NUMERICAL STUDY OF STANDING GAS DETONATION WAVES

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One of the most intriguing possibilities for supersonic propulsion is using a combustor based on a stabilized detonation wave (DW). This concept has substantial merits, however, the unstable nature of coupling between reaction zone and shock wave complicates its practical realization. Very rapid material and energy conversion is the key feature of detonations. This rapid burning or material conversion rate, typically tens of thousands of times faster than in flame, can offer several advantages for propulsion, such as more compact and efficient systems. Detonation engines should theoretically give the highest efficiency of transformation of thermal energy into kinetic energy. As shown by Zel'dovich [1], the combustion products have the minimal entropy in the case when combustion occurs in the detonation wave at the Chapman–Jouguet regime.

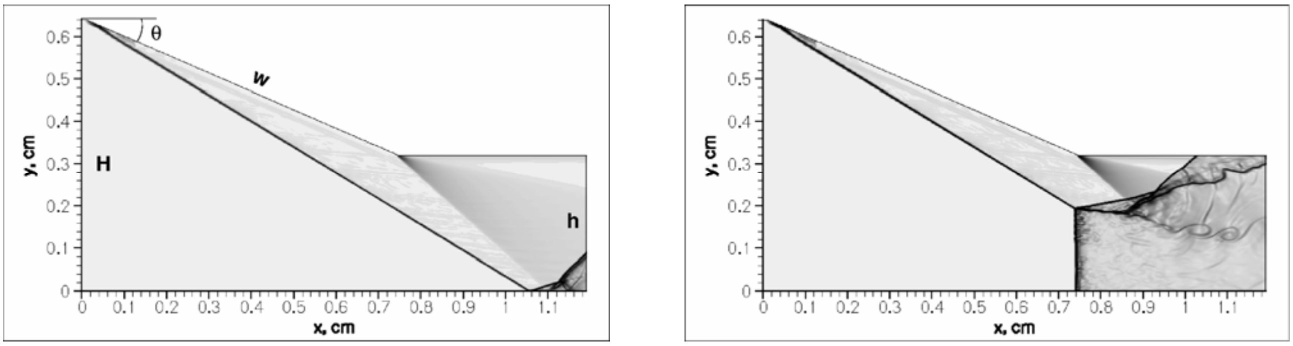
The proposals to use the detonation wave for propulsion appeared in the literature in the 1940s. Even in this early time, two different concepts were put forward. The use of standing (or stabilized) detonation waves was proposed in [1,2]. In the work [3], intermittent (or pulsed) detonation waves were explored in a propulsion device.

Subsequent evolution of the first approach led to development of various devices with the use of stabilized normal and oblique detonation waves. This field of extensive research is currently called the concept of Oblique Detonation Wave Engines (ODWEs). Application of such steady-state detonations to propulsion was explored, and performance comparable to conventional ramjets was reported for appreciably higher flight Mach numbers.

The works on the second approach, which are not less numerous, are united within the concept of Pulsed Detonation Engines (PDEs).

A number of experimental, theoretical, and numerical studies of these concepts were made during past years, and the interest in this subject has been recently renewed [4-14].

Little is known about steady detonation waves. The experimental evidence of their existence and stability are scant and contradictory [4], and the theory is far from definitive. Unfortunately, the most of experimental re-



(a) (b)

Fig. 1. Numerical Schlieren images of the flow field for M_{in}=7.0, θ=23.5°, and h/w=0.4: (a) regular reflection and (b) steady Mach reflection

sults can be properly interpreted as being shock-induced combustion rather than detonation phenomena [4].

The objective of the present study is to investigate numerically the feasibility of “stationary” detonation at the Mach reflection (MR) of an oblique shock wave generated by double wedge model a supersonic stream of hydrogen/oxygen mixtures. In nonreacting gas-dynamics, the flow structure in the case of regular (RR) and Mach reflection of shock waves (SW) and the criteria of transition between these types of reflection were studied in many theoretical, experimental, and numerical papers (see, e.g. [15-21]). As compared to reflection of oblique SW in inert mixture, the interaction of oblique SW and DW with each other, or a solid surface has not been adequately studied. We hope that numerical simulations can be used as a powerful tool for better understanding of this subject.

