Chemical Spike in Multiheaded Detonation

Anatoly A. Vasil'ev[1], Anatoly V. Trotsyuk[2]
[1]Lavrentyev Institute of Hydrodynamics SB RAS, Novosibirsk, Russia
[2]Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

Corresponding author, A.A. Vasil'ev: gasdet@hydro.nsc.ru

Introduction

Many years ago when the multifront DWs were observed in every gaseous mixtures the problem of application of one-dimensional ZND-model for description of parameters of multifront DW was discussed widely among specialists. It was established that some global parameters of multifront DW (velocity, products pressure,...) are well predicted by ideal ZND-model with plane DW-front. But such important parameters as local temperature, pressure, density, etc. are differed strongly for different segments of DW-front, and so the change of such strongly differed local states on state with homogeneous parameters as in ZND-model is incorrect. Nevertheless 1D calculations with schema of detailed kinetics are used widely up to now for estimation of induction and reaction zones in 1D-wave. Such calculations allow to estimate in principle the size of chemical spike in ideal ZND-model. The main question is the next: how this size of ideal 1D-wave correlates with size of chemical spike in real multifront DW? Another questions: how experimental size of chemical spike correlates with modern 2D calculation of multifront DW? These problems are the object of given paper.

Experimental investigation and results

Experimental investigation of chemical spike in multifront DW was carried out with the help of pressure gauges located along the detonation tube (diameter 80 mm, length 5500 mm) and on its end (DW-reflection). The gauge (zirconate-titanate-lead ceramics) for reflected DW was 10 mm diameter, 0.25 mm thickness, capacity about 700 pF, sensitivity 0.25 V/atm, resolution time 50 nsec. Oscilloscope has input resistance 1 MOm, bandwidth 25 MH, RC constant 700 μs. Typical oscillogram is demonstrated on Fig.1 (scanning 0.5 μs/div).

On Fig.2 the dimensionless ratio of size z_0 of chemical spike of multifront DW to cell size *a* is demonstrated for investigated mixtures at different initial pressure P_0 (atm). Value z_0 defines as $z_0 = Dt_0$, where D – velocity of multifront DW, t_0 – duration of zone with pressure higher then CJ pressure on oscillogram type as on Fig.1.

One can see that dimensionless ratio values differ for investigated mixtures, what means that cells in such mixtures are not strongly similar ones another. Such conclusion follows also from inconstancy of this ratio at increasing of initial pressure.

Two points of view are known on cell problem: first was based on assumption about some proportionality among cell size and length of induction zone of ideal CJ DW with plane front (Tshelkin, Westbrook, ...); second was based on assumption that such proportionality was artificial and the real multifront structure must be take into account at calculation of cell size. In first case the simplicity of calculation of length of induction time for ZND DW with plane front and assumption about linearity are the main arguments of application of such

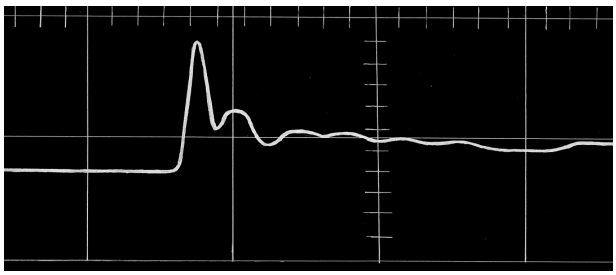

Figure 1.

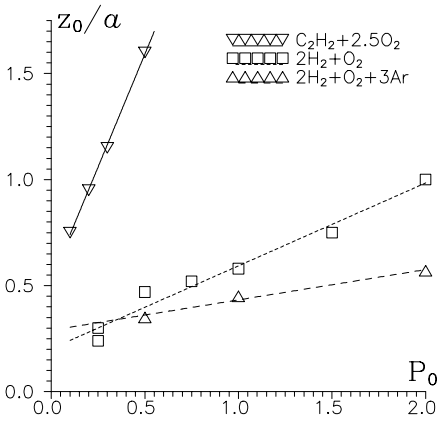

Figure 2.

method for estimation of cell size. Of course, this method and coefficient value were checked on some mixtures: among experimental cell size and calculated length of induction zone for ideal Chapman-Jouguet DW the proportionality can be ascertained in some range of defined parameters, for example, at near-stoichiometric concentrations. But the coefficient of such proportionality is not constant for wide range of parameters. Second point of view is based on real structure of multifront DW and not considered the stationary ZND model.

