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Calculation of Detonation Initiation in a Hydrogen/Oxygen/Argon Mixture in by a Small-Diameter Spherical Projectile

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Abstract. The initiation of detonation in a reactive mixture by a small-diameter spherical projectile launched at supersonic velocity was studied for a reduced kinetic scheme of chemical reactions. A mathematical technique based on the ANSYS Fluent package was developed for this purpose. Numerical and experimental data on the flow regimes and detonation cell sizes are compared. There is agreement between the calculated and experimental flow patterns and detonation cell sizes for each regime.

INTRODUCTION

The initiation and stabilization of detonation by supersonic-velocity projectiles is important from both scientific and technological viewpoints. This subject covers a wide field of science from issues related to the development of a ramjet engine with fuel combustion in shock waves to the estimation of detonation initiation energy.

Vasiljev [1] performed an experimental study of the initiation of detonation by a high-speed body. The experiments were carried out for a mixture of $C_2H_2 + 2.5O_2$ and a hemispherical or blunt cylinder with a velocity of about 800–1400 m/s. A new mechanism of the transformation of shock waves to detonation waves was observed in near-critical regimes. An analytical correlation between the aerodynamic characteristics of the high-speed body and the physicochemical parameters of the explosive mixture was proposed as a criterion for the initiation of gaseous detonation. Analytical and experimental data agreed well with each other.

Liu et al. [2] carried out numerical studies of a prompt oblique detonation wave (PODW) sustained by a finite-length wedge. The results show that a PODW can be stabilized on a finite-length wedge shorter than the induction length of the mixture behind the inert shock. Fully coupled and partially coupled PODWs were observed. For fully coupled PODWs, upstream facing transverse waves (UF TW) were swept downstream and, consequently, a fully coupled PODW could persist. For partially coupled PODWs, UF TWs propagated upstream, and downstream facing transverse waves were weakened by the expansion wave emanating from the corner. The stability of partially coupled PODWs was found to be low. The configuration of partially coupled PODWs can be altered by local explosions occurring downstream.

Miltiadis and Papalexandris [3] numerically examined the structure of detonations generated by flow of an ignitable mixture over a wedge. The simulations were performed using a recently designed unsplit algorithm which integrated the convective and reaction source terms simultaneously and chemical kinetics which followed a simple one-step Arrhenius law. Two different geometrical configurations were considered: a long wedge whose top corner could not affect the structure of the reaction zone and a short wedge whose corner could influence the reaction zone. A stable detonation and a steady flow-field were established near the wedge. It is observed that for moderate wedge angles, the leading shock curved smoothly until it reached a final angle. For higher wedge angles, an explosion occurred at the leading shock and the detonation became unstable.

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Michael et al. [4] reported experimental results for the initiation and stabilization of an oblique detonation by a projectile 25 mm in diameter with a velocity of 2700 m/s into stoichiometric H2–O2–N2 mixtures at pressures between 0.1 and 2.5 bar. Initiation events similar to DDT in propagating waves were observed after 300 mm of travel in H2–O2 mixtures diluted with 25% N2. A more direct initiation process was observed in H2–air mixtures. A stabilized but overdriven oblique detonation was observed in a stoichiometric H2–air mixture at an initial pressure of 2.5 bar.A critical threshold in initial pressure was found to be required for the establishment of detonation.

Kasahara et al. [5] experimentally studied self-sustained oblique detonation waves around projectiles as part of a fundamental investigation of the application of an oblique detonation wave engine and a high-efficiency detonation wave combustor as a power generator. In this study, the criticality for detonation waves was investigated. The first expression of the criticality was a mean-curvature coefficient, a ratio of 5.03 between the detonation cell width and the mean-curvature radius at which the normal velocity component was the Chapman–Jouguet (C–J) velocity. A mean curvature coefficient of 7.8 was determined to be the most important value for stabilizing self-sustained oblique detonation waves around multidimensional bodies. Based on experimental results obtained for high- and low-projectile-velocity ranges, it was concluded that a lower-velocity projectile could stabilize a self-sustained oblique detonation wave more effectively than could a higher-velocity one.

