Numerical Simulation of Irregular and Double-Cellular Detonation Structures

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1 Introduction

Extensive experimental and theoretical researches of detonation in gases [1,2] showed that the real structure of the detonation front is significantly different from that predicted by the one-dimensional theory [3]. The flow behind a plane front of a detonation wave (DW) is unstable. Because of the growth of initial disturbances the leading front is no longer smooth and acquires a complex structure repeated in time. The main element of this structure is a triple configuration consisting of the Mach stem (overdriven DW), incident wave (decaying wave), and reflected (transverse) wave adjacent to them at the triple point [1,2].

Collisions of transverse waves moving over the DW front in opposing directions lead to the reproduction of the front structure in time. The trajectories of triple points are two intersecting families of lines that form a network of diamond cells. These detonation structures are fixed in the experiment on the soot imprints [1,2,4]. The transverse size of the cell, a_0, determined as the average distance between the trajectories of one family measured in the direction normal to DW propagation, is a characteristic size of the DW front structure.

Depending on their chemical composition and initial pressure in the reactive mixture, gas systems display different degrees of regularity of the cellular structure. Particularly irregular patterns are observed in the methane-air mixture, where it is rather problematic to identify a typical ordered spatial structure. The detonation cell size a_0 in this mixture can only be considered as a quantity averaged over various segments of the detonation tube and over numerous experiments.

An unconventional double-scale cellular structure of the detonation wave (DW) was observed in [5,6,7] in mixtures of nitromethane (CH_3NO_2)-oxygen and hydrogen-nitrogen oxide (NO_2/N_2O_4). In our previous publications [8,9], we put forward a hypothesis about the nature of the double-scale cellular structure; such a structure was first observed in numerical studies of hydrogen-oxygen mixtures with addition of hydrogen peroxide (H_2O_2). The proposed hypothesis facilitates the search for new mixtures with a double-cellular (bifurcational) DW structure.

The present work is aimed at numerical simulation of the multifront (cellular) structure of the DW in methane-based mixtures and mixtures such as H_2-O_2-H_2O_2 and H_2-O_2-O_3, based on approximate models of detonation kinetics for these mixtures.

2 Problem Formulation and Physical Model

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The dynamics of the compressible medium was described by two-dimensional unsteady Euler equations.

Chemical conversion of matter in the DW was described in accordance with approximate kinetic models that we developed for the above-noted gas mixtures within the framework of the two-stage mechanism of detonation kinetics (induction stage plus subsequent stage of main heat release), which was first proposed in [10]. The induction stage was described by empirical relations derived from the analysis of experimental data on ignition delays. The induction period for methane-based mixtures was calculated by the empirical formula obtained in [11]. The main heat release took place after the induction period. The changes in internal energy and all thermodynamic parameters of the gas were described at this stage by the equations of the model [12, 13], which was modified to be applied to the above-noted reactive gas systems.

The proposed models of detonation combustion kinetics are consistent with the second law of thermodynamics; the model constants have a clear physical meaning and are calculated from tabulated thermodynamic parameters of mixtures before 2D numerical calculations. The calculations of the Chapman-Jouguet DW parameters show that the models are fairly accurate. An advantage of this model is its simplicity and convenience of its using in multidimensional numerical gas-dynamic codes.

The system of governing equations was closed by the known thermal equation of state for an ideal gas.

DW propagation in a two-dimensional straightline channel was studied. The slip conditions (impermeable solid wall) were imposed on the upper, lower, and left boundaries of the channel [14], and the right boundary was subjected to the condition of an undisturbed initial state of the gas. The detonation wave was initiated near the left closed end of the channel and propagated from left to right along the x axis. The size and energy of the initiation source [15] were chosen sufficiently large to ensure a supercritical regime of DW initiation in examined mixtures. The problem of determining the minimum critical initiation energy was not considered in this study.