The cell size and length of induction zone demonstrate the more complex dependence then linear. Possibly, it connects with assumption that cell size is proportional only induction zone without taking into account the reaction zone. Because in DW the two character times are existed, then the account of both times is physically more correct. The reaction time can be ignored when its value is much lower the induction time. For example, it can be registered in mixture with high effective promoter, because the promoter practically not influence on reaction time, but can decrease sufficiently the induction time. And at some parameters the induction and reaction times become commensurable.

Numerical simulations

Two-dimensional numerical simulations of the multi-front (cellular) structure of DW in the stoichiometric hydrogen-oxygen-argon gaseous mixture were performed in a wide range of initial pressure and argon concentrations [2,3]. A good agreement between calculated detonation cell width a_0 and experimental data was obtained. The objective of the present study is to investigate numerically the reflection of the multifront DW (propagating in a plane rectangular channel with width $H=a_0$) from the closed end at different phases of transverse waves movement on the leading front. The history of the pressure value on the reflected wall of averaged over the channel width H, obtained in these simulations, is similar to experimental data on Fig.1 (see also [1]).

The dynamics of the compressible medium was described by two-dimensional unsteady Euler equations. Chemical transformation in gas mixture was described by a two-step reaction model (including the induction step and the heat release step). The resultant hyperbolic system of equations was solved numerically using the finite-volume scheme with the fourth-order MUSCL TVD reconstruction and the advanced HLLC algorithm for an approximate solution of the Riemann problem. For the implementation of this algorithm for the case of a chemically reacting mixture, the ”energy relaxation method” was used. Integration in time

was performed with second-order accuracy by using recently developed additive semi-implicit Runge-Kutta methods. The use of adaptive moving grids with local refinement allowed us to have a fine resolution where necessary (in our case – in the vicinity of a leading shock front), using a significantly smaller number of cells, as compared with a uniform splitting of the computational domain. Implementation of these kinetic models and numerical methods for 2D numerical simulations of multifront (cellular) structure of detonation waves is described in more details in [2,3].

Results of computations

Figure 3 shows the front structure of the DW in $2H_2 + O_2$ mixture at the initial pressure p_0=0.2 bar and temperatureT_0= 298.15 K. The DW propagates in a channel with a width equal to the detonation cell size, $H=a_0$=0.64 cm. The different stages of the transverse waves periodically movements on the leading shock front are shown on the distance, equals the detonation cell length. The DW front positions from initiation source are 13.48 cm, 13.75 cm, 14.03 cm, 14.30, and 14.58 cm, respectively (see Fig.3). At these distances a reflection of DW from rigid wall, normal to the channel, are simulated.

The pressure history on the reflecting wall, averaged over channel width *H*, is obtained for each of the front structures shown on Fig3. It is found, that for all cases the difference between the pressure profiles is very low. The most deviation is found for the front structures Fig.3a and 3b (see Fig.4). From these data, it was estimated the value of duration t_0 of elevated pressure at normal reflection of DW: $t_0 \approx 5.0$ μs (see Fig.4).

At present, the numerical study of DW reflections is being carried out for the larger distances of DW front and different values of initial pressure p_0.

Conclusion

The results of experimental investigation and 2D numerical modelling on chemical spike in multifront detonation wave are presented. It was established, that dimensionless ratio of length of chemical spike in multifront DW to detonation cell size increases with growth of initial pressure value.

Acknowledgements

Work has partial financial support from Russian Foundation of Basic Researches.

References

1. Vasil'ev A.A. "Length of chemical spike in multifront detonation"(in Russian), *Combustion, Explosion and Shock Waves*, vol. 14, No. 4, pp. 138–140 (1978).
2. Trotsyuk A.V. "Numerical simulation of the structure of two-dimensional gaseous detonation of an $H_2 – O_2 – Ar$ mixture" (in Russian), *Combustion, Explosion and Shock Waves*, vol. 35, No. 5, pp. 549–558 (1999).
3. Trotsyuk A.V. "Numerical simulation of the structure of two-dimensional detonations in $H_2 – O_2 – Ar$," In: *Gaseous and heterogeneous detonations: Science to Applications*. Eds. G. Roy, S. Frolov et al., ENAS Publ., Moscow, 163–178 (1999).