Li et al. [6] performed time-dependent numerical simulations to investigate detonation structures generated by wedge-induced oblique shocks in hydrogen–oxygen–nitrogen mixtures. The simulations showed the existence of a multidimensional detonation structure consisting of the following elements: a nonreactive oblique shock, an induction zone, a set of deflagration waves, and a reactive shock, in which the shock front was closely coupled with energy release. In a wide range of flow and mixture conditions, this structure was stable and very resilient to disturbances in the flow, but if a part of the flow behind the structure was subsonic, the entire structure could become detached from the wedge and moved upstream continuously.

Wang et al [7] used the reactive Euler equations with a detailed chemical reaction model to simulate two-dimensional, oblique detonations induced by a wedge. The oblique shock-to-detonation transition in a stoichiometric hydrogen–air mixture at low pressure and high temperature corresponding to the realistic inflow conditions in oblique detonation wave engines was studied. Numerical results suggested that oblique detonation initiation was achieved through a smooth transition from a curved shock. The formation mechanism of this smooth transition was discussed and a quantitative analysis was carried out by defining a characteristic length for the initiation process. The dependence of the initiation length on different parameters including the wedge angle, flight Mach number, and inflow Mach number was discussed.

Muralidharan and Menon [8] investigated the initiation of detonation by supersonic projectiles and the stabilization of oblique detonation waves (ODWs) using a high-order adaptive Cartesian cut-cell method developed for simulations of compressible viscous flows. The cut-cell scheme for supersonic viscous flows was additionally validated by comparing the results for Mach 2 turbulent flow over a sphere with the corresponding experimental data. Also, the method was used to investigate the detonation initiation and stabilization mechanisms for a 3.18 mm diameter high-density polyethylene sphere which was launched into a detonable hydrogen–oxygen mixture with a velocity approximately 1.2 times the Chapman–Jouguet (C–J) velocity. The effect of the filling pressure on the stabilization mechanism was studied, and a qualitative comparison of the results with the experimental data was made.

Yang et al. [9] numerically investigated oblique detonation structures formed by semi-infinite cones. Unsteady, two-dimensional and axisymmetric Euler equations with a one-step irreversible Arrhenius reaction model were used. It was shown that a novel wave structure characterized by two distinct points where there was close-coupling between the shock and the combustion front occurred when either the cone angle or the incident Mach number was reduced. The initiation mechanism behind the conical shock was discussed to investigate the interplay between the effect of the Taylor–Maccoll flow, front curvature, and energy releases from the chemical reaction in conical oblique detonations. The observed flow fields were interpreted in terms of the energetic limit as in the critical regime for initiation of detonation.

Belanger et al. [10] presented the results of experimental studies on the initiation of detonations by in hydrogen–oxygen–nitrogen mixtures by projectiles of 25-mm diameter with speeds of around 3000 m/s. Flow visualization and pressure measurements for several mixture conditions were made. A clear transition between shock-induced combustion and detonation was observed. Transition to detonation was observed with an overtaking wave occurring in the shocked but unreacted gas.

Maeda et al. [11] performed experimental studies of the stabilization of oblique detonation waves (ODWs) by launching a spherical projectile of 3.18-mm diameter with a velocity 1.2–1.4 times the Chapman–Jouguet (C–J) velocity into detonable mixtures at rest. The detonable mixture used was a stoichiometric oxygen mixture and hydrogen diluted with 50 vol% argon. The detonation stability was discussed in terms of the curvature effect arising from the three-dimensional nature of the stabilized ODW around the projectile. The dimensionless projectile diameter was found to be a unique parameter for the stabilizing criticality regardless of the projectile diameter.

In the present study, the mathematical model for the problem of detonation initiation by a small-diameter projectile was verified against experimental data [11]. This was done to select the constants of the kinetic scheme for the further use of this model in numerical simulations of combustion and detonation. In studies of such problems, it is necessary to ensure that the chosen mathematical model fits the chemical reaction kinetic scheme.

PROBLEM FORMULATION

A schematic of the simulation is shown in Fig. 1. A premixed stoichiometric hydrogen–oxygen mixture diluted with argon ($2H_2 + O_2 + 3Ar$) having a velocity $V=1.24\pm0.03\ D_{CJ}$, a static temperature T_{st} = 295 K, and an initial pressure P_{st} = 121–141 kPa was supplied to the inlet of the simulation domain.

