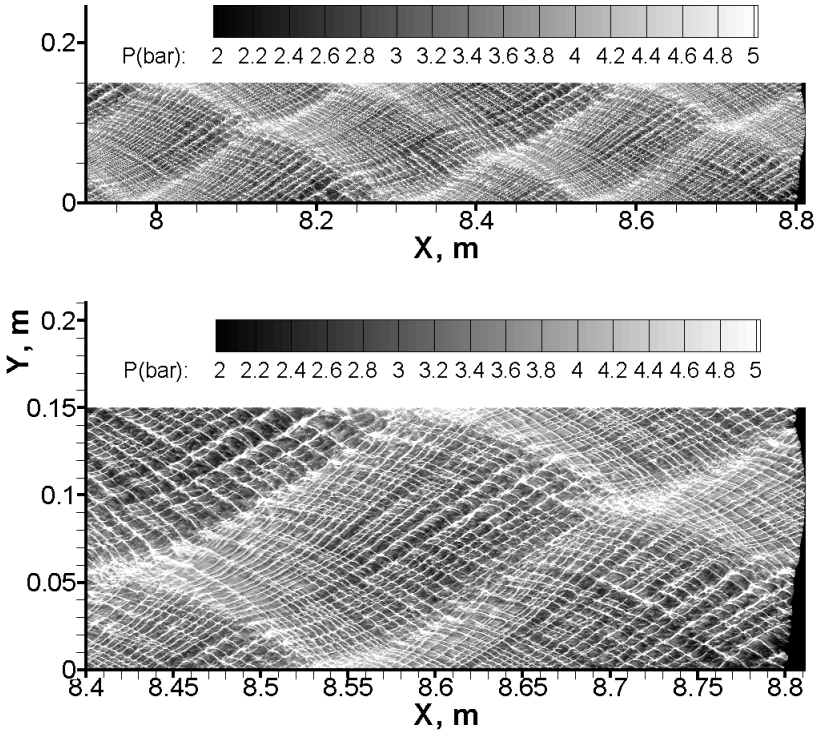

Figure 2. Detonation structure in the standard case (above) and its zoom (below)

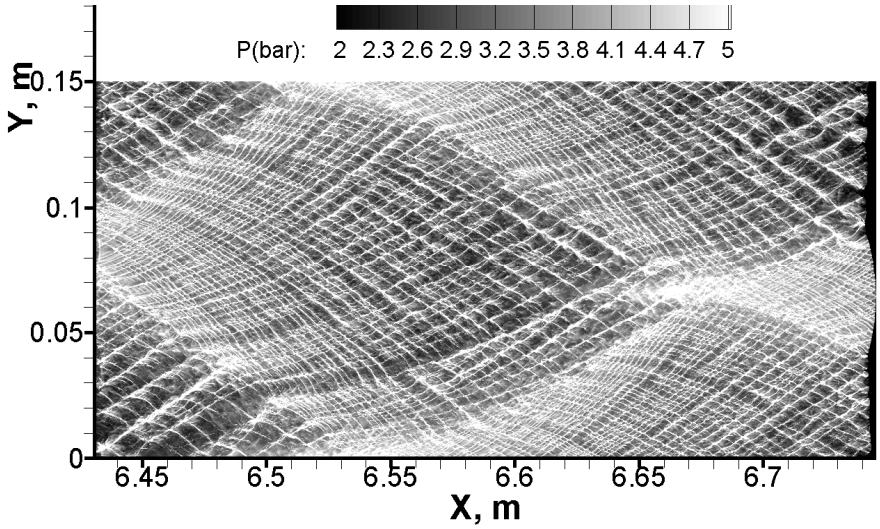

Figure 3. The detonation structure in the same standard case as in Fig.2, but at two times better resolution.

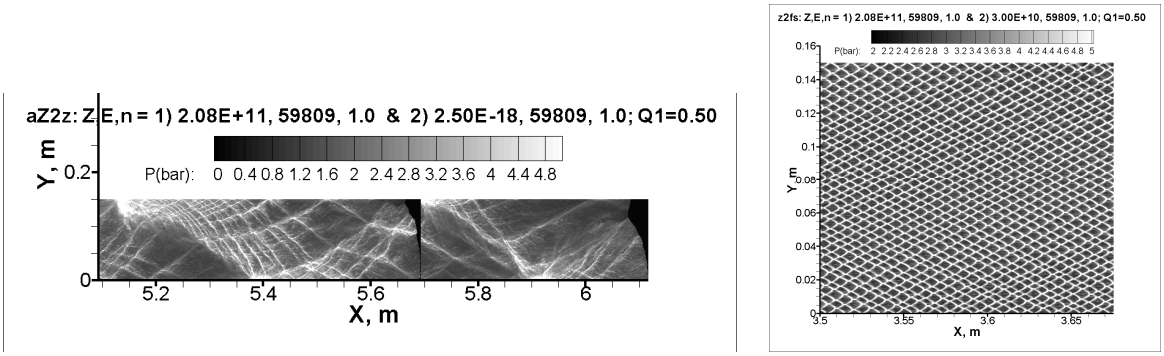

Figure 4. Extreme detonation structures at very small (left) and very large Z_2 =3E10 (right).

