Shock-wave structures of prospective combined jet engine

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Abstract. The paper presents numerical analysis of typical model flows with Mach reflection. For example, flows in narrowing channels between two triangles and long narrowing channels are discussed. The obtained results can serve as reference data for various approximate theoretical models, in particular, for a newly proposed approximate analytical model, which should take into account combustion and detonation.

1. Introduction
Development of jet aerospace vehicles and jet technologies requires the theoretical analysis of flows with irregular (Mach) reflection of oblique shock waves. Such flows, for example, occur in inlets of high-speed flying vehicles, in supersonic jet flows and in nozzle devices. Quick size prediction of Mach stems in the investigated flow field, with their increased losses in total pressure and corresponding increase in the gas stream entropy allows control of the jet engine parameters, as well as the jet flow length range in various engineering devices.

Approximate analytical models elaborated earlier (see, for example, in [1-4]) agreed that the main problem is in computation of the key parameter (the height of the triple point in the Mach reflection), and decide this problem with rather different accuracy. New interest in adjustment of existing models or in development of modernized ones, appeared recently, see in [5-8]. This new interest is connected with the practical design of apparatus for flights at high supersonic speeds, as well as the ramjet detonation engines and the combined engines [9-12].

In the presented study, we provide a numerical analysis of typical model flows with Mach reflection, such as flows in narrowing channels between two triangles and long narrowing channels. The results achieved can serve as reference data for various approximate theoretical models such as proposed in [1-8].

The reached high temperature of the gas stream (or the fuel-oxidizer one), downstream the Mach shock can be several times higher than the temperature behind the incident oblique shock wave and the reflected one [13, 14]. This fact can initiate the impulse energy release due to the chemical reactions and due to combustion or detonation behind the Mach shock wave.

Development in design of vehicles for hypersonic flights [15], their ramjet engines [16], detonation engines [9, 10] and combined ones [12] requires fast and reliable estimation of Mach shock size. This is so because crucial features of the resulting flow depend on the Mach shock size [13, 14]. Meanwhile, there is a lack of reliable experimental data even for the supersonic flow of the perfect gas (for example, the letter [8] published in 2021 uses the experimental data of a widely-known study [17] obtained almost 40 years ago). Before proposing the modernized theoretical models that include chemical reactions due to combustion and detonation, it is necessary to provide a series of numerical experiments that can obtain reference data. The aim of the present paper is to simulate reliably a steady Mach reflection in high supersonic flow with impulse heat influx due to chemical reactions and to get reference data for future analytical models.
2. Model and methods

The numerical simulation of the process under consideration is based on the Reynolds-averaged Navier-Stokes equations for a compressible perfect gas (in the following the signs indicating averaging are omitted):

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0
\]

\[
\frac{\partial (\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot (\tau_m + \tau_t)
\]

\[
\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho \vec{u} H) = \nabla \cdot \left[ \alpha_e \nabla T - \sum_j h_j \vec{J}_j + \vec{u} \cdot (\tau_m + \tau_t) \right] + S_h
\]

In (1), \( \vec{u} \) is the averaged flow velocity vector while \( u, v \) and \( w \) are its components; \( \tau_m + \tau_t \) are molecular and turbulent components of the viscous stress tensor, correspondingly; \( E = C_v T + 0.5(u^2 + v^2 + w^2) \) and \( H = E + p / \rho = C_p T + 0.5(u^2 + v^2 + w^2) \) are the total energy and the total enthalpy, correspondingly; \( T \) is the static temperature, \( C_v = (C_p - R) \) is the gas specific heat at constant volume, \( C_p \) is the specific heat at constant pressure, \( R \) is the gas constant, \( \alpha_e = \alpha + \alpha_t \) is the effective thermal conductivity coefficient, \( \vec{J}_j \) is the diffusion flux, \( h_j \) is the formation enthalpy of the corresponding components of the gas mixture, \( S_h \) belongs to quantitative characteristics of the energy source (it allows taking into account the process of formation and absorption of thermal energy).

The relationship between turbulent stresses and averaged flow parameters can be determined using various turbulence models. Presently, the turbulence model “k-ε Realizable” [18] is applied. This model satisfies the exact mathematical constraints on Reynolds stresses arising from the physical properties of turbulent fluid flows.

Taking into account the chemical reactions, a one-stage chemical reaction of methane with an air mixture, in which the values of mass concentration set by stoichiometry, was applied:

\[
CH_4 + 2O_2 \Rightarrow 2H_2O + CO_2
\]

For analysing chemical reactions, a Finite-Rate / No TCI model is used. This implies that the code includes a finite rate kinetics model for calculating chemical components, using general expressions for the reaction rate, such as the Arrhenius reaction rates, without attempts to consider the effects of turbulent oscillations.

