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Numerical simulation of hypersonic flow with non-equilibrium chemical reactions around sphere

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Abstract

High-temperature effects have a significant impact on the characteristics of aircraft moving at super- and hypersonic speeds. Due to the complexity of setting up a physical experiment, methods of mathematical modelling play an important role in finding the characteristics of hypersonic aircraft. Numerical modelling of super- and hypersonic air flow around the sphere is carried out taking into account high-temperature effects and non-equilibrium chemical reactions. The mathematical model includes equations of gas dynamics, equations of the turbulence model and equations of chemical kinetics. A critical review of the various models that are used to find the stand-off distance is provided. The results of numerical calculations on the distribution of flow quantities in the shock layer and the stand-off distance at different freestream Mach numbers are presented. The results of numerical calculations in a wide range of freestream Mach numbers are compared with the experimental data and computational results of other researchers. Standoff distance is computed at various Mach number and heights during a flight in the atmosphere at hypersonic speed.

Keywords

Flight safety, hypersonic flow, high-temperature effects, shock wave, chemical reactions, sphere.

1 Introduction

The evaluation of drag and heat flux during hypersonic flight is of interest for design and optimization of future operational hypersonic vehicles [1]. Ground based experiments and flight tests are encountered with significant problems and in many cases are not able to provide relevant information to the thermal protection system. The methods of computational fluid dynamics (CFD) are potentially useful in hypersonic research allowing to reduce the risk in flight tests and requirements to ground based experiments.

The main features of hypersonic flows are a significant increase in temperature behind the front of bow shock, strong deceleration of flow in the shock layer and aerodynamic heating of aircraft surface. The complexity of the phenomena accompanying the flight of hypersonic aircraft practically excludes the possibility of full simulation of full-scale flow conditions in shock tubes, in connection with which the methods of mathematical modelling become important. Numerical modelling of hypersonic flows relies on the use of complex mathematical models which include equations of unsteady three-dimensional compressible flow, equations of turbulence model, equations of state and equations of chemical kinetics.

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The choice of level of complexity of fluid model is usually based on comparison of CFD results with experimental data [2, 3].

Many studies consider flow regimes at moderate Mach numbers. The pattern of the flow around the blunt head of an object flying in the Earth atmosphere (or in a gaseous medium that simulates it), obtained by numerically integrating the Euler or Navier–Stokes equations, has a fairly typical form in a wide range of parameters. During high-speed flight in the atmosphere, a strong shock arises in front of aircraft, and intensity of shock (it represents the ratio of pressures before and behind gas dynamic discontinuity) significantly depends on the flight speed. The maximum pressure and temperature are reached at the stagnation point of the flow. At a supersonic flight speed, the front of the bow shock wave has a small thickness, and for its mathematical description a model of an infinitely thin discontinuity is adopted, upon passing through which the flow quantities change in an abrupt manner. The influence of viscosity during supersonic flight affects only a thin boundary layer adjacent to the surface of the streamlined body [4, 5].

The change in gas properties during hypersonic flow determines the change in flow characteristics. In hypersonic flow, the bow shock wave has a diffuse front, which is associated not only with physical effects (excitation of vibrational degrees of freedom in diatomic and polyatomic gases), but also with gas-dynamic processes (a decrease in the density of the gaseous medium when flying at high altitudes). With increasing flight altitude, the Reynolds number decreases, and the thickness of the boundary layer increases. A closed viscous shock layer is formed, which is a single structure integrated from the shock layer of the free-flow deceleration (thin bow shock at supersonic) and from the wide region of interaction of the flow with the surface (rather thin boundary layer at supersonic).

The simplest body with a streamlined surface of constant curvature is the sphere. The problem of hypersonic flow around a sphere is of independent importance, since the nose of many hypersonic aircraft has a blunt shape, and is also used to test various computational algorithms. The dependence of drag coefficient of sphere is discussed in [6–8] in a wide range of Mach numbers. Dependence of standoff distance on Mach number is discussed in [9, 10]. A hypersonic flow of a perfect gas around a sphere is considered at Mach numbers up to 20 in [11]. The numerical method is based on splitting the system of equations for the dynamics of a viscous compressible gas into two groups of equations. The Navier–Stokes equations are integrated using AUSM finite difference schemes, and the energy conservation equation is integrated using the implicit method and a five point finite difference scheme. The assumption of a perfect gas leads to an overestimated temperature of the compressed layer [12]. The influence of numerical dissipation on the accuracy of calculations at hypersonic speeds is discussed in [13]. A study of steady state and unsteady flows around bodies of various configurations with model of inviscid gas (Euler equations) and model of viscous gas (Navier-Stokes equations) is carried out in a wide range of parameters. The carbuncle phenomena discovered in computer modelling of the aerodynamics of high-speed flight is considered in [14].

Experimental and numerical data on hypersonic flow around a sphere are given in [15–17]. Experimental and computational results are used to design a semi-empirical method for evaluation of aerodynamic characteristics of complex geometry bodies [18, 19]. Analysis of the local formulae through the comparison of other results show that these correlations have a good match of the pressure and skin friction coefficients at high altitudes. Semi-empirical correlations developed in [18, 19] have to be corrected in continuum low density regime. The global bridging formula to compute the aerodynamic force coefficients is proposed in [20].