Formulation of the problem and physical model

The simulation was performed for a flow of a combustible mixture $2H_2 + O_2$ for p_0= 0.2 bar, T_0= 298.15 K, and different inflow Mach numbers M_{in}. A two-dimensional supersonic flow of the mixture over a compression body, which was a wedge with an angle θ and a length of the compression surface w, in a channel with an input cross section H and output cross section h was considered (Fig. 1a). In contrast to simulation of SW reflection in an inert medium, for chemically reacting flows there is some characteristic velocity, namely, the DW velocity in the Chapman-Jouguet (C-J) regime D_{CJ}, and an intrinsic length scale. The detonation cell width a_0 is often used as this length scale. Another commonly used length is the calculated thickness of an idealized one-dimensional steady reaction-zone structure of DW. For the given mixture and initial conditions, we have D_{CJ} = 2757 m/s and M_{CJ} = 5.13. A standing DW can be formed only under the condition that the inflow Mach number is greater than M_{CJ}. If this condition is violated, the DW (if detonation arises in the channel) propagates upstream, and the formation of a steady configuration is impossible. In the present simulation, we retained the value of H constant for any changes in θ and h/w. Thus, the mass flow rate entering the channel, i.e. $m_{in} = \rho_0 c_0 M_{in} H$, was constant for different channel geometries.

The dynamics of the compressible medium was described by two-dimensional unsteady Euler equations. Chemical transformations in the gas mixture were described by a two-step reaction model (including the induction step and the heat release step) [22]. The first (induction) stage was simulated in accordance with the experimental kinetics [23].

After the induction period, the stage of heat release was described using the model of generalized kinetics of chemical reactions at high temperatures [24,25] and the caloric equation of state [25], correlated with the adopted kinetic model with allowance for the second law of thermodynamics. We note that the proposed approach makes it possible to take into account substantial variations in the values of the mean molar mass of the mixture, heat release, specific heats, and their ratio in the course of chemical reactions. The system of equations was closed by the thermal equation of state for an ideal gas. Implementation of these kinetic models is described in more details in [32,33].

The boundary conditions on the different sides of the computational domain were as follows (see Fig. 1): a uniform supersonic flow is imposed on the left upstream side; supersonic outflow conditions are implemented on the right downstream side; nonpermeable conditions are specified on the upper solid wall; the lower side is an axis of symmetry so in the case of Eulerian approach it is equivalent to a perfect wall and nonpermeable conditions are taken at it. In implementation of these boundary conditions in the computational code, we used procedures described in [26].

Numerical method

The resultant hyperbolic system of equations was solved numerically using the finite-volume scheme with the fourth-order MUSCL TVD reconstruction [27] and the advanced HLLC algorithm [28] 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’’ [29] 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 [30]. In the present simulations, the values of the Courant number were CFL=0.2-0.3.

A body-fitted quadrilaterial grid was used with values of node numbers about N_x=600 and N_y=200 in the x and y directions, respectively. To ensure the independence of computational results on grid resolution, some of the runs were repeated with a doubled number of points in each direction. We found that the agreement between the coarse and fine grid results was very close.

Results of computations

Regular and Mach reflections of oblique shocks were analyzed by using detonation and shock polars (see Fig. 2). To obtain a detonation curve, a single-front model of the detonation wave was used for a model mixture with γ_0=1.4, γ_{CJ}=1.2, and M_{CJ}=5.13. The point IS in Fig. 2 indicates the state behind the incident oblique shock wave. This point is the origin of the reflected oblique SW polar, which intersects the detonation polar at the point MR. If Mach reflection with the detonation wave as MS is formed, this point determines the parameters behind MS and behind the reflected SW in the vicinity of the triple point. As is seen from Fig. 2, however, the same reflected SW polar intersects the ordinate axis at the point RR. This point corresponds to regular reflection and indicates parameters behind the