In simulating the air flow, it is necessary to take into account that the air is multicomponent and reactive. So the equation for changing the concentration of the \( i \)-th component of the mixture is written in the following form:

\[
\frac{\partial (\rho C_i)}{\partial t} + \nabla (\rho \vec{u} C_i) = -\nabla \vec{g}_i + \omega_i + S_i.
\]

Here \( \omega_i \) is the rate of formation of the \( i \)-th component in chemical reactions; it is determined by the following relation:

\[
\omega_i = \mu_m \sum_{j=1}^{N_k} R_{ij}.
\]

Here \( \mu_m \) is the molar mass of the \( i \)-th component of the mixture, \( N_k \) is the number of the considered chemical reactions, \( R_{ij} \) is the molar formation / decay rate of the \( i \)-th component in reaction \( r \), calculated by the following equation of chemical kinetics:

\[
R_{ij} = \Gamma \left( \nu_{jr} - \nu_{ij} \right) \left( k_p \prod_{j=1}^{N} \left[ X_{jr} \right]^{-\nu_{jr}} - k_p \prod_{j=1}^{N} \left[ X_{jr} \right]^{-\nu_{ij}} \right).
\]

In the preceding formula, \( \Gamma = \sum_j \gamma_{jr} X_j \) is the coefficient that takes into account the influence of third bodies on the rate of chemical reactions, \( \nu_{jr} \) is the exponent for product \( j \) in reaction \( r \), \( \nu_{ij} \) is
the stoichiometric coefficient for reagent \( j \) in reaction \( r \); \( k_p \) and \( k_w \) are rate constants of forward and inverse reactions, respectively, \( X_p \) is the molar concentration of a component \( j \) in reaction \( r \); \( \eta_p \) is the exponent for reagent \( j \) in reaction \( r \); \( \gamma_p \) is the efficiency of the component \( j \) in reaction \( r \) as a third body.

The rate constants of the forward and inverse reactions are calculated according to the Arrhenius law:

\[
k_{f,r} = A_r T^{\beta_r} e^{-E_r/RT}
\]

Here \( A_r \) is pre-exponential factor, \( T^{\beta_r} \) is the dimensionless temperature indicator, \( E_r \) is the reaction activation energy, \( R \) is the universal gas constant.

Combustion model “Species Transport”, Finite-Rate / No TCI was used in all calculations of flows with chemical reactions as recommended in [19]. In the “Species Transport” model, the local mass of each of the reactants is calculated by solving the following convective-diffusion equation:

\[
\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \mathbf{v} Y_i) = \nabla \cdot (\mathbf{J}_i) + R_i + S_i.
\]

Here \( R_i \) is the rate of additional production of reagent \( i \) during a chemical reaction, \( S_i \) is user-specified rate of reagent production. This equation is to be solved for \( N-1 \) reagents (\( N \) is the number of all included reagents into the system). The mass of reagent \( N \) is equal to the difference between the total mass of the system and the mass of the rest of the calculated \( N-1 \) reagents. To avoid numerical errors, it is recommended to set the \( N \)-th reagent to a substance having the maximum mass fraction in the system, for example, nitrogen for reactions in air flow [20].

Numerical simulation of a supersonic flow with complicated shock-wave structure was carried out using the ANSYS software package for engineering analysis and the Fluent computational fluid dynamics model. The associated “Density-Based” solver was selected for the solver settings. Equation discretization scheme was as follows: “Implicit” – implicit iterative solver, “Roe-FDS” – numerical scheme for calculating numerical fluxes through the faces of computational cells, “Least Squares Cell Based” – method for approximation of gradients of flow parameters; second order of discretization of all other equations.

The computational mesh was refined near the body walls to improve the computation’s quality in areas having large gradients in the flow parameters. The computational grid has about 900 thousand cells.

3. Numerical results and discussion

In the first series of the present numerical experiments, the flow in the entrance part of the supersonic inlet was simulated. The Mach number of the undisturbed flow was \( M=5 \), and the gas specific heats ratio was \( \gamma=1.4 \). The following parameters corresponded to the well-known von Neumann criterion [21, 22] of regular / Mach reflection transition which is recognized to be preferable for steady flows: flow deflection angle (wedge angle) \( \beta_1=20.862^\circ \), incident shock slope angle \( \alpha_i=30.796^\circ \), incident shock strength (ratio of static pressures across the shock) \( J_i=7.479 \). To obtain Mach reflection with sufficient size of the Mach stem, we specified the flow deflection angle (wedge angle) to be \( \beta_i=31^\circ \).

Flow field simulation (distribution of local flow Mach numbers) is shown in Figure 1. The height of the forming Mach stem is about half of the width of the entrance section. The flow behind the Mach stem strongly resembles a quasi-one-dimensional flow in a de Laval (“convergent – divergent”) nozzle, having a shift from subsonic flow velocity to supersonic flow in the narrowest section of that “virtual nozzle” [5, 23, 24]. The turn of the slipstream that bounds the “virtual nozzle” occurs under the influence of the expansion waves that falls from the tail (the rear edge) of the streamlined triangle.