The results of numerical simulation of a hypersonic flow around a sphere taking into account equilibrium and non-equilibrium chemical reactions are discussed in [21–24]. High-
temperature effects are taken into account in [25]. At low Knudsen numbers, the Navier–Stokes equations are solved, and calculations in a rarefied flow are carried out using the Monte Carlo method. A mathematical model describing the processes of heat and mass transfer occurring on the surface of a blunt body during flight in the atmosphere at hypersonic speed is presented in [26]. Air is treated as a mixture of reactive gases. In [27, 28], the air model proposed in [29] is used to simulate hypersonic flow around a sphere taking into account high-temperature effects.

The influence of equilibrium and non-equilibrium chemical reactions on the aerodynamic characteristics of a descent spacecraft of segmental and conical shape is studied in [30]. The non-equilibrium of chemical reactions manifests itself in a narrow gradient layer behind the shock wave due to the initial conditions for the constancy of the gas composition on the shock wave. The influence of chemical reactions, non-equilibrium excitation of internal degrees of freedom of molecules and multi-component diffusion on flow parameters and convective heat transfer are considered in [31]. Dissociation and ionization absorb up to 75% of the flow energy, which makes many results of the gas dynamics of a perfect gas inapplicable. Finite difference schemes for solving the Euler equations describing flows of real gases are discussed in [32]. A number of benchmark problems are proposed in [33] to test the performance of turbulence models in hypersonic flows.

One of the main problems of hypersonic aerodynamics is the problem of numerical modelling of hypersonic gas flows taking into account real physical and chemical processes occurring in the shock layer near blunt bodies. Numerical modelling of complex three-dimensional problems of hypersonic flow, taking into account chemical processes that depend on many defining parameters, requires high computational resources [34]. Investigation of the dependencies of aerodynamic and thermal characteristics on altitude and flight speed, angle of attack, geometric shape of the body requires calculations of numerous variants. In this regard, it is important to develop effective numerical methods that can reduce computational costs and obtain solutions that are useful for setting up experiments and interpreting the results of numerical modelling, allowing their use in parametric calculations.

This study discusses the construction and implementation of a mathematical model intended for numerical simulation of hypersonic flow around a sphere taking into account non-equilibrium chemical processes occurring in high-temperature air. The results of numerical calculations for the shock layer thickness obtained with various approaches are presented. The results obtained make it possible to establish the extent to which it is possible to use the basic principles of ideal gas thermodynamics for a non-perfect gas.

## 2 Mathematical model

Flow simulation with the full Navier–Stokes equations allows to study the structure of complex three-dimensional flows with zones of viscous and inviscid interaction, shock waves, separation regions.

### 2.1 Main assumptions

The hypersonic flow around the body at high altitudes has a number of specific features associated with the rarefaction of atmosphere, which must be taken into account when developing a mathematical model. Under such conditions, it is necessary to establish the possibility of applying the model of a continuous medium and the use of Navier–Stokes equations. In a compressed boundary layer, air loses the properties of an ideal gas. In
this case, chemical reactions of dissociation, recombination and ionization begin to play an essential role.

The Knudsen number represents the ratio of the mean free path of molecules or atoms, \( l \), and the characteristic linear size, \( L \), and expressed as \( \text{Kn} = l/L \). The continuum condition is satisfied when the Knudsen test is in the range \( 0 < \text{Kn} < 0.01 \). The flow is described with Navier–Stokes equations, and no-slip condition for the tangential velocity component is used on the surface. Navier–Stokes equations are also applied in the transient mode, which is realized in the range of variation of the Knudsen criterion \( 0.01 < \text{Kn} < 0.1 \). The slip condition is used for the tangential velocity on the wall [35]. For Knudsen numbers exceeding 0.1, the flow is free molecular and is not described by the Navier–Stokes equations.

For the calculation conditions, the mean free path of particles in a shock layer (\( l = 2.31 \cdot 10^{-4} \text{ m} \)) is approximately one order of magnitude less than the characteristic size of the body (\( L = 1.27 \cdot 10^{-2} \text{ m} \)). The flow is described with Navier–Stokes equations, and no-slip and no-penetration boundary conditions for the tangential and normal velocities are applied to the wall.

2.2 Governing equations

The modelling of air flow around a sphere with non-equilibrium chemical reactions is considered. The mathematical model includes equations describing the flow of a viscous compressible gas taking into account the dissociation, recombination, exchange reactions and ionization. An equilibrium distribution of the mixture components over the translational and all internal degrees of freedom is assumed. The system of equations includes:

— continuity equation for component \( i \)

\[
\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}) = R_i, \tag{1}
\]

— momentum equation

\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + p) = 0, \tag{2}
\]

— total energy equation

\[
\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot [(\rho \varepsilon + p) \mathbf{v}] = 0. \tag{3}
\]

Here, \( \rho \) and \( \rho_i \) are densities of the mixture and component \( i \) of the mixture.

The equation of state is

\[
p = nkT = \rho \frac{RT}{M} = \sum_i \rho_i \frac{R}{M_i} T = \sum_i X_i RT, \tag{4}
\]

where \( n \) is numerical density of the mixture, \( R \) is universal gas constant, \( M_i \) and \( M \) are molar mass of mixture component and molar mass of the mixture, \( X_i = \rho_i/M_i \) is molar fraction of component \( i \), \( k \) is Boltzmann constant.