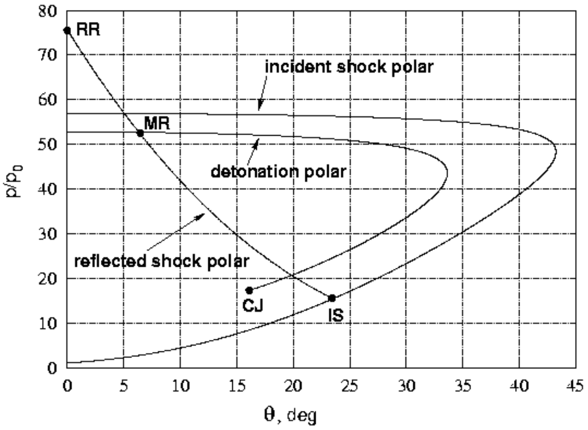
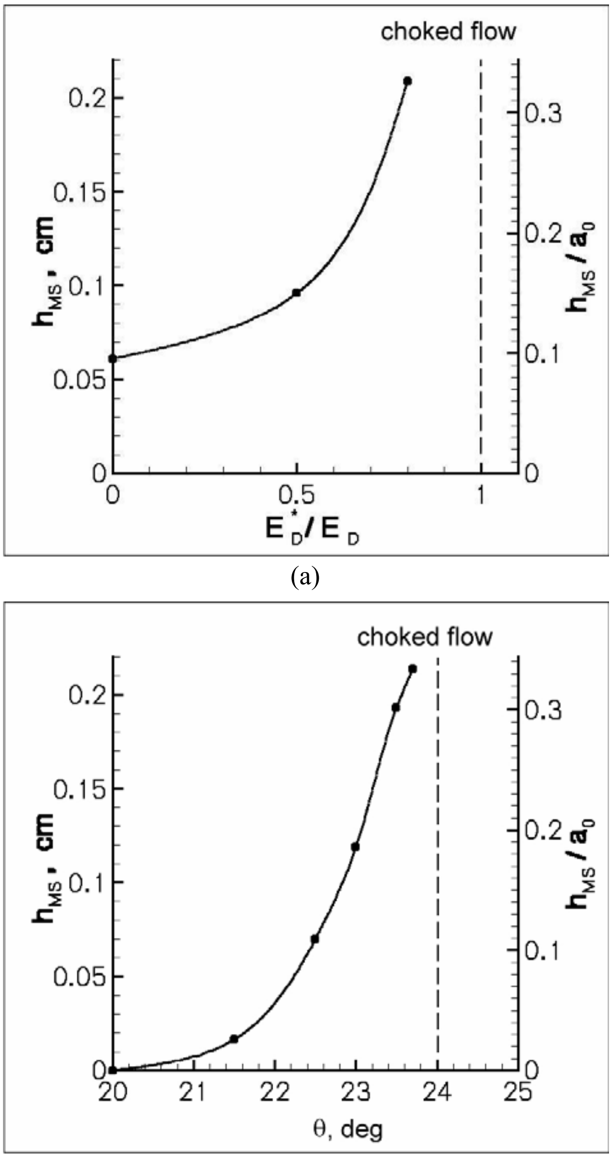


Fig. 2. Pressure vs deflection angle polar diagrams for M_{in}=7.0 and θ=23.5



(a)

(b)

Fig. 3. Mach stem height, h_{MS}, for M_{in}=7.0 and h/w=0.4 as a function of: (a) the amount of heat release in the model mixture (for θ=24.5°), (b) the wedge angle (for the normal mixture)