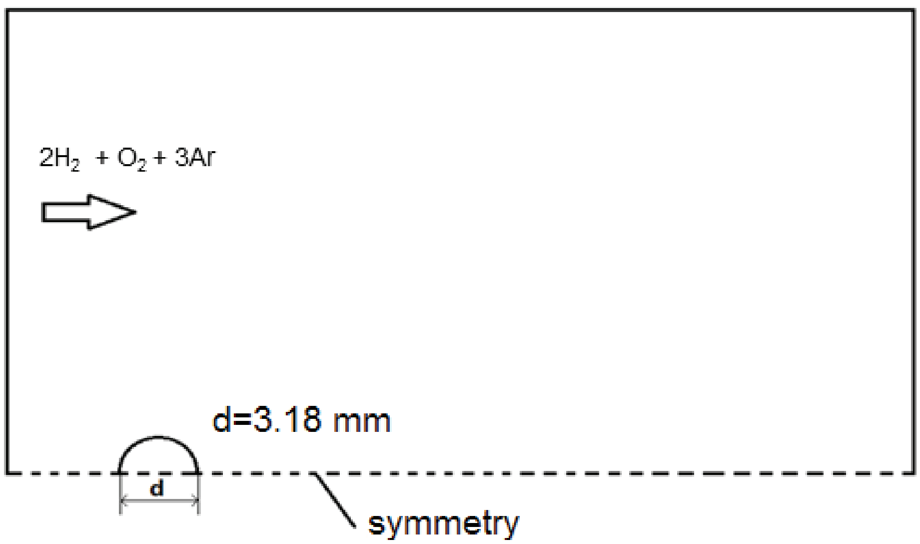


FIGURE. 1. Schematic of the simulation

MATHEMATICAL MODEL AND NUMERICAL ALGORITHM

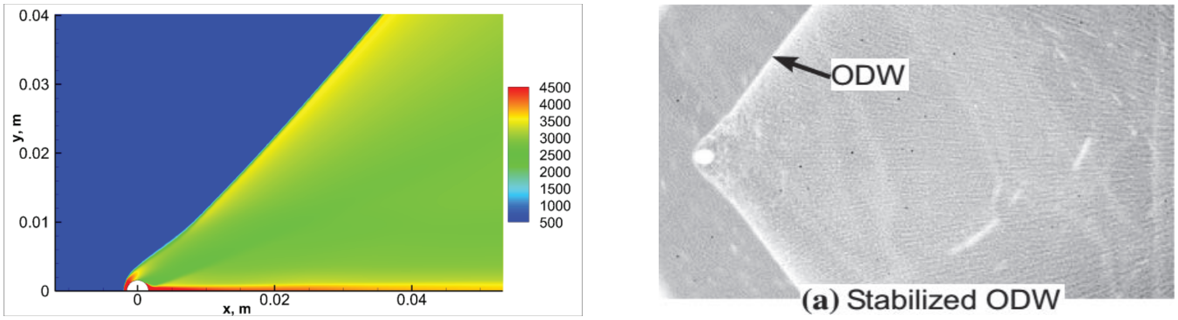
The mathematical model includes the Favre-averaged Navier–Stokes equations for a multicomponent gas mixture with chemical reactions, supplemented by the SST modification of the k-ω turbulence model.

In modeling flows with detonation waves, as in any problem with chemical reactions, one has to select a kinetic scheme for an adequate description of the combustion process. Reduced and detailed combustion kinetic schemes are distinsguished. In contrast to detailed kinetics, reduced kinetics does not accurately reproduce parameters such as the ignition delay and combustion time of the mixture, especially for the limiting regimes, but it requires less computing time. In this work, the kinetics was modeled using a reduced kinetic scheme with one reaction for four species. In [12], this kinetic scheme was verified against experimental data on the ignition delay and the propagation velocity of the detonation wave under different conditions.

The ANSYS Fluent software package was used as the solver. In the unsteady case, an implicit second-order scheme was used for temporal approximation, and the AUSM flux vector splitting method with a second-order upwind scheme for spatial approximation.