The total energy per unit mass of the mixture is the sum of the internal and kinetic energies

\[
\varepsilon = u + \frac{1}{2} v^2. \tag{5}
\]
The internal energy per unit mass of the mixture is the sum of the specific translational $e_{tr}$, rotational $e_{rot}$, vibrational $e_{vibr}$, electron $e_{el}$ energies, and the formation energy $e_f$

$$\rho u = e_{tr} + e_{rot} + e_{vibr} + e_{el} + e_f.$$  \hspace{1cm} (6)

Here

$$e_{tr} = \frac{3}{2} \rho \frac{R}{M} T, \quad e_f = \sum_i \varepsilon^i_f N_a X_i,$$

$$e_{int} = e_{rot} + e_{vibr} + e_{el} = \sum_i \frac{X_i}{Z_i} \sum_{naj} g^i_n g^i_q g^i_j \varepsilon^i_{naj} N_a \exp \left( -\frac{\varepsilon^i_{naj}}{k_B T} \right),$$

$$\varepsilon^i_{naj} = \varepsilon^i_n + \varepsilon^{in}_q + \varepsilon^{inq}_j,$$

where $N_a$ is Avogadro number, $\varepsilon^i_n$ is energy of formation of particle $i$, $\varepsilon^i_q$ is energy of electron level $n$, $\varepsilon^{in}_q$ and $\varepsilon^{inq}_j$ are vibrational and rotational energies of molecules on vibrational level $q$ and rotational level $j$. The internal statistical sum, taking into account electronic excitation, has the form:

— for molecules

$$Z^i_{int} = \sum_{naj} g^i_n g^i_q g^i_j \exp \left( -\frac{\varepsilon^i_{naj}}{k_B T} \right);$$

— for atoms

$$Z^i_{int} = \sum_n g^i_n \exp \left( -\frac{\varepsilon^i_n}{k_B T} \right).$$

Here $g^i_n$, $g^i_q$ and $g^i_j$ are electronic, vibrational and rotational weights.

The source term in the right hand side of the equation (1) is written as

$$R_i = M_i \sum_r (\nu^+_{i,r} - \nu^-_{i,r}) \left( k_{f,r} \prod_{j=1}^{L} X^{
u^+_{i,r}}_j - k_{b,r} \prod_{j=1}^{L} X^{
u^-_{i,r}}_j \right).$$  \hspace{1cm} (7)

Stoichiometric coefficients $\nu^+_{i,r}$ and $\nu^-_{i,r}$ of direct and reverse reactions with number $r$ are found from the relations

$$\sum_{i=1}^{L} \nu^+_{i,r} A_i = \sum_{i=1}^{L} \nu^-_{i,r} A_i.$$  

The rate coefficients of the forward and reverse reactions, $k_{f,r}$ and $k_{b,r}$, are related by the relation for the equilibrium constant

$$K_r = \frac{k_{b,r}}{k_{f,r}} = \frac{\prod_i Z_i^{\nu^+_{i,r}}}{\prod_i Z_i^{\nu^-_{i,r}}} \exp \left( -\frac{Q_r}{kT} \right).$$ \hspace{1cm} (8)

The total statistical sum included in the ratio (8) is the product of the statistical sums of the translational and internal degrees of freedom

$$Z_i = Z^i_{tr} Z^i_{int}.$$
The progressive statistical sum is calculated by the formula

\[ Z^{tr}_i = \left( \frac{2\pi m_i k_B T}{h^2} \right)^{3/2} \frac{RT}{\rho}, \]

where \( m_i \) is mass of particle \( i \), and \( h \) is Plank constant.

The heat release of the reaction is represented as

\[ Q_r = \sum_{i \in \text{reagents}} D_i - \sum_{i \in \text{products}} D_i, \]

where \( D_i \) is energy of dissociation of component \( i \).

In calculations, the generalized Arrhenius law is used to describe the rate coefficients of chemical reactions

\[ k_{f,r} = A_{f,r} T_{b,r} \exp \left( -\frac{E_{f,r}}{k_B T} \right). \quad (9) \]

To simplify the numerical implementation, the energy of the internal degrees of freedom is found using the reference data [36] based on the relationship between the internal energy of the mixture and the specific enthalpy of its components

\[ u = h - \frac{p}{\rho} = \sum_i \frac{p_i}{\rho} h_i - \frac{p}{\rho}. \quad (10) \]

It is also possible in the calculations to use the temperature dependencies of the equilibrium constants for various processes.