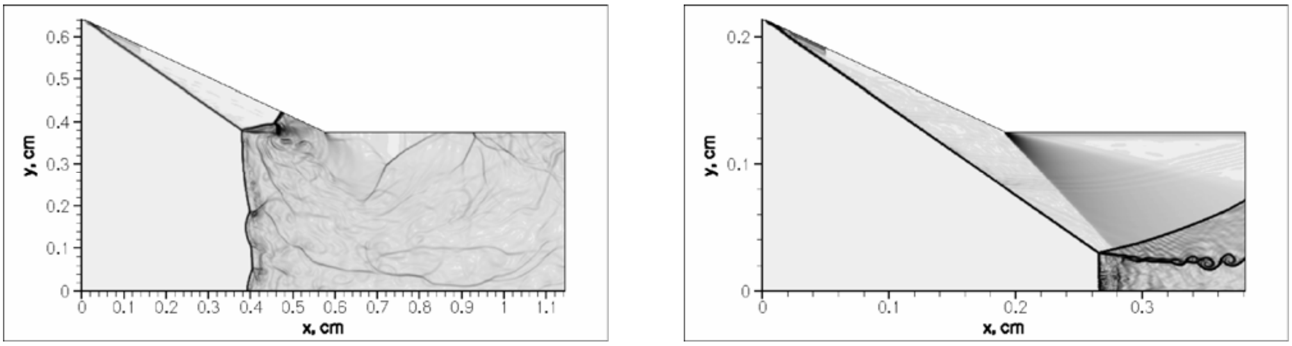
reflected SW in the vicinity of the reflection point. Thus, from Fig. 2, one can clearly see that the existence of both RR and MR is possible for identical flow parameters. This problem was investigated numerically in subsequent 2D simulations.

Figure 1a shows the numerical Schlieren visualization [31] of regular reflection of an oblique shock wave for a wedge angle θ=23.5° and inflow Mach number M_{in}=7.0. The flow structure is similar to RR in an inert medium [15, 19-21], except that there is a heat-release zone behind the reflected wave. The channel height was H=a_0, i.e., it was chosen to be equal to the transverse size of the detonation cell in a freely propagating unsteady multifront DW. The cell size predicted by our 2D numerical simulations [32] of the DW front structure for the specified mixture and initial conditions is a_0=0.64 cm. This value is in very good agreement with the experimental results.

Steady MR configurations were obtained for Mach numbers M_{in}=7.0 and M_{in}=8.0. In this case, the Mach stem is a smooth shock wave similar to the shock in an inert medium, with a subsequent induction zone and heat-release zone (see Fig. 1b). There are no transverse waves on the Mach stem; the stem is a standing and stable overdriven DW. The influence of the amount of heat release in the reaction zone on the MS height was studied (see Fig. 3a). For this purpose, simulations were performed for a flow of a model mixture with constants E_D smaller than E_D for the normal $2H_2$+O_2 mixture. This constant enters the heat-release kinetic model we use and determines the maximum value of heat that can be released in the reaction zone (see eqs. in [21, 22]); E_D =0 refers to an inert medium. The MS height increases with increasing amount of heat released, see Fig. 3a. Figure 3b shows the dependence of the MS height on the wedge angle θ for the normal mixture.

In Fig. 4a, one can see the case of Mach reflection for M_{in}=5.5. The flow structure behind the Mach stem is similar to the flow structure behind the front of a multifront (cellular) unsteady propagating DW [32]. There are unsteady transverse waves on the Mach stem, which are periodically reflected from the plane of symmetry and from the flow region in the vicinity of the triple point. The motion of these waves along the Mach stem changes its shape significantly.

In contrast to MR in an inert medium, the Mach stem for a chemically reacting flow is un-



(a) (b)