CALCULATIONS RESULTS

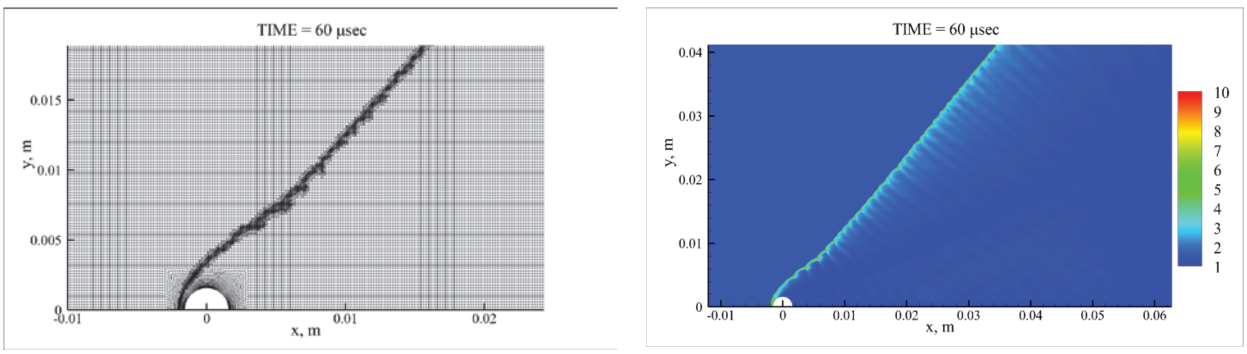
In the initial stage of the study, steady-state calculations were performed. Figure 2 shows the calculated fields of the static temperature and an experimental shadowgraph from [11] for the static pressure of the free stream P_{st} = 141 kPa.



(a) (b)

FIGURE. 2. Oblique detonation wave at P_{st} = 141kPa. Steady-state calculation: (a) static temperature field; (b) experimental shadowgraph from [11]

As can be seen from the comparison, the calculated and experimental flow patterns coincide, but steady-state calculation does not resolve the fine structure of the cellular detonation. Figure 3 presents the results of modeling this problem in an unsteady formulation.

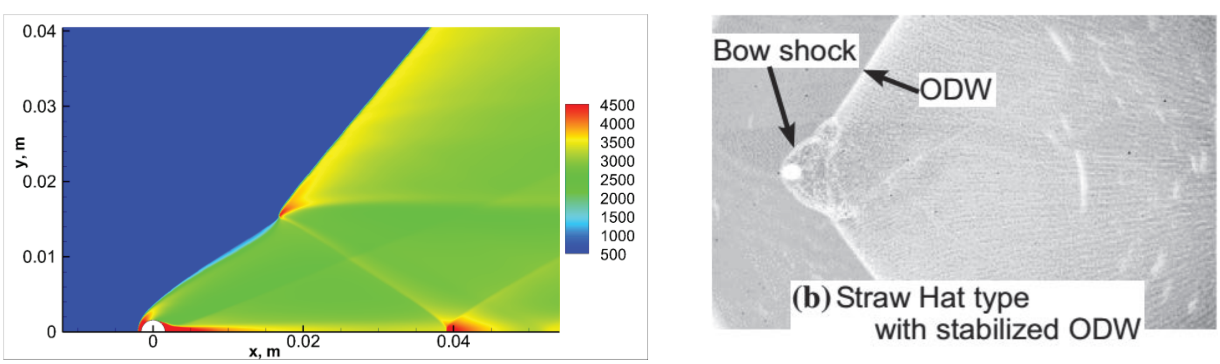


(a) (b)

FIGURE. 3. Fragment of the grid (a), and the calculated density fields at P_{st} = 141 kPa (b)

For the unsteady calculation, we performed a dynamic adaptation of the computational grid to the density gradient. As an example, Fig. 3a shows a fragment of the adapted grid. The unsteady formulation of the problem makes it possible to obtain the cellular detonation structure, with the cell size being consistent with the available experimental data for hydrogen–oxygen mixtures diluted with argon at the given pressures.

Figure 4 shows the static temperature fields for the steady-state calculations at P_{st} = 136 kPa and the shadowgraph from the experiment [11].



