

NUMERICAL INVESTIGATION OF INTERACTION OF OBLIQUE SHOCK AND DETONATION WAVES IN A STEADY SUPERSONIC FLOW OF A CHEMICALLY REACTIVE GASEOUS MIXTURE

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Introduction

In studying the detonation phenomenon in gas mixtures, much attention is traditionally paid to investigation of the multifront (cellular) structure of a self-sustained unsteady detonation wave (DW) propagating in a mixture at rest, determination of the critical conditions of detonation initiation (critical value of the initiation energy), and marginal regimes of DW propagation.

Development of new promising scramjets that use the detonation combustion mode requires a detailed study of interaction of oblique shock waves (SW) and detonation waves in steady flows. These studies are also necessary to create effective RAM accelerators, since oblique DW are the most important element in the flow structure around an accelerated body in the accelerator barrel.

In nonreacting gas-dynamics, the flow structure in the case of regular (RR) and Mach (MR) reflection of shock waves and the criteria of transition between these types of reflection have been studied in many theoretical, experimental, and numerical papers. It is known that there are two principal conditions, the von Neumann criterion α_N and the detachment criterion α_D , at which the transition from one type of reflection to the other occurs in steady flows. Here α is the angle between the SW and the free-stream velocity vector, and $\alpha_N < \alpha_D$. There is a dual solution domain $\alpha_N < \alpha < \alpha_D$, where both types of reflection are possible. A hysteresis phenomenon is also possible, where the transition from RR to MR and back occurs at different values of the flow parameter being changed (the angle α or the flow Mach number).

At the Institute of Theoretical and Applied Mechanics (ITAM) of the Siberian Branch of the Russian Academy of Sciences a hysteresis of the RR to MR transition (both in terms of the wave angle and the Mach number) was obtained for the first time [1, 2]; the effect of the Reynolds number on the Mach stem height was shown [3]; stability of RR and MR to perturbations was examined [3,4]; three-dimensional MR of shock waves was calculated for the first time [4], and the wave and Mach surface shapes were shown; a hysteresis was obtained for the three-dimensional case [4], and a new type of three-dimensional reflection of shock waves (combined reflection) was found [5]. The latter type of reflection was experimentally confirmed in investigations performed at ITAM [5].

As compared to reflection of oblique SW, the interaction of oblique DW with each other, SW, or a solid surface has not been adequately studied.

The main objective of the present work is to study the flow structure with reflection of oblique SW and DW in a steady supersonic flow of a chemically reacting mixture and the transition from regular to Mach reflection.

Formulation of the problem and physical model

The simulation was performed for a flow of a uniformly mixed mixture $2\text{H}_2 + \text{O}_2$ for $p_0 = 0.2$ bar, $T_0 = 298.15$ K, and inflow Mach number $M_{\text{in}} = 5.5$. A two-dimensional supersonic flow of the mixture over a compression body, which was a wedge with an angle θ and a length

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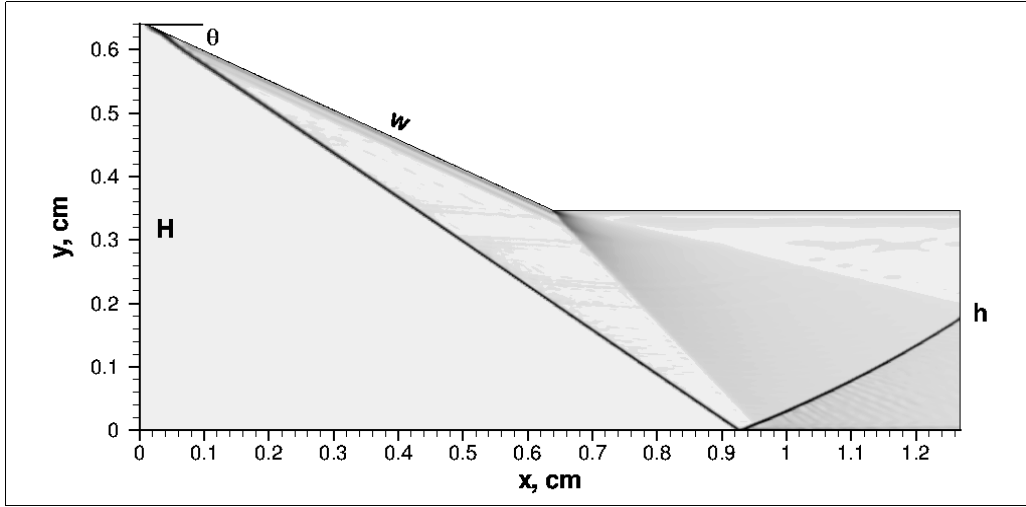