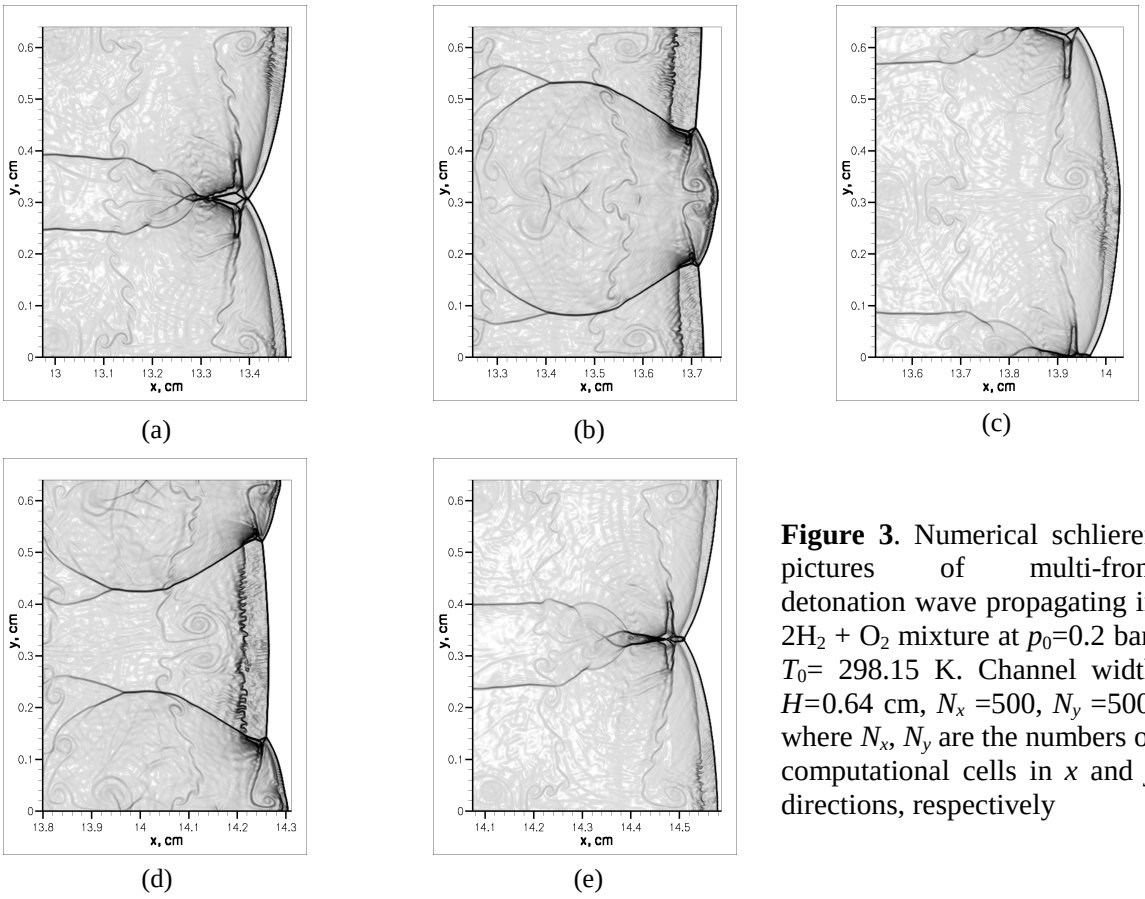

Figure 3. Numerical schlieren pictures of multi-front detonation wave propagating in $2H_2 + O_2$ mixture at p_0=0.2 bar, T_0= 298.15 K. Channel width H=0.64 cm, N_x =500, N_y =500. where N_x, N_y are the numbers of computational cells in x and y directions, respectively

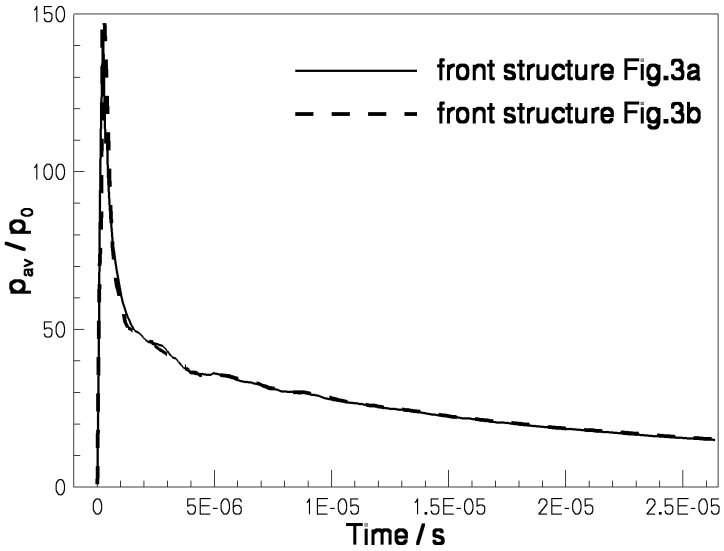

Figure 4. Dependency of the pressure p_{av} on the right rigid boundary, averaged over channel width H, on the time, when the detonation wave reflects from the closed channel end with the front structures, shown on Fig.3a and Fig.3b.