2.3 Turbulence model

The Spalart–Allmares turbulence model solves one equation for the transfer of the modified turbulent viscosity \( \tilde{\nu} \), which has the form

\[ \frac{d\tilde{\nu}}{dt} = P^{\nu} - D^{\nu} + \frac{1}{\sigma} [\nabla \cdot \{ (\nu + \tilde{\nu}) \nabla \tilde{\nu} \} + C_{l2} \{ (\nabla \tilde{\nu}) \cdot (\nabla \tilde{\nu}) \}] + f_{t1} \Delta u^2. \]

Modified turbulent viscosity is defined in terms of kinematic turbulent viscosity

\[ \tilde{\nu} = \frac{\nu_t}{f_{\nu1}}, \]

where

\[ f_{\nu1} = \frac{\chi^3}{\chi^3 + c_{\nu1}^3}, \quad \chi = \frac{\tilde{\nu}}{\nu}. \]

The turbulence generation term \( P^{\nu} \) and the dissipative term \( D^{\nu} \) are defined by the following expressions

\[ P^{\nu} = c_{b1} (1 - f_{t2}) \tilde{S}_\nu, \quad D^{\nu} = \left( c_{w1} f_w - \frac{c_{b1}}{k^2 f_{t2}} \right) \left( \frac{\tilde{\nu}}{d_w} \right)^2. \]

Here

\[ \tilde{S} = \Omega + f_{w2} \frac{\tilde{\nu}}{(kd_w)^2}, \quad f_{\nu2} = 1 - \frac{\chi}{1 + \chi f_{\nu1}}. \]
Correction function are

\[ f_w = g \left( \frac{1 + c_{w3}^6}{g^6 + c_{w3}^3} \right)^{\frac{1}{6}}, \quad g = r + c_{w2}(r^6 - r), \quad r = \frac{\nu}{S(kd_w)^2}, \]

where \( d_w \) is distance to the wall, \( \kappa = 0.41 \) is von Karman constant. The rate of vorticity tensor is found from the relation

\[ \Omega = (2\Omega_{ij}\Omega_{ij})^{1/2}, \quad \Omega_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right). \]

The function \( f_{t2} \) is responsible for the suppression of a spontaneous or numerical laminar-turbulent transition in the boundary layer and is determined by the expression

\[ f_{t2} = C_{t3} \exp \left( -C_{t4} \chi^2 \right). \]

The source term \( f_{t1} \Delta u^2 \) in the turbulent viscosity transfer equation is responsible for the initiation of the laminar-turbulent transition at a given point. The constants defining the model have the following values \( \sigma = 2/3, c_{b1} = 0.1355, c_{b2} = 0.622, c_{w2} = 0.3, c_{w3} = 2, c_{w1} = 7.1, c_{t3} = 1.2, c_{t4} = 0.5 \). Wherein

\[ c_{w1} = \frac{c_{b1}}{k^2} + \frac{1 + c_{b2}}{\sigma}. \]

2.4 Thermodynamics properties of air

Air is considered as a multi-component gas consisting of \( n \) components. The partial density of the \( i \)th air component is found from the equation of state

\[ \rho_i = \frac{p_i}{R_i T}, \]

where \( p_i \) is partial pressure of component \( i \), \( R_i \) is gas constant of component \( i \) in the mixture. The gas constant is found from \( R_i = R_0 / M_i \), where \( R_0 \) is universal gas constant, \( M_i \) is molar mass of component \( i \). The density of the mixture is found from the equation of state

\[ \rho = \frac{p}{RT}, \]

where \( p \) is the pressure of the mixture, \( M \) is the molar mass of the mixture. The mixture pressure is found from Dalton law

\[ p = \sum_{i=1}^{n} p_i. \]

The molar mass of the mixture is found from the ratio

\[ M = \sum_{i=1}^{n} c_i M_i. \]

where \( M_i \) is molar mass of component \( i \), \( c_i \) is mass fraction of component \( i \) of the mixture \( (c_i = \rho_i / \rho) \).

The enthalpy of the mixture is

\[ h = \sum_{i=1}^{n} c_i h_i. \]
The enthalpy of the component $i$ of the mixture is found from the relation

$$h_i = \int_{T_1}^{T_2} c_{pi}dT.$$ 

The specific heat capacity of each component $i$ of the mixture is specified as a piecewise linear dependence as a function of temperature and pressure. The average specific heat of the gas mixture is calculated using the relation

$$c = \sum_{i=1}^{n} c_i C_{pi},$$

where $c_{pi}$ is specific heat capacity of component $i$.

The viscosity and thermal conductivity of the gas mixture are determined by the formulas

$$\mu = \sum_{i=1}^{n} \frac{x_i \mu_i}{\sum_{j=1}^{n} x_j \varphi_{ij}}, \quad \lambda = \sum_{i=1}^{n} \frac{x_i \lambda_i}{\sum_{j=1}^{n} x_j \varphi_{ij}},$$

where $x_i$ is molar fraction of component $i$. The factor $\varphi_{ij}$ is calculation using the relation

$$\varphi_{ij} = \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{1/2} \left( \frac{M_{wj}}{M_{wi}} \right)^{1/4} \right]^2 \left[ 8 \left( 1 + \frac{M_{wi}}{M_{wj}} \right) \right]^{-1/2}.$$

The viscosity of each component is calculated using the Sutherland formula

$$\mu_i = \mu_{0i} \left( \frac{T}{T_0} \right)^{3/2} \frac{T_0 + S}{T + S},$$

where $\mu_{0i}$ is dynamic viscosity of component $i$ at temperature $T_0$, $S$ is effective temperature (Sutherland constant, $S = 110.4$ K). For air, $\mu_0 = 1.76 \cdot 10^{-5}$ Pa s at $T_0 = 273.14$ K. The thermal conductivity of each component is determined using the relationship from the kinetic theory of gases

$$\lambda_i = \frac{15}{4} \frac{R_0}{M_i} \mu_i \left( \frac{4 \ c_{pi} M_i}{15 \ R_0} + \frac{1}{3} \right).$$