3 Numerical Method

The resultant systems of equations were solved numerically using the code based on the finite-volume scheme [14] with the fourth-order MUSCL TVD reconstruction [16] and the advanced HLLC algorithm [17] for an approximate solution of the Riemann problem. In implementation of this algorithm for the case of a chemically reacting mixture, the ”energy relaxation method” [18] was used. This method eliminates the problem of numerical solution of the Riemann problem for a medium with a complicated nonlinear equation of state (including that with a variable ratio of specific heats). Integration in time was performed with second-order accuracy by using recently developed additive semi-implicit Runge-Kutta methods [19]. The use of adaptive moving grids with local refinement in the vicinity of a leading shock front allowed us to have a fine resolution where necessary, using a significantly smaller number of cells, as compared with a uniform splitting of the computational domain. The special preliminary computations have been performed for studied mixtures to determine required numerical grid resolution that is needed to get grid-independent results. The time step was determined at each time layer of the solution from the stability condition [14]. In the present simulations, the values of the Courant number were CFL=0.3–0.4. The codes are parallelized with MPI library using the domain decomposition technique.

4 Results of Calculations

The numerical simulation was performed for a stoichiometric methane-air mixture under standard initial conditions. The simulated results are illustrated in Figs. 1-2, which show the numerical schlieren visualization of the flow field. The density gradient clearly features not only the shape of the leading shock front of the DW and the structure of transverse waves, but also the contact discontinuities. Significant changes in density at the end of the induction period, which are associated with the beginning of the main heat release stage, clearly show the two-dimensional structure of the DW induction region. The x and y coordinates are given in centimeters.

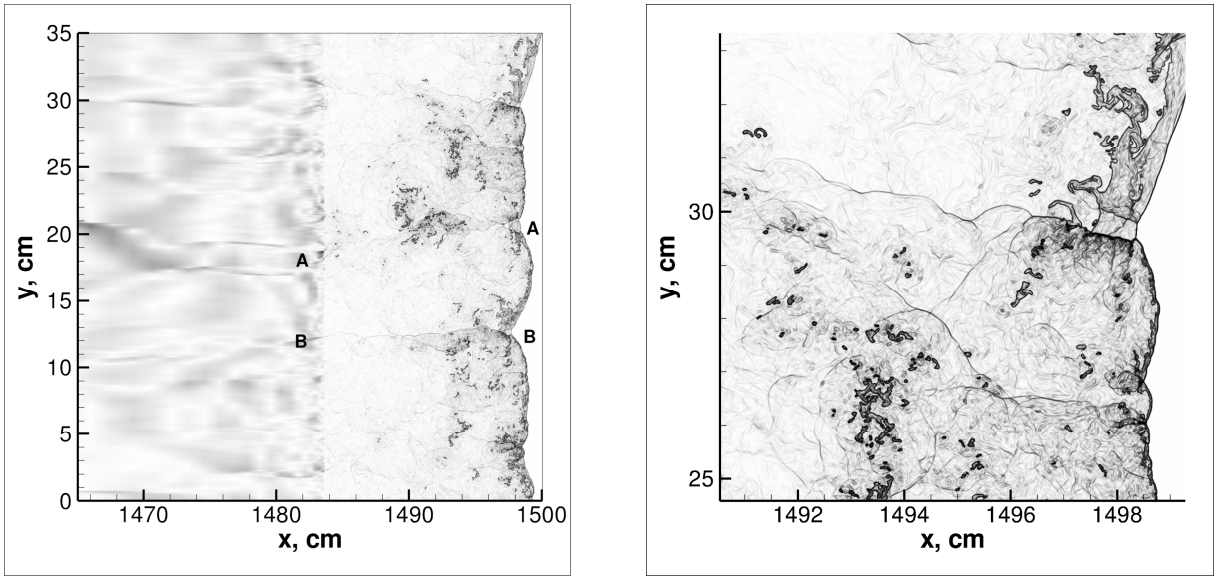

Figure 1. Detonation wave structure in a stoichiometric methane-air mixture in channel with H=35 cm at x_{front}=1500 cm. Left: Numerical Schlieren-visualization of all flowfield, one pair of primary transverse wave AA and BB. Right: Magnified fragment of the flowfield near an upper wall of a channel.

The detonation cell size for the methane-air mixture was determined in a procedure similar to that used in the numerical study of regular and double-scale cellular structures [8,9,15]. The two-dimensional DW structure was numerically simulated in a wide range of channel height H. Variation of the H in the computations affected the number of primary transverse waves (compare Figs. 1 and 2) remaining on the DW front after it reached the self-sustained Chanpam-Jouguet regime; thus, the cell size was determined.