Fig.1 Numerical Schlieren picture of the flow field for RR of SW in $2\text{H}_2 + \text{O}_2$ mixture. $p_0 = 0.2$ bar, $T_0 = 298.15$ K, $M_{\text{in}} = 5.5$, $\theta = 25^\circ$, $h/w = 0.5$

of the compression surface w , in a channel with an input cross section H and output cross section h was considered (see Fig.1). In contrast to simulation of SW reflection in a inert medium, for a chemically reacting flows there is some characteristic speed, namely, the DW speed in the Chapman-Jouguet 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 the DW. For the given mixture and initial conditions, we have $D_{\text{CJ}} = 2757$ m/s and $M_{\text{CJ}} = 5.13$. Hence, the value of M_{CJ} is the lower limit of M_{in} . 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. $m_{\text{in}} = \rho_0 c_0 M_{\text{in}} H$, 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-stage model of chemical kinetics [6]. The first (induction) stage was modeled in accordance with the experimental kinetics [7]:

$$\tau_{\text{ind}} = 4,17 \cdot 10^{-14} \cdot \exp \frac{18100}{RT} \times [\text{O}_2]^{-1/2} [\text{H}_2]^{-1/2} \left[\frac{\text{mole} \cdot \text{s}}{\text{cm}^3} \right]. \quad (1)$$

After the induction period, the stage of heat release was described using the model of generalized kinetics of chemical reactions at high temperatures and the caloric equation of state correlated with this kinetics [8,9]. 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 [15].

The boundary conditions on the different sides of the computational domain were as follows (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 [10].

Numerical method

The hyperbolic system of equations was solved numerically using the finite-volume scheme with the fourth-order MUSCL TVD reconstruction [11] and the advanced HLLC algorithm [12] 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” [13] 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 a second-order accuracy by using new, recently developed, additive semi-implicit Runge-Kutta methods [14]. In this case, the characteristic values of the Courant number were $CFL=0.2-0.3$.

A body-fitted quadrilateral grid was used with typical values of points $N_x=600$ and $N_y=200$ in the x -direction and y -direction, respectively. To ensure the independence of the computational results on grid resolution, some of the runs were checked with the 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

As in the case of nonreacting SW, there is a dual solution domain, where the existence of both regular and Mach reflections are possible under identical boundary conditions. Figure 1 shows the numerical Schlieren visualization of regular reflection of an oblique shock wave for a wedge angle $\theta=25^\circ$. The study of reflection of nonreacting SW shows that h/w is one of the governing parameters; in the present case, it had the value $h/w=0.5$. For an inert SW for a given combination of M_{in} , θ (or shock-wave angle α), and γ , there is an upper limit of h/w , i.e. h/w_{max} . This limit is determined by h_{max} , i.e. the situation when the leading characteristic of the expansion fan, which is formed at the trailing edge of the wedge, intersects the incident SW. For the present simulation, we have $h/w_{max}=0.6145$. 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 results of our studies the cell size is $a_0=0.64$ cm for the above mixture under the initial conditions mentioned. This value is in very good agreement with the experimental results (see [15]). The computation described shows that, for the above parameters, the temperature behind both the incident and reflected waves is not sufficiently high, and the induction region length is greater than the computational domain. In this case, the flow structure is similar to RR in a inert medium [1–5].