### 2.5 Chemical kinetics

Taking into account the real properties of the gas mixture formed near the streamlined body due to heating during deceleration of the flow increases the number of differential equations in accordance with the number of the mixture components under consideration. For each of the components of the gas mixture $i = 1, \ldots, N - 1$, an equation of mass concentration is solved

$$\frac{\partial p_i c_i}{\partial t} + \nabla (\rho_i \mathbf{v} c_i) = -\nabla J_i + \omega_i,$$

where $J_i$ is the vector of the diffusion flux of the $i$ component, $\omega_i$ is the mass rate of formation of the $i$ component in chemical reactions. To describe the model of the reacting gas, the $N - 1$ diffusion equations are used, to which the condition is added

$$\sum_{i=1}^{N} c_i = 1,$$
where $N$ is the number of mixture components.

The diffusion flux of the component $i$ is calculated from Fick law

$$
\mathbf{J}_i = -\rho D_{i,m} \nabla c_i - D_{T,i} \frac{\nabla T}{T},
$$

where $D_{i,m}$ and $D_{T,i}$ are coefficients of diffusion and thermodiffusion of component $i$.

The mass rate of formation of component $i$ is calculated using a finite-rate chemical model (the influence of turbulent fluctuations is ignored). The relationship between temperature and the rate constant of a chemical reaction is found from Arrhenius equation. The rate of formation of component $i$ in chemical reactions is expressed as

$$
\omega_i = M_i \sum_{r=1}^{N_r} \tilde{\omega}_{i,r},
$$

where $M_i$ is molar mass of component $i$, $\tilde{\omega}_{i,r}$ is molar rate of formation/decay of the $i$ component in $r$th reaction. The summation takes place over the reactions in which the component $i$ is involved ($N_r$ is understood as the number of such chemical reactions). In general, the reaction $r$ is written as

$$
\sum_{i=1}^{N} \nu'_{i,r} S_i \left( k_{f,r} \prod_{j=1}^{N} C'_{j,r} - k_{b,r} \prod_{j=1}^{N} C''_{j,r} \right),
$$

where $\nu'_{i,r}$ is stoichiometric coefficient of reagent $i$ in reaction $r$, $\nu''_{i,r}$ is stoichiometric coefficient of product $i$ in reaction $r$, $k_{f,r}$ is the rate coefficient of forward reaction, $k_{b,r}$ is the rate coefficient of reverse reaction, and $S_i$ denotes the $i$th component.

The molar rate of formation/decay of $i$th component in reaction $r$ is determined from the formula

$$
\tilde{\omega}_{i,r} = \Gamma_r \left( \nu''_{i,r} - \nu'_{i,r} \right) \left( k_{f,r} \prod_{j=1}^{N} C'_{j,r} - k_{b,r} \prod_{j=1}^{N} C''_{j,r} \right),
$$

where $C_{j,r}$ is the molar concentration of component $j$ in reaction $r$, $\nu'_{i,r}$ is the rate coefficient of component $i$ in reaction $r$, $\nu''_{i,r}$ is the rate coefficient of product of component $i$ in reaction $r$, $k_{f,r}$ is the rate coefficient of forward reaction, $k_{b,r}$ is the rate coefficient of reverse reaction. The coefficient $\Gamma_r$ takes into account the effect of the third bodies on reaction $r$. It is found from equation

$$
\Gamma_r = \sum_{j=1}^{N} \gamma_{j,r} C_{j,r},
$$

where $\gamma_{j,r}$ is the efficiency of component $j$ in reaction $r$ as a third body. When using a model of air consisting of 5 components, the coefficient $\Gamma_r$ differs from unity in reactions involving a third non-reactive particle, for example, in the reaction of dissociation of an oxygen molecule by a nitrogen molecule that does not decompose ($O_2+N_2 = 2O+N_2$). This makes it possible, instead of a set of reactions of the form $O_2+M=2O+M$, where $M=N$, $O$, $N_2$, $O_2$, $NO$, to write just one reaction (in the Arrhenius formula for these reactions only the pre-exponential factor is different), introducing the efficiency coefficient of the third particle in this reaction $\gamma_{j,r}$. In other reactions $\Gamma_r = 1$. The effectiveness of each chemical component as a third body is shown in Table 1.
Table 1. The effectiveness of chemical components as a third body

<table>
<thead>
<tr>
<th>Reaction</th>
<th>O&lt;sub&gt;2&lt;/sub&gt;</th>
<th>N&lt;sub&gt;2&lt;/sub&gt;</th>
<th>NO</th>
<th>N</th>
<th>O</th>
</tr>
</thead>
<tbody>
<tr>
<td>O&lt;sub&gt;2&lt;/sub&gt;+M=2O+M</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>N&lt;sub&gt;2&lt;/sub&gt;+M=2N+M</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>4.28</td>
<td>4.28</td>
</tr>
<tr>
<td>NO+M=N+O+M</td>
<td>1</td>
<td>1</td>
<td>22</td>
<td>22</td>
<td>22</td>
</tr>
</tbody>
</table>