Based on the analysis of the numerical Schlieren flow fields at different H, as well as density, temperature, and pressure fields, the detonation cells size in a stoichiometric methane-air mixture was found to be 33±3 cm. This value is in good agreement with all available experimental data for methane-air mixtures (see in [4,20,21]). The computations reproduced the irregular DW structure with all its basic specific features observed in experiments: random motion of the primary transverse waves, presence of secondary transverse waves on the leading shock front, which have a smaller size, but commensurable intensity, etc. Figure 1 (left) shows a pair of the primary transverse waves (AA and BB) forming the detonation cell. Multiple secondary transverse waves composing a hierarchy of DW front disturbances decreasing in size are clearly visible. Figure 1 (right) shows the fine cellular structure of the front of one transverse wave and multiple regions of the unburned mixture at a significant distance behind the DW front. Modeling of the irregular multifront structure was performed for the first time for a real hydrocarbon-air mixture with an adequate description of all thermophysical and chemical parameters of this mixture. The computations were performed on a fine grid with the grid cells size $h_y=h_x\approx$ 80 μm, and 256 co-processors were used.

2D numerical modeling of the multifront DW structure in a stoichiometric hydrogen-oxygen mixture containing additives of hydrogen peroxide (H_2O_2) and argon was performed. The computations were conducted at the initial pressures of the mixture p_0= 0.066 − 0.4 atm, H_2O_2 and argon concentrations up to 10 and 70 %, respectively, and initial temperature of 298.15 K. Figure 3 shows typical results of such computations. Figure 3 (left) shows the DW front structure in a mixture with addition of H_2O_2. Apart from a pair of intense and extended symmetric primary transverse waves, the leading shock front of the detonation wave has smaller and less intense secondary transverse waves (having approximately identical sizes and amplitudes). As is seen in Fig. 3 (right), these secondary transverse waves form their own cellular structure, which is fairly regular and is "nested" into the primary detonation cell.

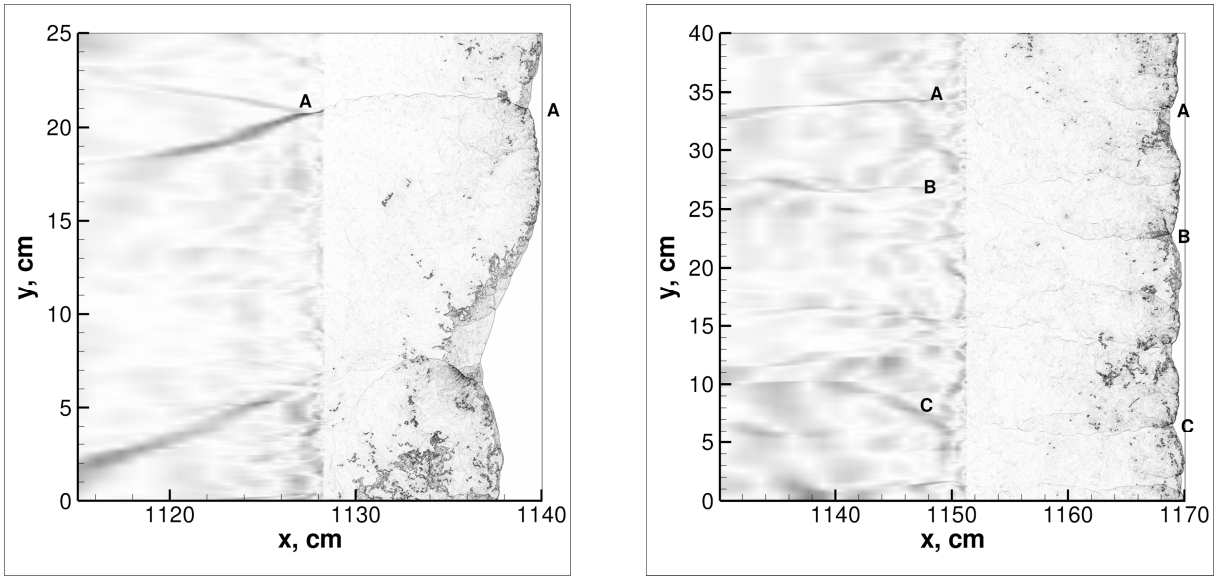

Figure 2. Numerical Schlieren-visualization of detonation wave structure. Left: In channel with H=25 cm at x_{front}=1140 cm, one primary transverse wave AA. Right: In channel with H=40 cm at x_{front}=1170 cm, three primary transverse waves AA, BB, and CC.