(a) (b)

FIGURE. 4. Straw-hat regime with an oblique detonation wave at P_{st} = 136 kPa. Steady-state calculation: (a) static temperature field; (b) experimental shadowgraph from [11]

The steady-state calculation reproduces the so-called straw-hat type detonation wave observed in experiments [11]. However, as in the previous case, the steady-state calculation does not identify the detonation cell. Figure 5 shows the simulation results for the unsteady problem. The unsteady calculation reveals the cellular detonation structure and the agreement in the cell size, the flow structure is consistent with the experimental pattern.

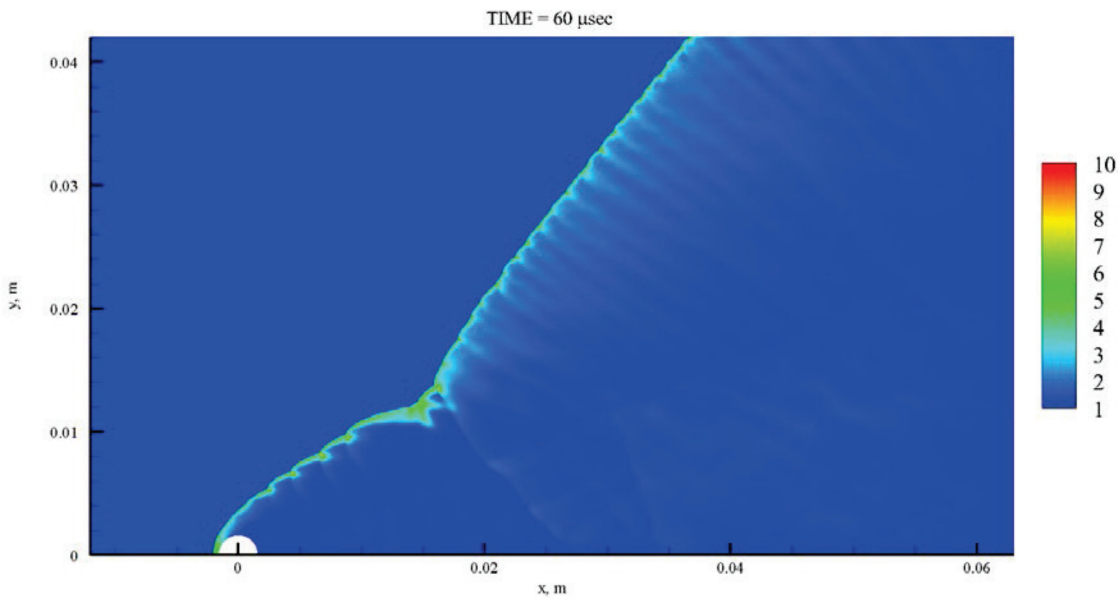
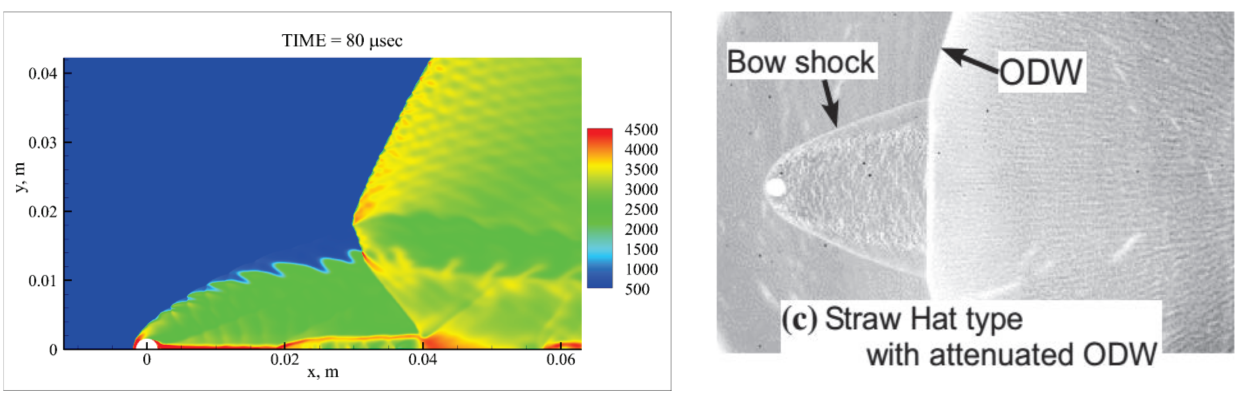


FIGURE. 5. Density fields at P_{st} = 136kPa

For the flow regime at P_{st} = 131 kPa, steady-state calculation was not carried out since, under these conditions, a detached detonation wave is formed. In [11], this regime is called the straw-hat regime with an attenuated ODW. Figure 6 shows the static temperature fields for the unsteady calculation and an experimental shadowgraph.