The direct reaction rate coefficient $k_{f,r}$ is calculated using the Arrhenius equation

$$k_{f,r} = A_r T^{\beta_r} \exp \left( -\frac{E_r}{R_0 T} \right),$$

where $A_r$ is the pre-exponential factor, $\beta_r$ is the temperature exponent, $E_r$ is the activation energy of the reaction, $R_0$ is the universal gas constant. In the case of a reversible reaction, the reverse reaction rate coefficient is calculated using the forward reaction rate constant by the formula

$$k_{b,r} = \frac{f_{f,r}}{K_r},$$

where $K_r$ is the equilibrium constant of the reaction $r$. The equilibrium constant is determined by the following relationship

$$K_r = \exp \left( \frac{\Delta S_r^0}{R} - \frac{\Delta H_r^0}{RT} \right) \left( p_{\text{atm}} \right)^{\sum_{i=1}^{N} (v'_{i,r} - v''_{i,r})},$$

where $p_{\text{atm}}$ is the atmospheric pressure. The exponent expresses the change in the Gibbs energy, and the entropy and enthalpy factors are determined, respectively, by the expressions

$$\Delta S_r^0 = \sum_{i=1}^{N} (v''_{i,r} - v'_{i,r}) S_i^0;$$

$$\Delta H_r^0 = \sum_{i=1}^{N} (v''_{i,r} - v'_{i,r}) h_i^0;$$

Here $S_i^0$ and $h_i^0$ are entropy of standard state and enthalpy of standard state.

An additional source term is introduced into the right side of the energy equation, which takes into account the release of thermal energy

$$S_h = -\sum_{j=1}^{n} \frac{h_j^0}{M_j} \omega_j,$$

where $h_j^0$ is enthalpy of formation of component $j$.

3 Model of high-temperature air

The code developed considers air as a mixture of five species (O<sub>2</sub>, N<sub>2</sub>, O, N and NO), and assumes that 17 forward/reverse chemical reactions take place between these species (there are 15 dissociation and recombination reactions and 2 exchange reactions). The chemical models taking into account dissociation, recombination and exchange reactions are proposed in [37–39].
3.1 Dissociation and recombination chemical models

For the model proposed in [37], the forward rate coefficient, \( k_f \), and the reverse rate coefficient, \( k_r \), are expressed using the Arrhenius equation

\[
k_s = C_s T^{n_s} \exp \left( -\frac{E_{a,s}}{kT} \right).
\]

Here, \( C_s \) is the pre-exponential factor, \( n \) is the temperature exponent, \( E_a \) is the specific activation energy, \( k \) is Boltzmann constant. The ratio \( E_{a,s} / (kT) \) represents the characteristic temperature of chemical reaction. Subscript \( s = f \) corresponds to forward reaction \((s = f)\), and subscript \( s = r \) corresponds to reverse reaction. The chemical reactions, reaction rates and activation energies are reported in Table 2.

<table>
<thead>
<tr>
<th>No</th>
<th>Reaction</th>
<th>( C_f ) [m^3/(mol s)]</th>
<th>( n_f )</th>
<th>( E_{a,f}/k ), K</th>
<th>( C_r ) [m^6/(mol^2 s)]</th>
<th>( n_r )</th>
<th>( E_{a,r}/k ), K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( O_2+N=O+O+N )</td>
<td>3.99 \times 10^{-12}</td>
<td>-1</td>
<td>59500</td>
<td>8.30 \times 10^{-45}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>( O_2+NO=O+O+NO )</td>
<td>5.99 \times 10^{-12}</td>
<td>-1</td>
<td>59500</td>
<td>8.30 \times 10^{-45}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>( O_2+N_2=O+O+N_2 )</td>
<td>1.20 \times 10^{-11}</td>
<td>-1</td>
<td>59500</td>
<td>1.66 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>( O_2+O_2=O+O+O_2 )</td>
<td>5.39 \times 10^{-11}</td>
<td>-1</td>
<td>59500</td>
<td>7.47 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>( O_2+O=O+O+O )</td>
<td>1.50 \times 10^{-10}</td>
<td>-1</td>
<td>59500</td>
<td>2.07 \times 10^{-43}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>( N_2+O+N+O )</td>
<td>3.18 \times 10^{-13}</td>
<td>-0.5</td>
<td>113200</td>
<td>3.01 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>( N_2+O_2=N+O+N_2 )</td>
<td>3.18 \times 10^{-13}</td>
<td>-0.5</td>
<td>113200</td>
<td>3.01 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>( N_2+NO=O+N+O )</td>
<td>3.18 \times 10^{-13}</td>
<td>-0.5</td>
<td>113200</td>
<td>3.01 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>9</td>
<td>( N_2+N_2=O+N+O )</td>
<td>7.97 \times 10^{-13}</td>
<td>-0.5</td>
<td>113200</td>
<td>7.51 \times 10^{-44}</td>
<td>-0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>( N_2+N=N+N+N )</td>
<td>6.90 \times 10^{-8}</td>
<td>-1.5</td>
<td>113200</td>
<td>6.42 \times 10^{-39}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>11</td>
<td>( NO+NO=O+O+N_2 )</td>
<td>6.59 \times 10^{-10}</td>
<td>-1.5</td>
<td>75500</td>
<td>2.78 \times 10^{-40}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>12</td>
<td>( NO+O_2=N+O+O_2 )</td>
<td>6.59 \times 10^{-10}</td>
<td>-1.5</td>
<td>75500</td>
<td>2.78 \times 10^{-40}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>( NO+NO=O+O+NO )</td>
<td>1.32 \times 10^{-8}</td>
<td>-1.5</td>
<td>75500</td>
<td>5.57 \times 10^{-39}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>( NO+O=O+O+O )</td>
<td>1.32 \times 10^{-8}</td>
<td>-1.5</td>
<td>75500</td>
<td>5.57 \times 10^{-39}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>( NO+N=O+N+O )</td>
<td>1.32 \times 10^{-8}</td>
<td>-1.5</td>
<td>75500</td>
<td>5.57 \times 10^{-39}</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
</tbody>
</table>

