Self–Organisation of Multifront Structure in Expanding Detonation Wave

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Origin and destruction of ordered structures in chemically active medium is the major problems of the theory of dynamic systems. The multifront detonation wave (DW), stationary propagated in reacting gas mixture, is an example of such system with complicated threedimensional cellular structure of DW-front. The experimental fact is known that the cellular structure is observed in expanding (divergent) DW of any symmetry also, and the cell size *a* in such wave practically does not vary at increasing of a wave radius. Nontriviality of similar periodicity for divergent DW must be especially underlined, because of it requires as a minimum of the co-ordinated origin of new microexplosions and new transverse waves, ensuring a constancy of a multifront structures characteristic size at increase of a wave radius.

Many physical aspects and mechanisms of non-stationary interactions of the elements of DW-front remain not clear with reference to expanding waves. At the same time two-dimensional modelling of DW-structure in the channel of a constant cross-section has achieved such level, when the basic parameters of DW-cell are calculated quite surely [1-3].

In this paper the physical mechanisms of self-organisation of an ordered structure of DW– front at its constant expansion are discussed on the base of experimental investigations and numerical modelling of cylindrically expanding DW. In experiments these DWs are formed at transition of DWs from the channel of a constant cross-section into expanding channel with linear generatrix.

In present paper the dynamics of compressible chemically reacting medium is described by two-dimensional Euler equations. Chemical transformation of substance is modeled by the two-step model: induction and energy-release stages. For induction stage the experimental kinetics [4] governed by Arrhenius equation is used. When the induction period ends, the stage of heat-release has to be started. This stage is described by approximate model of chemical reactions at high temperatures [5-7] together with the caloric equation of state [8]. The equation of state for an ideal gas is used as the thermal equation of state. The application of this model is described in more details in [2].

The given hyperbolic system of equations has been solved numerically. The following space discretization has been performed. The adaptive moving stretched grid [2] has been used in the *x* direction (along the plane channel). A part of the grid with a uniform distribution of nodes formed a zone with small cells and covered the flow region near the DW front with large gradients of parameters. The remaining cells with a non-uniform distribution of nodes occupied the region from the closed left end of the channel to the beginning of the first zone. In each vertical section of the channel, the nodes along the *y*-axis were arranged non-uniformly so as to make possible a periodic increasing a number of cells as channel width increased. The maximum number of grid cells was $N_x \times N_y = 150 \times 400$.



The system of governing equations was solved with the application of MUSCL TVD schemes. We used the fourth-order scheme [9, 10] to calculate the fluxes along the x-axis in the uniform grid zone, and a third-order scheme [11, 12] was used in the non-uniform grid zone. The fluxes along the y-axis were calculated by the scheme [11, 12]. The details on the numerical method and time integration can be found in [2].

Implementation of the MUCL scheme requires the solution of the Riemann problem for finding the fluxes through the control volume faces. The new modern algorithm of solving this problem has been used in present calculations – the HLLC method [13]. Its realisation for a case of chemically reacting gas has been conducted using an Energy Relaxation Method [14].

The results of simulation of DW propagation from a channel with initial width $H = a = a_0$ to linearly expanding channel are shown on Figs.1–4. All tests have been performed for a $2H_2+O_2$ mixture at $p_0=0.2$ bar and $T_0=298.15$ K. In [2] the detonation cell size for this mixture at this initial condition is calculated as a=0.6 cm. An angle of a divergent is 10°. In all figures, the density isolines, which refer to the level $\rho / \rho_0 = 1$, 1.5, 1.5·1.1, 1.5·1.1², ... are shown. A visualisation of density field fixes all flow singularities more precisely. The scales of the x and y-axes are equal, but the y-axis is labelled in a_0 units.

Figure 1 shows initial stage of DW propagation in expanding channel. One can see the reflections from top and bottom channel walls of two equivalent transverse waves moving in opposite direction over the leading DW front. Channel width at this moment is $H = 1.1 a_0$. On Fig.2 it is seen still only one pair of transverse waves instead of two pair that must be formed in channel with constant $H = 2 a_0 [2]$. The intensity and shape of these waves are different.