Temperature field (Figure 2) shows that high temperature is reached in several times (up to 1800 K) downstream of the Mach stem, than behind the reflected wave. It creates favourable conditions for ignition, combustion, and detonation of fuel that penetrates through the Mach stem. However, for the flow downstream the reflected shock, such conditions are not so appropriate. But the distribution of stagnation pressures (Figure 3) reveals that the flow behind the reflected oblique shock has total pressure several times higher than the total pressure in a “virtual nozzle” flow, behind the Mach stem.
Therefore, the flow downstream of the reflected shock can be more effectively applied to the combustion chamber of a “classical” ramjet.

**Figure 1.** Distribution of flow Mach numbers in the narrowing channel between two wedges.

**Figure 2.** Distribution of static temperature in the narrowing channel between two wedges.

**Figure 3.** Total pressure distribution in the narrowing channel between two wedges.

For separating the flows, solid walls are needed; contours of those separating walls must correspond to the shape of the flow slipstream emanating from the triple point of Mach reflection. Approximate analytical models [3-8] were elaborated to predict the Mach stem height and contour of the slipstream in a flow without chemical reactions. A new analytical model is necessary for taking into account the heat efflux (for example, impulse efflux due to detonation behind the Mach stem).
Dependence of dimensionless (i.e., divided to the width of inlet entrance section) Mach stem size on the wedge angle at situations shown in Figures 1-3 is presented in Table 1.

Table 1. Dependence of the dimensionless Mach stem height $y_T$ on the wedge angle $\beta_1$.

| Case No. | $\beta_1$, deg. | $y_T$  |
|----------|----------------|--------|
| 1        | 26.96          | 0.05   |
| 2        | 27.96          | 0.13   |
| 3        | 28.96          | 0.19   |
| 4        | 29.96          | 0.28   |
| 5        | 30.96          | 0.36   |
| 6        | 31.10          | 0.37   |
| 7        | 31.20          | 0.38   |
| 8        | 31.30          | 0.39   |
| 9        | 31.50          | 0.41   |
| 10       | 31.70          | 0.44   |

For simulating the gas flow in the channel downstream of the triangular entrance, we adopted the geometrical model of a long channel (see Figure 4, all sizes are given in millimetres).

Figure 4. Geometry of simulated channel, all sizes are given in millimetres.

The flowfield in the absence of fuel supply (distribution of static temperatures) is shown in Figure 5 with “multi-barrel” and gradually smearing shock-wave structure, typical for non-isobaric supersonic jet flow are evident in this figure.
The method adopted for simulating the flow behind the Mach stem (shown in Figure 5); that includes chemical reactions excited by the high temperature is to be described in the following. First, we consider the case of air flow at Mach number $M=5$ as, presented earlier, but the geometry of the long channel is as shown in Figure 4. After completing all computations of steady flow without chemical reactions, we introduce fuel (hydrocarbons) through a small planar slot ($A$ in Figure 4); half-width of this fuel entrance slot is equal to 10 millimeters. We added the fuel (methane) source to the steady air flow-field obtained for the flow without taking the chemical reactions into account, and, after some transient process, we reached a new steady state of the reacting flow (see Figures 6-8).

Addition of combustible fuel (methane) into the reacting flow is shown in Figure 6 via distribution of its mass fraction. It is evident that almost all methane added through a thin chink reacts with the formation of carbon dioxide (see also Figure 7).
Figure 8. Distribution of gas static temperature in reacting flow in long channel.

Distribution of the gas static temperature, shown in Figure 8, reveals that the highest value of temperature is equal to 3320 K. Distribution of the carbon dioxide mass fraction, shown in Figure 7, shows that gas-fuel mixture reacts only behind the central part of the main shock (i.e., after the almost normal Mach stem). Consequently, it is the Mach stem that provoked the mixture ignition. Since the region of fuel combustion does not touch the channel’s walls, problems of heat protection are avoided.

Due to the chemical reactions, the Mach stem is conveyed upward facing the stream flow, unlike the case of no chemical reactions (non-reactive flow, shown in Figures 1-5). The distance from planar slot to the Mach stem is about 2.6 meters, and in this distance the methane flow becomes dispersed. But the concentration of methane in the fuel-air mixture is enough for igniting the mixture. The length of the flame plume behind the Mach stem reaches almost 6 meters.

Change in the shock configuration due to chemical reactions can also be seen. The reflected shock approaches the trail edge of the wedge, and the Mach shock shifts upstream. Nevertheless, the triple point structure observed in a single Mach reflection in steady supersonic flow remains qualitatively unchanged.

4. Conclusion
Heat energy efflux due to the chemical reactions downstream of the Mach stem causes changes in the triple point height, the total pressure losses, and the shape of the Mach stem. To analyze the influence of the heat energy efflux on the Mach reflection structure, it is necessary to elaborate on the engineering analytical model used for simulating Mach reflection with impulse energy release. The results obtained in the present study could be used as benchmarks for newly-created approximate analytical models and their application in simulating ramjets and combined jet engines flows.

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