The forward reaction rate coefficients of the model proposed in [38] are found from Arrhenius equation

\[
k_f = C_f T_c^{n_f} \exp \left( -\frac{E_{a,f}}{kT_c} \right).
\]

The temperature \( T_c \) controls the reaction. It takes into account the vibrational degrees of freedom and found as the mean of the transitional and vibrational temperatures \( T_c = T^\phi T_v^{1-\theta} \), where \( \theta = 0.5 \) for dissociation and recombination reactions and \( \theta = 1.0 \) for exchange reactions [38].

The reverse coefficient is found as the ratio of coefficient of forward reaction and equilibrium constant, \( k_r = k_f / K_e \). It is then interpolated by polynomial fitting curves. For reactions from 1 to 10 and for reactions from 16 to 17 in the model proposed in [38], the equilibrium constant is found as

\[
K_e(T) = \exp \left[ \frac{A_1}{Z} + A_2 + A_3 \ln(Z) + A_4 Z + A_5 Z^2 \right].
\]

For reactions from 11 to 15, the equilibrium constant is computed as

\[
K_e(T) = \exp \left[ A_1 + A_2 \ln(Z) + A_3 Z + A_4 Z^2 + A_5 Z^3 \right].
\]

Here, \( Z = 10000/T \). The pre-exponential factors, temperature exponents, activation energies and equilibrium constants are reported in Table 3.
Table 3. Reaction model from [38]

<table>
<thead>
<tr>
<th>No</th>
<th>Reaction</th>
<th>$C_i$ [m³/(molecule s)]</th>
<th>$n_f$</th>
<th>$E_{a_f}$/K</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
<th>$A_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Dissociation/Recombination</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>reactions</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>O₂+N=O+O+N</td>
<td>1.66 × 10⁻⁸</td>
<td>-1.5</td>
<td>59500</td>
<td>2.85</td>
<td>0.988</td>
<td>-6.181</td>
<td>-0.023</td>
<td>-0.001</td>
</tr>
<tr>
<td>2</td>
<td>O₂+NO- O+O+NO</td>
<td>3.32 × 10⁻⁹</td>
<td>-1.5</td>
<td>59500</td>
<td>2.85</td>
<td>0.988</td>
<td>-6.181</td>
<td>-0.023</td>
<td>-0.001</td>
</tr>
<tr>
<td>3</td>
<td>O₂+N₂=O+O+N₂</td>
<td>3.32 × 10⁻⁹</td>
<td>-1.5</td>
<td>59500</td>
<td>2.85</td>
<td>0.988</td>
<td>-6.181</td>
<td>-0.023</td>
<td>-0.001</td>
</tr>
<tr>
<td>4</td>
<td>O₂+O₂=O+O+O₂</td>
<td>3.32 × 10⁻⁹</td>
<td>-1.5</td>
<td>59500</td>
<td>2.85</td>
<td>0.988</td>
<td>-6.181</td>
<td>-0.023</td>
<td>-0.001</td>
</tr>
<tr>
<td>5</td>
<td>N₂+O=N+O+O</td>
<td>1.66 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>6</td>
<td>N₂+O₂=N+O+N+O</td>
<td>4.98 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>7</td>
<td>N₂+O₂=N+N+O₂</td>
<td>1.16 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>8</td>
<td>N₂+NO=O+N+N+NO</td>
<td>1.16 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>9</td>
<td>N₂+O₂=N+O+N+O₂</td>
<td>1.16 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>10</td>
<td>N₂+O=N+O+N</td>
<td>4.98 × 10⁻⁸</td>
<td>-1.6</td>
<td>113200</td>
<td>1.85</td>
<td>-1.325</td>
<td>-9.856</td>
<td>-0.174</td>
<td>0.008</td>
</tr>
<tr>
<td>11</td>
<td>NO+O₂=N+O+O₂</td>
<td>8.30 × 10⁻¹⁵</td>
<td>0.0</td>
<td>75500</td>
<td>0.792</td>
<td>-0.492</td>
<td>-6.761</td>
<td>-0.091</td>
<td>0.0</td>
</tr>
<tr>
<td>12</td>
<td>NO+O₂=N+O+O₂</td>
<td>8.30 × 10⁻¹⁵</td>
<td>0.0</td>
<td>75500</td>
<td>0.792</td>
<td>-0.492</td>
<td>-6.761</td>
<td>-0.091</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>NO+O=N+O+NO</td>
<td>1.83 × 10⁻¹³</td>
<td>0.0</td>
<td>75500</td>
<td>0.792</td>
<td>-0.492</td>
<td>-6.761</td>
<td>-0.091</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>NO+O=N+O+O</td>
<td>1.83 × 10⁻¹³</td>
<td>0.0</td>
<td>75500</td>
<td>0.792</td>
<td>-0.492</td>
<td>-6.761</td>
<td>-0.091</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>NO+O+N=NO+O</td>
<td>1.83 × 10⁻¹³</td>
<td>0.0</td>
<td>75500</td>
<td>0.792</td>
<td>-0.492</td>
<td>-6.761</td>
<td>-0.091</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Forward and reverse reaction rate coefficients depend on temperature. These dependencies are shown in Figures 1 and 2 if temperature varies from 3000 to 13000 K. These reactions are the most frequent. The results show that both models proposed in [37] and [38] provide comparable values of reaction rate coefficients for the most frequent reactions.