Figure 2 shows the case of Mach reflection; all geometric dimensions and flow parameters are similar to Fig. 1. The flow structure behind the Mach stem is similar to the flow structure behind the front of a multifront (cellular) unsteady DW [15]. 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. The behavior of these transverse waves corresponds to the behavior of transverse waves behind the front of an unsteady multifront DW. This gives grounds to consider that the Mach stem is a section of the front of an overdriven DW with a degree of overdrive approximately equal to $M_{in}/M_{CJ}=1.07$.

In contrast to MR in a inert medium, the Mach stem for a chemically reacting flow is unsteady. 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 $\theta=25^\circ$.

For values of h/w up to 0.7 (that is greater than h/w_{max}), the Mach stem inevitably moves upstream up to the inflow boundary. For this case, we have an unstarted two-dimensional

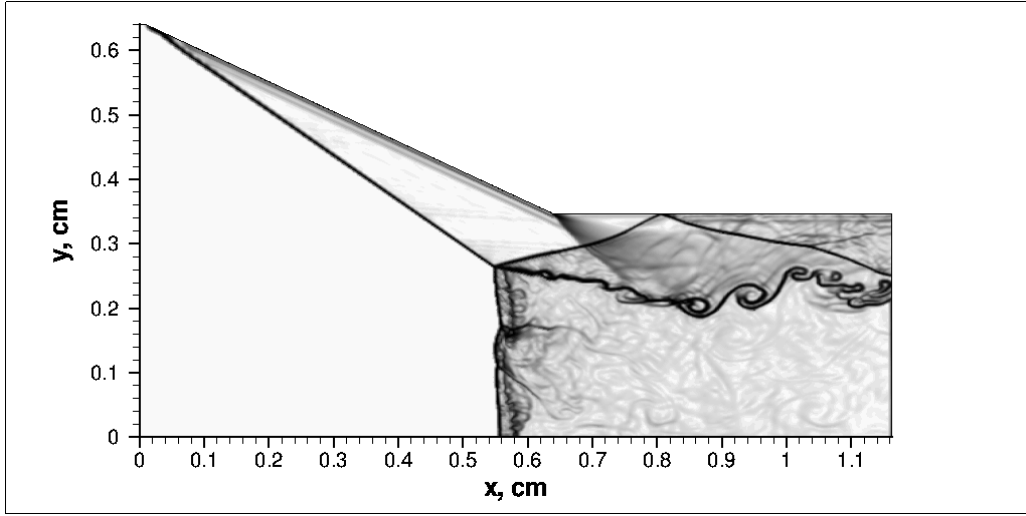


Fig.2 Numerical Schlieren picture of the flow field for MR of SW in $2\text{H}_2 + \text{O}_2$ mixture. $p_0 = 0.2$ bar, $T_0 = 298.15$ K, $M_{\text{in}} = 5.5$, $\theta = 25^\circ$, $h/w = 0.5$

converging nozzle. If h/w exceeds some 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 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. The results of numerical simulation of Mach reflection make us formulate the following problem: for a given mixture and chosen value of H , which combinations of M_{in} and θ can ensure the existence of a steady MR configuration (as for nonreacting SW) in the some range of h/w ?

In the study described above, we had regular reflection as an initial steady flow configuration. An RR configuration was formed if the computations were started under the initial condition that there was a uniform flow with the same gas parameters in the computational domain as at the inflow boundary. To obtain an MR, we used a technique that was applied in investigations of reflection of nonreacting SW [3,4].