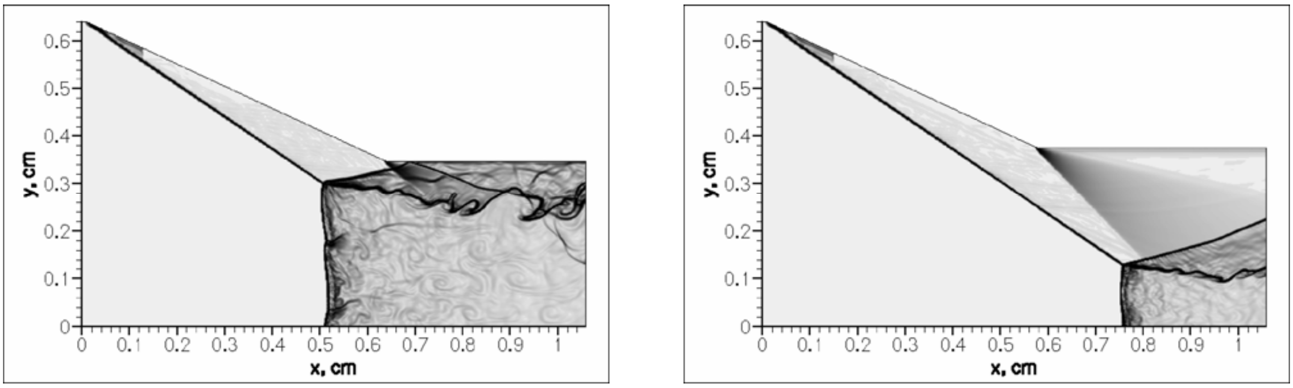
Fig. 4. Numerical Schlieren images of the flow field for M_{in}=5.5, θ=25°, and h/w=0.6: (a) unsteady multifront Mach stem at $H=a_0$ and (b) standing Mach stem with a suppressed multifront structure at $H=a_0/3$

steady for M_{in}=5.5. When Mach reflection is formed, the detonation front moves upstream or downstream. Our study revealed that, for fixed values of M_{in} and θ, h/w is the governing parameter. The simulations were performed for θ =25°. For values of h/w up to 0.7, the Mach stem inevitably moves upstream up to the inflow boundary. For this case, we have an unstarted two-dimensional converging nozzle (or choked flow). If h/w exceeds a certain critical value, the Mach stem arises, goes downstream, and vanishes, so we have RR as the final stationary configuration. This evolution of the flow was obtained for h/w=0.8. Hence, the critical value of h/w is between 0.7 and 0.8. The closer h/w to this value, the lower the velocity of upstream or downstream motion of the unsteady Mach stem, and the greater the CPU time needed for calculation of the final flow configuration. Based on these considerations, we believe that the Mach stem is in the state of unstable equilibrium for h/w exactly equal to the critical value. In addition, we cannot exclude the possibility of existence of a very narrow range of h/w values, where a standing MS can be formed for this value of M_{in}.

Subsequent studies showed that there may exist a standing MS with a system of unsteady transverse waves on its front, like that shown in Fig. 4a. The results of MR modeling for M_{in}=6.0 are shown in Fig. 5. Despite the existence of transverse shocks and their motion along MS and periodic changes in the stem shape, MS, on the average, is a standing wave that slightly oscillates near some equilibrium point. Comparing the MS front structures in Fig. 4a and Fig. 5, one can see that transverse waves in the second case are less pronounced and have a smaller length in the x direction (especially in Fig. 5b) than in the first case. This is explained by the higher degree of MS overdrive (i.e., M_{in}/M_{CJ}) for M_{in}=6.0. It was assumed that it is the existence of intense and extended transverse waves on the MS front for M_{in}=5.5 that leads to MR instability.

To verify the validity of this assumption, we simulated MR for two channels with the same θ and h/w and with identical flow parameters but different H, see Fig. 4. For the case $H=a_0$ (Fig. 4a), we have an unsteady multifront MS moving upstream up to the inflow boundary. For $H=a_0/3$, however, the flow structure is qualitatively different. The standing and stable MS has a smooth front, and there are no transverse waves at all (cf. Fig. 5b). Thus, a change in the flow scale leads to the formation of a steady MS. The characteristic flow size (MS height) in the second case is smaller than the intrinsic length scale of DW (i.e., detonation cell width on the front of the overdriven DW). This was the reason for suppression of the development of MS front instability and, as a consequence, for flow steadiness as a whole.