(a) (b)

FIGURE. 6. Straw-hat regime with an oblique detonation wave at P_{st} = 136 kPa. Steady-state calculation: (a) static temperature field; (b) experimental shadowgraph from [11]

The dynamically adapted grid and unsteady formulation of the problem, as in the previous cases, made it possible not only to reproduce the regime observed in the experiment, but also to follow the motion of the detonation wave in time. Figure 6 shows the density fields for different times. In this case, the oblique detonation wave is not stable and moves downstream with time. Thus, this regime is transient between the so-called straw-hat regime at P_{st} = 136 kPa and shock-induced combustion at P_{st} = 121 kPa.

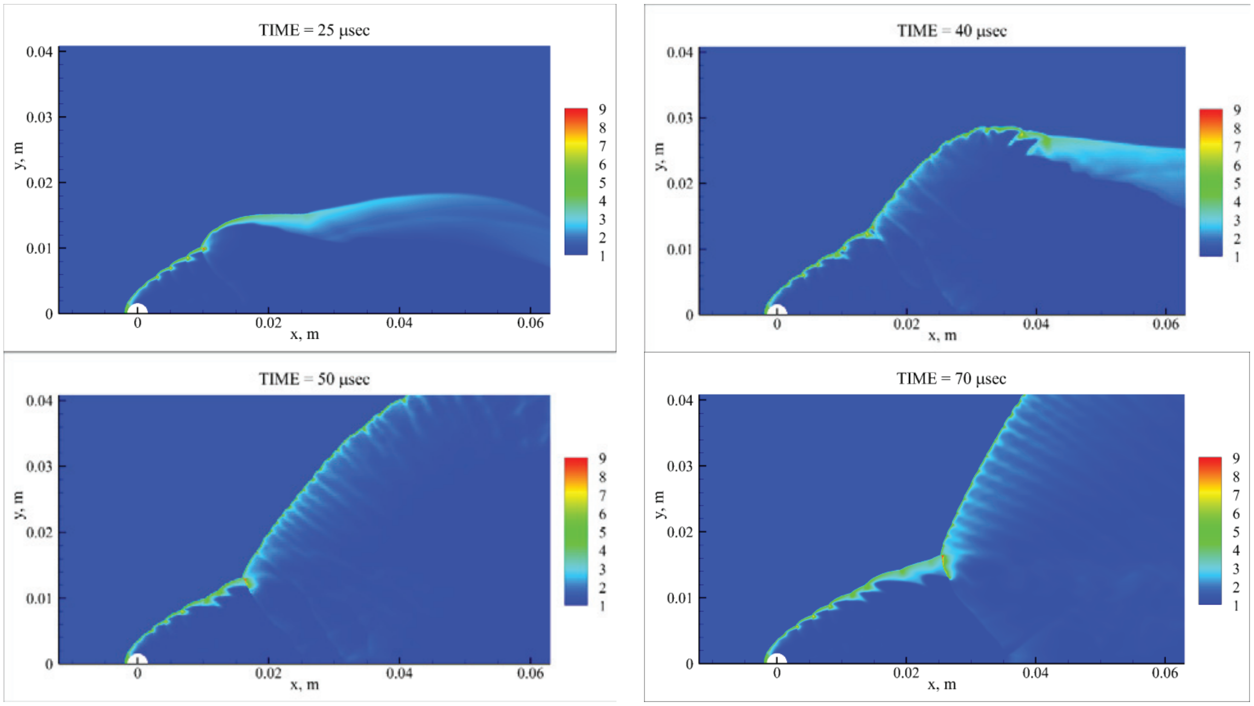


FIGURE. 7. Density fields at P_{st} = 131 kPa at different times. Unsteady calculation

Figure 8 shows the calculation and experimental results for shock-induced combustion at P_{st} = 121 kPa. In this case, a steady-state calculation is sufficient to obtain agreement with the experimental flow pattern. Since the detonation wave is not formed, combustion is initiated behind the shock wave and the regime is steady in time.