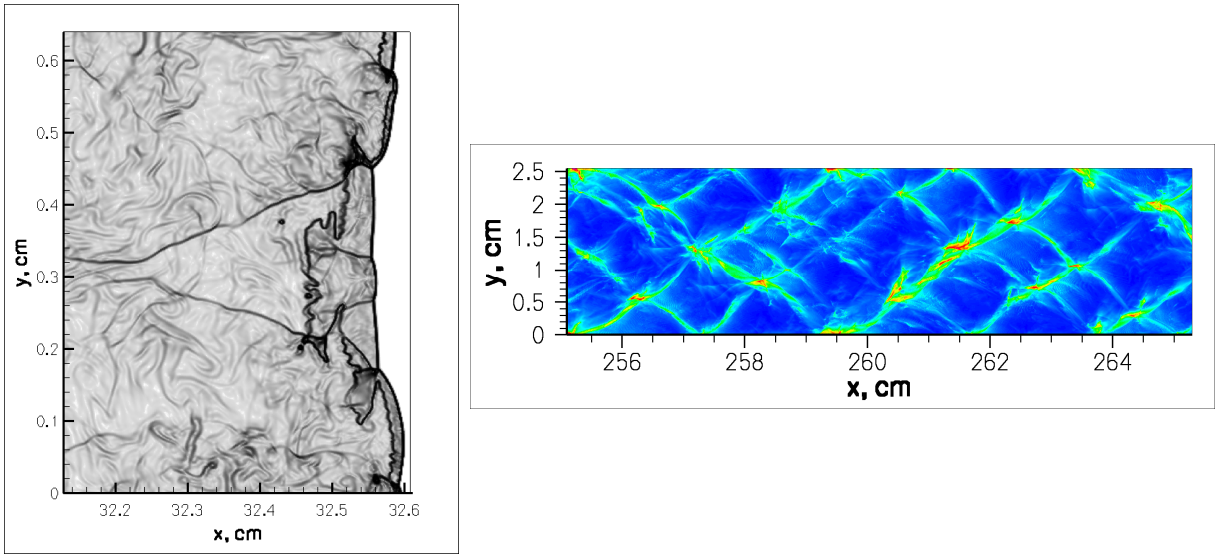

Figure 3. Mixture $2H_2+O_2+7Ar+1.1111\ H_2O_2$. Left: Numerical Schlieren-visualization of detonation wave structure in a channel with H=0.64 cm, p_0=0.2 atm. Right: Numerical soot tracks of detonation in a channel with H=2.55 cm, p_0=0.066 atm=50 Torr.

4 Conclusion

The conducted two-dimensional numerical simulation of the detonation front structure in a stoichiometric methane-air mixture revealed good agreement of the transverse size of the cell with available experimental data. The irregular cellular structure with all basic specific features (random motion of the primary transverse waves, multiple secondary transverse waves, which form a hierarchy of disturbances of the leading shock front of the detonation wave decreasing in size, regions of the unburned mixture at significant distances behind the DW front, and fine (cellular) structure of the transverse wave proper) was reproduced in computations for the first time for a mixture with realistic

thermophysical and chemical properties. The particular features of chemical kinetics in methane-air mixtures can be described by two-stage kinetic model. The use of this proposed model provides realistic results for the two-dimensional cellular structure of DW.

A multifront (cellular) DW structure with two sets (scales) of cells was obtained in hydrogen-oxygen mixtures with addition of hydrogen peroxide. Two-scale detonation structures were found in all examined mixtures with addition of H_2O_2 at different degrees of dilution by argon and at different initial pressures. We consider [8,9] that decomposition of H_2O_2 in induction zone, accompanies the process of heat release, leads to formation of double-cell detonation structure.

At present numerical experiments on detonation of hydrogen mixtures with addition of ozone O_3 are underway. We expect to obtain two-scale detonation cell structure in these mixtures.

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