The influence of initial conditions to obtained final steady flow configurations, and the



(a) (b)

Fig. 5. Numerical Schlieren images of the flow field with a standing multifront Mach stem for M_{in}=6.0 and θ=25° at: (a) h/w=0.5 and (b) h/w=0.6

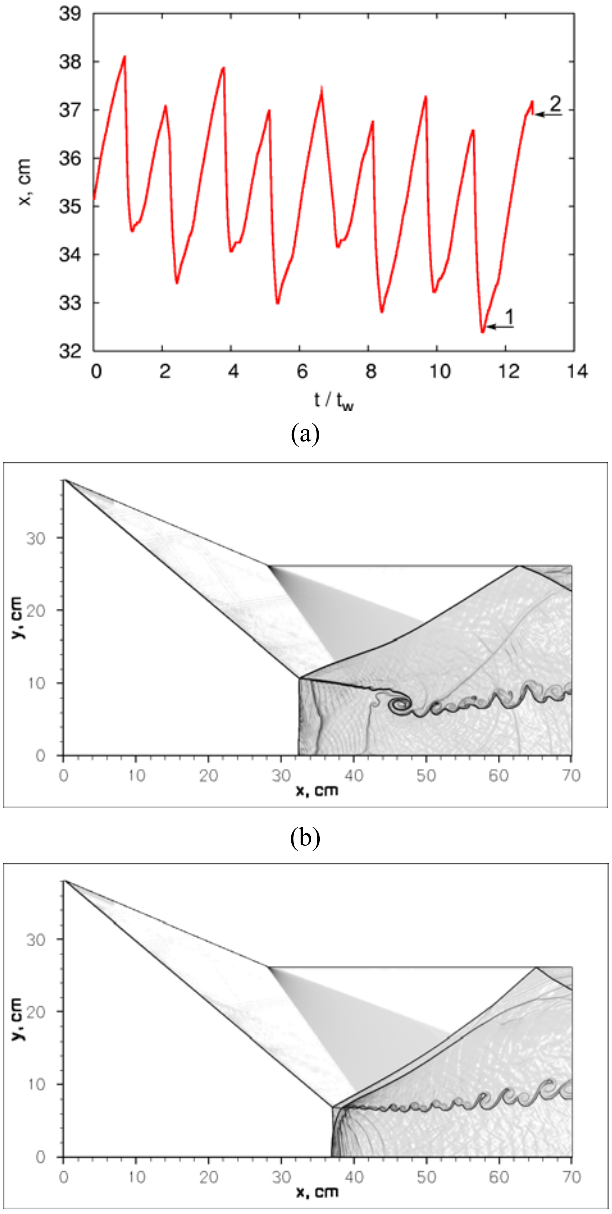
investigation of the transition from RR to MR under the local perturbations of the free-stream flow are described in [33].

We also simulated the flow of hydrogen-air mixtures. The size and geometry of the computational domain were chosen to correspond to the test section of the high-temperature, steady-flow, Mach 3 tunnel described by Gross and Chinitz [34,35]. We have θ=23°, h/w=0.8655, h=5.25 cm, and H=7.62 cm. These values were reconstructed with the maximum possible accuracy from photographs and schemes from the above-mentioned papers. For the lean hydrogen-air mixture $0.4H_2$ + 4.772 Air (equivalence ratio 0.2, M_{CJ}=3.04), the free-stream Mach number and stagnation conditions were chosen to be identical to the test conditions of [34,35], M_{in}=3.15, p_{00}=7.485 atm (=110 psi), and T_{00}= 1033.15 K(=1400 F). For the chosen from parameters and computational domain size, no chemical reactions were registered behind the reflected wave or Mach stem in numerical experiments with both RR and MR reflection configurations. The flow structure corresponded to the regular and Mach reflection in an inert medium. A threefold increase in the linear size of the computational domain (with an unchanged geometry of the channel) produced similar results. In the case of a fivefold increase in size, a very interesting mode of the Mach reflection with a strongly intermittent Mach stem was observed (see Fig. 6). The oscillations of the Mach stem position have a significant amplitude and are periodic in time, Fig. 1a. With these oscillations, the front of the Mach stem always remains smooth, and no transverse waves or perturbations were registered. This mode is rather similar to the regime of one-dimensional oscillations of a detonation wave propagating freely in a narrow tube (near-critical galloping detonation mode).