As for these previous simulations, the present study showed that a different local perturbation of the free-stream flow might initiate the transition from RR to MR in the dual-solution domain. Here we did not set the problem of finding the minimum size and amplitude of perturbations for the successful transition from RR to MR, i.e., the critical conditions for such transformation. A rectangular “spot” with dimensions from $0.2h$ to $0.5h$ in both directions was placed at the axis of symmetry. This disturbance was introduced into the flow upstream of the reflection point. The computations were performed for two different types of perturbations. The first type of disturbances consisted of instantaneous changes in density from ρ_0 to $0.1\rho_0$ in this region; all the remaining flow parameters remained unchanged. The physical reason for the MR formation is a refraction of an incident SW on this low-density region and temporary existence

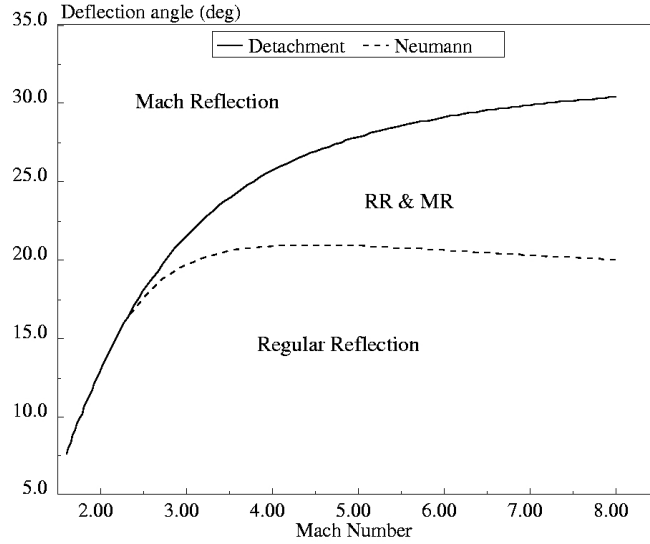


Fig.3 The transition criteria in terms of deflection angle θ vs. inflow Mach number M_{in} for the case of nonreacting shock waves in $2H_2+O_2$ mixture, $\gamma_0=1,397$

of an SW with a larger angle of incidence than the detachment criterion angle α_D determined for the perturbed “spot” parameters [4].

We also used another type of disturbances. All flow parameters in the region described above were changed to those behind the normal steady SW. There is one more variant of this type of perturbations [3]. In this variant, the velocity in the perturbed “spot” is set to zero. In both cases, the local normal SW is formed near the axis of symmetry and interacts with the existing steady SW structure of the flow.

The creation of the normal SW by both types of disturbances is the key mechanism of transition from RR to MR in chemically reacting mixtures. The temperature behind the normal SW is much greater than that behind the incident oblique SW. Thus, due to the strong dependence of an induction period τ_{ind} on temperature (see Eq. (1)), the value of this quantity is low behind the normal SW. Hence, the heat release process successfully starts at a short distance (short induction zone) behind the leading SW. This rapid release of energy forces the formation of an unsteady multifront DW – Mach stem.

For this value of M_{in} , choosing the wedge angle (i.e. flow deflection angle) $\theta=25^\circ$ leaves us approximately in the middle of the dual solution domain (Fig.3) for nonreacting shock waves. Determination of the boundaries of this region for a flow of a chemically active medium is another problem of interest.

Numerical investigation of the von Neumann criterion is a severe problem for computational fluid dynamics methods. For finite volume schemes, the reason is that the Mach stem height becomes comparable with the computational cell size as θ approaches θ_N . Therefore, the detachment criterion was examined. For a nonreacting SW, the value of θ for the detachment criterion is $\theta_D=28.55^\circ$ at $M_{in}=5.5$ (see Fig. 3). The simulations started from $\theta > \theta_D$, and the initial conditions described above were used, $h/w=0.6$. We found that an unsteady MR was formed up to $\theta=28.60^\circ$. This result and analysis of the RR flow structure give grounds to

believe that the dual solution domain for the given size of the channel and M_{in} is very close or coincides with one for the nonreacting SW (see Fig. 3).