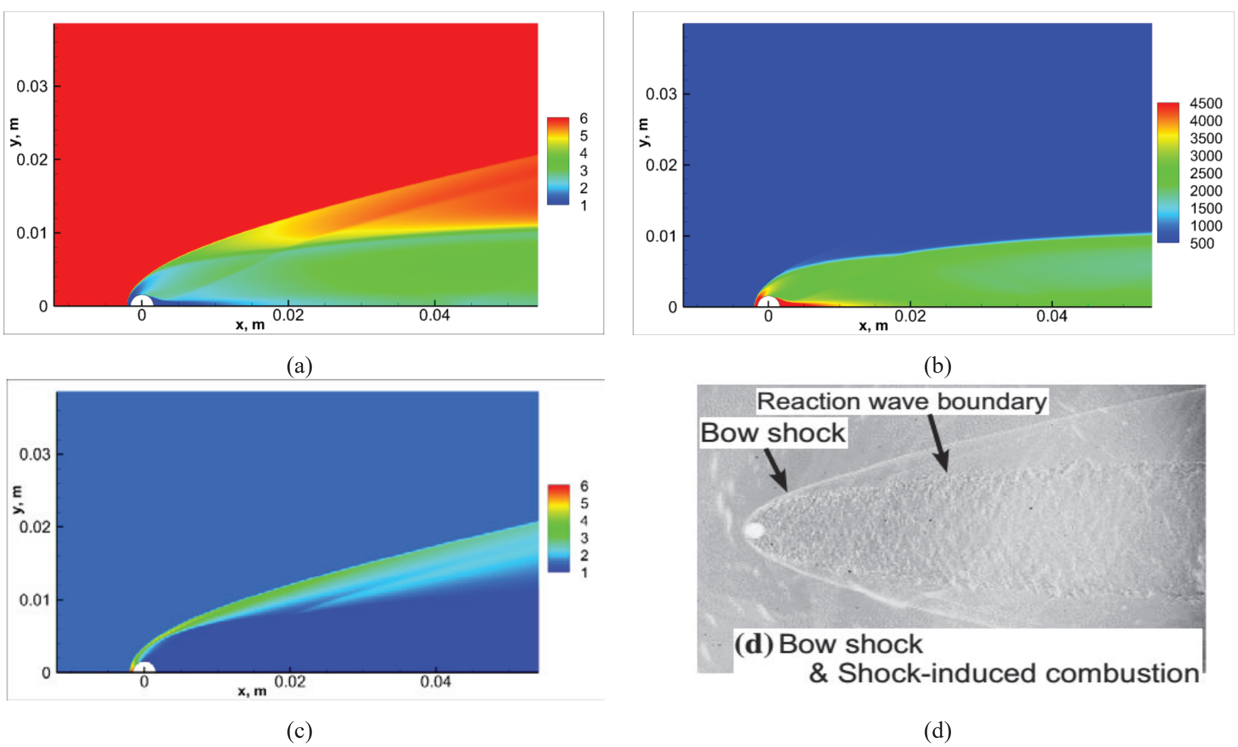


FIGURE. 8. Shock-induced combustion with P_{st} = 121 kPa. Steady-state calculation: (a) Mach number field; (b) static temperature field; (c) density field; (d) experimental shadowgraph [11]

The aforesaid is illustrated in Fig. 9, which shows the density fields obtained by unsteady calculation for shock-induced combustion. Some unsteadiness of the flow is observed only near the projectile and does not affect the flow structure as a whole. For these free-stream parameters, the detonation cell size increases to a certain critical value. In this case, the formation of an oblique detonation wave does not occur.