Figure3 can give the answer to a question about causes of origin of new transverse waves. In this moment ($H = 3.6 a_0$) the perturbations of flow parameters are fixed in the induction zone behind overdriven elements of detonation front (points A and B on Fig. 3). The further growth of these perturbations leads to formation of a new pair of transverse waves. Interaction of new transverse waves with already existing waves leads to distortion of the last and to process of further formation of newer transverse waves.

On Figure 4 channel width is $H = 4.5 a_0$. Here one can see much greater number of transverse waves (at least five), that are different in a size and intensities. These waves form the extremely irregular structure. Thus, sudden spasmodic magnification of number of



transverse waves in DW structure takes place during constant smooth growth of the channel width.

The possible mechanisms of origin and destruction of regular structures in expanding detonation wave are discussed also. Calculated results are compared with experimental data.

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References

- 1. Oran E.S. The structure of propagating detonations // Gaseous and Heterogeneous Detonations / G. Roy, S. Frolov et al. (Eds). Moscow: ENAS Publ., 1999, P.97 120.
- Trotsyuk A.V. Numerical simulation of the structure of two-dimensional detonations in H₂ - O₂ - Ar // Gaseous and Heterogeneous Detonations / G. Roy, S. Frolov et al. (Eds). Moscow: ENAS Publ., 1999, P.163 - 178.
- 3. Gamezo V.N., Vasil'ev A.A., Khokhlov A.M., Oran E.S. Fine cellular structures produced by marginal detonations // 28th Symposium. (Intern.) on Combustion, UK, 2000.
- 4. White D.R. Density induction times in very lean mixtures of D_2 , H_2 , C_2H_2 , and C_2H_4 with O_2 // 11th Symposium. (Intern.) on Combustion, Berkeley, P.147—154, 1966.
- 5. Nikolaev Yu. A. Model of chemical reactions at high temperatures // Combustion, explosion, and shock waves. 1978. V. 14, No.4, P. 468 471.
- 6. Nikolaev Yu. A., Fomin P. A. Analysis of equilibrium flows of chemically reactng gases // Combustion, explosion, and shock waves. 1982. V. 18, No.1, P. 53 – 58.
- Nikolaev Yu. A., Fomin P. A. Approximate equation of kinetics in heterogeneous systems of the gas--condensed-phase type // Combustion, explosion, and shock waves. 1983. V. 19, No.6. P. 737 – 745.
- Nikolaev Yu.A., Zak D.V. Agreement of models of chemical reactions in gases with the second law of thermodynamics // Combustion, explosion, and shock waves. 1988. V. 24, No.4, P. 461 – 464.
- Yamamoto S., Daiguji H. Higher-order-accurate upwind schemes for solving the compressible Euler and Navier-Stokes equations // Computer Fluids. 1993, V.22, No.2/3, P.259 - 270.

- 10. Daiguji H., Yuan X., Yamamoto S. Stabilization of higher-order high resolution schemes for the compressible Navier-Stokes equation //International Journal of Numerical Methods for Heat and Fluid Flow. 1997, V.7, No.2/3, P.250 274.
- 11. Lin S.-Y., Chin Y.-S. Comparison of higher resolution Euler schemes for aeroacoustic computations // AIAA Journal. 1995, V.33, No.2, P.237 245.
- Chakravarthy S. R., Osher S. A new class of high accuracy TVD schemes for hyperbolic conservation laws // AIAA 23rd Aerospace Sciences Meeting. Reno, Nevada, 1985. AIAA Paper No.85 - 0363.
- Batten P., Leschziner M. A., Goldberg U. C. Average-state Jacobians and implicit methods for compressible viscous and turbulent flows //J. Comput. Phys. 1997, V.137, P.38 - 78.
- Coquel F., Perthame B. Relaxation of energy and approximate Riemann Solvers for general pressure laws in fluid dynamics // SIAM J. Numer. Anal. 1998. V.35, No.6, P.2223 - 2249.