Conclusions

Numerical investigations of regular and Mach reflections in 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 boundary conditions. In the case of the MR, the Mach stem is a section of the front of an unsteady overdriven multifront DW. Our study has revealed that h/w is one of the governing parameters. Depending of its value, the Mach stem inevitably moves upstream up to the inflow boundary or vanishes. The simulations have showed that different local perturbations of the free-stream flow might initiate the transition from RR to MR. The detachment criterion has been examined. It has been found that, for the size of the computational domain under consideration and Mach number, the detachment wedge angle is very close or coincides with the value for a nonreacting SW.

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REFERENCES

1. **Ivanov M.S., Gimelshein S.F., Beylich A.E.** Hysteresis effect in stationary reflection of shock waves // *Physics of Fluids*. 1995. Vol. 7, No. 4. P. 685–687.
2. **Ivanov M.S., Ben-Dor G., Elperin T., Kudryavtsev A.N., Khotyanovsky D.V.** Flow-Mach-number-variation-induced hysteresis in steady shock wave reflection // *AIAA Journal*. 2001. Vol. 39, No. 5. P. 972–974.
3. **Ivanov M.S., Gimelshein S.F., Markelov G.N.** Statistical simulation of the transition between regular and Mach reflection in steady flows // *Computers Math. Applic.* 1998. Vol. 35, No. 1/2. P. 113–125.
4. **Ivanov M.S., Markelov G.N., Kudryavtsev A.N., Gimelshein S.F.** Numerical analysis of shock wave reflection transition in steady flows // *AIAA Journal*. 1998. Vol. 36, No. 11. P. 2079–2086.
5. **Ivanov M.S., Vandromme D., Fomin V.M., Kudryavtsev A.N., Hadjadj A., Khotyanovsky D.V.** Transition between regular and Mach reflection of shock waves: new numerical and experimental results // *Shock Waves*. 2001. Vol. 11, No. 3. P. 199–207.
6. **Korobeinikov V.P., Levin V.A., Markov V.V., and Chernyi G.G.** Propagation of blast waves in a combustible gas // *Astronaut. Acta*. 1972. Vol. 17. P. 529–537.
7. **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 Symp. (International) on Combustion: Proceedings. Berkeley, 1966. P. 147–154.
8. **Nikolaev Yu.A., Fomin P.A.** Analysis of equilibrium flows of chemically reacting gases // *Combustion, Explosion, and Shock Waves*. 1982. Vol. 18, No. 1. P. 53–58.
9. **Nikolaev Yu.A., Zak D.V.** The agreement of models of chemical reactions in gases with the second law of thermodynamics // *Combustion, Explosion, and Shock Waves*. 1988. Vol. 24, No. 4. P. 87–90.
10. **Godynov S.K. (Ed.)** Numerical solution of the multi-dimensional problems of gaseous dynamics. Moscow: Nauka, 1976.
11. **Yamamoto S., Daiguji H.** Higher-order-accurate upwind schemes for solving the compressible Euler and Navier-Stokes equations // *Comput. Fluids*. 1993. Vol. 22, No. 2/3. P. 259–270.
12. **Batten P., Leshziner M.A., Goldberg U.C.** Average-state Jacobians and implicit methods for compressible viscous and turbulent flows // *J. Comput. Phys.* 1997. Vol. 137. P.38–78.
13. **Coquel F., Perthame B.** Relaxation of energy and approximate Riemann Solvers for general pressure laws in fluid dynamics // *SIAM J. Numer. Anal.* 1998. Vol. 35, No. 6. P. 2223–2249.
14. **Shen J.W., Zhong X.** Semi-implicit Runge-Kutta schemes for non-autonomous differential equations in reactive flow computations. AIAA Paper No.96–1969, 1996.
15. **Trotsyuk A.V.** Numerical simulation of the structure of two-dimensional gaseous detonation of an $H_2 - O_2 - Ar$ mixture // *Combustion, Explosion and Shock Waves*. 1999. Vol. 35, No. 5. P. 549–558.