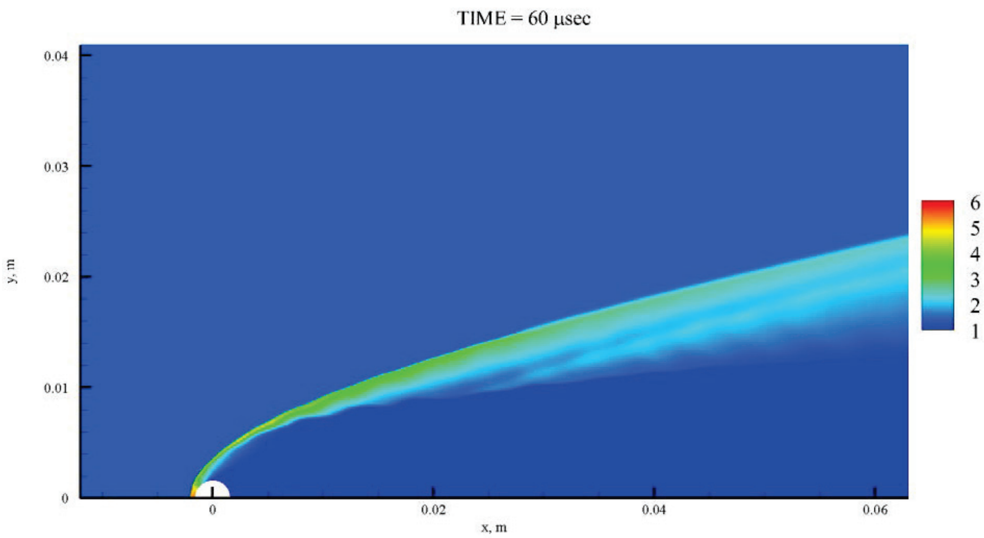
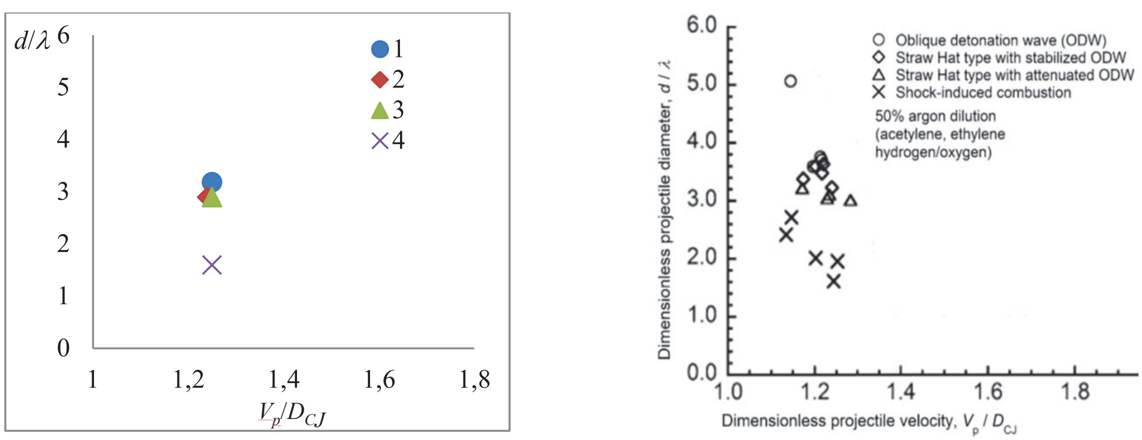


FIGURE. 9. Density fields at P_{st} = 121 kPa. Unsteady calculation

Figure 10 shows a comparison of the flow regimes obtained in the calculation and experiment [11] for different projectile diameters normalized to the detonation cell size and different projectile velocities normalized to the Chapman–Jouguet detonation velocity for experimental and calculated data. It can be seen from the comparison that simulated map of regimes is within the scatter of the experimental data, suggesting that the chosen mathematical model and kinetic scheme are adequate.



(a) (b)

FIGURE. 10. Maps of regimes: (a) simulation results; (b) experimental data

CONCLUSIONS

A mathematical model for calculating the initiation of detonation in a reactive mixture by a small-diameter supersonic projectile was developed, and a mathematical technique for its implementation based on the ANSYS Fluent package was designed.

The flow patterns for the steady-state and unsteady calculations were compared with experimental data. Comparative analysis showed that for problems of this type, it makes sense to conduct an unsteady calculation and a dynamic adaptation of the computational grid. Although this complicates the calculation and increases the data processing time, but provides a more realistic flow pattern and better agreement between experimental and simulation results.

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