In numerical experiments with a stoichiometric mixture $2H_2$ + 4.772 Air (M_{CJ}=4.4), the values of flow parameters were as follows: M_{in}=4.6, T_{00}= 1700 K, and p_{00}=110 psi. The simulation results showed that the Mach reflection has no specific features in this mixture, and the flow pattern is similar to that shown in Fig. 4b. The computations were performed with a large computational domain for which the intermittent Mach reflection mode was obtained in the lean mixture.

Conclusions

Numerical investigations of regular and Mach reflections in supersonic chemically reacting flows have been performed by a high-order MUSCL TVD scheme. It has been found that, as for nonreacting SW, there is a dual solution domain, where the existence of both RR and MR is possible under identical flow parameters and geometry. In the case of MR, MS is a section of the front of an overdriven DW.



(c)

Fig. 6. Oscillating Mach stem in lean mixture $0.4H_2$ + 4.772 Air (equivalence ratio 0.2 and M_{CJ}=3.04) for θ =23°, h/w=0.865, and M_{in}= 3.15: (a) Mach stem trajectory. Frequency is about 840 Hz.; (b) numerical Schlieren picture of the flow field at the front position 1, Fig.7a; (c) numerical Schlieren picture of the flow field at the front position 2, Fig.7a. Here $t_w=w/c_0$, where c_0 is a speed of sound at freestream condition

Simulations have been done for a series of inflow Mach numbers M_{in}.

For the case of M_{in}=5.5 (this value is slightly greater than M_{CJ}=5.13), the flow structure behind MS is similar to the flow structure behind the front of a freely propagating multifront unsteady DW. There is a system of strong transverse waves on the Mach stem. The motion of these transverse waves along MS corresponds to the motion of transverse waves on the front of cellular detonation waves in gaseous mixtures. The Mach stem is unsteady for M_{in}=5.5. Our study has revealed that h/w is one of the governing parameters. Depending of its value, for M_{in}=5.5, MS inevitably moves upstream up to the inflow boundary or vanishes.

For higher Mach numbers, M_{in}=6.0, M_{in}=7.0, and M_{in}=8.0, MR configurations with a standing MS have been obtained. In the case M_{in}=6.0, MS has a system of weak unsteady transverse waves on its front. For M_{in}=7.0 and M_{in}=8.0, the Mach stem is a smooth, standing, and stable overdriven DW without any transverse waves.

To explain the results obtained, a hypothesis has been put forward that the presence of strong transverse waves at the MS front violates MR steadiness. If the degree of overdrive M_{in}/M_{CJ} is high (high values of M_{in}), transverse waves do not appear or have low intensity. To suppress the emergence and growth of transverse disturbances at low Mach numbers M_{in}=5.5, it is necessary to change the MS height and make it smaller than the detonation cell width in the overdriven DW. Simulations conducted in a threefold reduced computational domain showed that steady MR can also exist at this value of M_{in}. In this case, transverse disturbances on the MS front are very weak, and the Mach stem is smooth and steady.

The dependences of the MS height on the wedge angle θ and on the amount of heat released have been found.

For a lean hydrogen-air mixture, an extremely interesting regime of Mach reflection with a strongly oscillating Mach stem was obtained for the first time. The upstream and downstream oscillations of the Mach stem relative to its equilibrium position have a significant amplitude and are rigorously periodic in time.

The simulations have shown that certain types of local perturbations of the free-stream flow might initiate the transition from RR to MR.

Acknowledgments

This research was supported by the Russian Foundation for Basic Research under Grant 05-03-32131.

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