Table 1: Governing parameters and resulting detonation structure (channel thickness H=150 mm)

Z_2 / Z_2^*	q_1 / 0.5	λ_1, mm, ≈	λ_2, mm	Comment on the structure
1	1	5	150	Standard case: large cells are quite irregular
0.125	1	5	-	Single structure
0.167	1	10	300	Weak double structure, half-cell case
0.25	1	5	300	Half-cell per channel width
0.5	1	5	150	Double structure is more regular than the "standard" one
0.833	1	5	150	"Good" double structure
1.5	1	7.5	100	Double structure but weaker than standard one
1	1.4	5	-	No double structure
1	1.2	5	100	"Good" double structure but weaker than in the standard case
1	0.8	-	150	Sharp double structure but λ_1 could not be measured (insufficient resolution)
1	0.6	-	-	Single Manzhalei kind structure
0	1	300	-	LVD at D=1636 m/s: very irregular single structure of Manzhalei kind, half-cell in the channel
100	1	5	-	Single very regular structure

It is clear that the double detonation structure should disappear if the fraction of heat released by a first step (q_1) becomes too small or approaches 1. Hence this energetic parameter also has some optimum range of values most favorable for observing the double cellular detonation structures. Apparently, here it is close to 0.5, but it is worth to remind that in our example the mixture did not change its properties in the course of chemical reaction.

Conclusions

The numerical study of detonation structure in the model but typical example of two-step heat release demonstrates the change of the quality of the double-level structure, from "sharp" to "weak" up to its complete disappearance. It is shown that double structure exists when the ratio of induction zone lengths of the first and second reaction step ranges from ≈0.01 to ≈0.1. The optimum ratio of heat effects of both reaction stages seems to be close to 1.

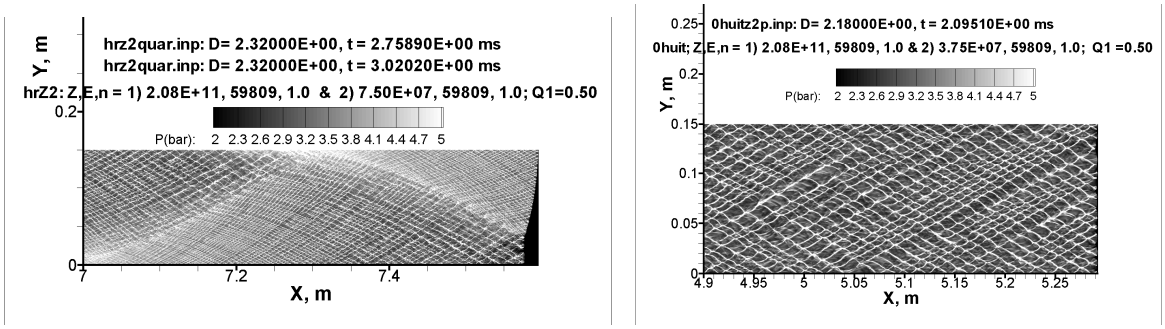

Figure 5. Detoantion structures at a) $Z_2 / Z_2^* = 0.25$ (left) and b) $Z_2 / Z_2^* = 0.125$ (right).

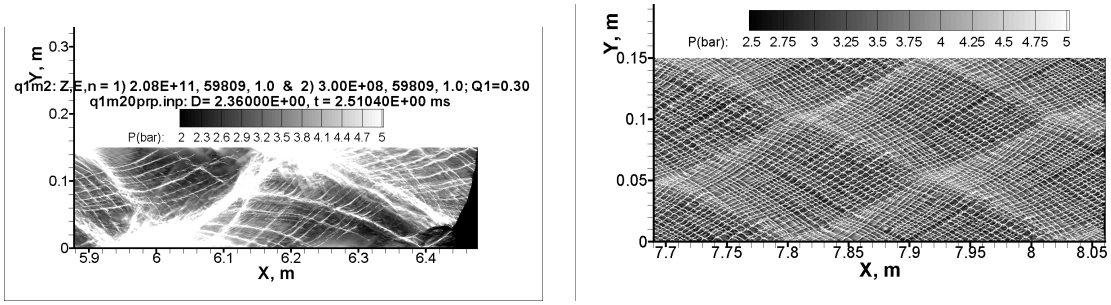

Figure 6. a) Detonation structure at q_1=0.3 (left) and b) q_1 =0.6 (right).

References

[1] Presles HN, Desbordes D, Guirard M, Guerraud C (1996). Gaseous nitromethane and nitromethane-oxygen mixture, a new detonation structure, Shock Waves 6:111-114.

[2] Desbordes D, Presles HN, Joubert F, Gbado Douala C (2004). Etude de la détonation de mélanges pauvres H_2-NO_2/N_2O_4, C.R. Mécanique 332, 993-999.

[3] Joubert F, Desbordes D, Presles HN (2008). Detonation cellular structure in NO_2/N_2O_4–fuel gaseous mixtures, Combustion and Flame, 152, 482-495.

[4] Presles HN, Virot F, Desbordes D, Khasainov B (2010). Double cellular structure in the detonation of lean mixtures containing NO_2 groups. 19th International Shock Interaction Symposium, Moscow.

[5] Djeballi N, Chaumeix S Abid, Paillard CE (1997) Shock tube study of the nitro-methane decomposition and oxidation, 21st Symposium on Shock Waves, 1, 121-126.

[6] Vasil'ev A, V.Vasiliev V (2009) Ammonia: Detonation Hazards, Multi-Structure. Proceedings of the ECM 2009 FOURTH EUROPEAN COMBUSTION MEETING, 14 - 17 April 2009, Vienna University of Technology, Vienna, Austria, paper No 057.

[7] Guilly V, Khasainov B, Presles HN, Desbordes D (2005) Numerical Simulation of Detonations with Double Cellular Structure. C. R. Mecanique XXX.

[8] Oran ES, Boris JP (2001). Numerical Simulation of Reactive Flow, 2nd edn. Cambridge University Press, Cambridge.

[9] Manzhalei VI (1977) Fine Structure of the Leading Front of a Gas Detonation. Fizika Gorenia i Vzryva 13(3): 470-472.