![Figure 1](image1.png)

Figure 1. Distributions of forward rate coefficients for chemical models proposed in [37] (lines 1) and [38] (lines 2)
3.2 Ionization chemical models

The chemical models proposed in [37] and [38] consider air as a mixture of 11 species (O₂, N₂, O, N, NO, O⁺, N⁺, NO⁺, e⁻). Table 2 provides coefficients for neutral species. The coefficients given in Table 4 are related to ionization process.

Table 4. Kinetic model from [37] for ionization reactions

<table>
<thead>
<tr>
<th>No</th>
<th>Reaction</th>
<th>(C_{f,\cdot}) [m³/(molecule s)]</th>
<th>(n_f)</th>
<th>(E_{a,f}/k,) K</th>
<th>(C_{r,\cdot}) [m³/(molecule s)]</th>
<th>(n_r)</th>
<th>(E_{a,r}/k,) K</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>N + O = NO⁺ + e⁻</td>
<td>1.50 × 10⁻²⁰</td>
<td>0.5</td>
<td>32400</td>
<td>2.99 × 10⁻¹⁴</td>
<td>-1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>O + e⁻ = O⁺ + e⁻</td>
<td>5.98 × 10</td>
<td>2.91</td>
<td>158000</td>
<td>3.65 × 10⁹</td>
<td>-4.5</td>
<td>0.0</td>
</tr>
<tr>
<td>3</td>
<td>N + e⁻ = N⁺ + e⁻</td>
<td>1.83 × 10⁻¹⁰</td>
<td>-3.14</td>
<td>169000</td>
<td>3.65 × 10⁹</td>
<td>-4.5</td>
<td>0.0</td>
</tr>
<tr>
<td>4</td>
<td>O + O₂⁺ = O⁺ + O⁺</td>
<td>2.66 × 10⁻¹³</td>
<td>-0.98</td>
<td>80800</td>
<td>1.35 × 10⁻⁸</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>5</td>
<td>O + O₂⁺ = O₂⁺ + O⁺</td>
<td>4.85 × 10⁻¹²</td>
<td>-1.11</td>
<td>28900</td>
<td>1.30 × 10⁻¹⁸</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>6</td>
<td>N₂⁺ + N⁺ = N₂⁺ + N⁺⁺</td>
<td>3.35 × 10⁻¹⁹</td>
<td>0.81</td>
<td>13000</td>
<td>1.30 × 10⁻¹⁸</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>7</td>
<td>N + N = N₂⁺ + e⁻</td>
<td>2.32 × 10⁻¹⁷</td>
<td>0</td>
<td>67800</td>
<td>2.49 × 10⁻⁸</td>
<td>-1.5</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>O + NO⁺ = NO⁺ + O⁺</td>
<td>6.03 × 10⁻¹⁵</td>
<td>-0.6</td>
<td>50800</td>
<td>2.49 × 10⁻¹⁷</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>9</td>
<td>N₂⁺ + O⁺ = O⁺ + N₂⁺⁺</td>
<td>5.65 × 10⁻¹¹</td>
<td>2</td>
<td>23000</td>
<td>4.12 × 10⁻¹¹</td>
<td>-2.2</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>O₂⁺ + NO⁺ = NO⁺ + O₂⁺⁺</td>
<td>2.99 × 10⁻¹⁵</td>
<td>0.17</td>
<td>33000</td>
<td>2.99 × 10⁻¹⁷</td>
<td>0.5</td>
<td>0.0</td>
</tr>
<tr>
<td>11</td>
<td>O + NO⁺ = O⁺ + N⁺⁺</td>
<td>2.23 × 10⁻¹⁷</td>
<td>0.31</td>
<td>77270</td>
<td>1.66 × 10⁻¹⁶</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>12</td>
<td>O₂⁺ + N₂⁺ = NO⁺ + O₂⁺⁺</td>
<td>2.29 × 10⁻¹⁰</td>
<td>-1.84</td>
<td>141000</td>
<td>1.66 × 10⁻⁶</td>
<td>-2.5</td>
<td>0.0</td>
</tr>
<tr>
<td>13</td>
<td>NO + O₂⁺ = NO⁺⁺ + e⁻ + O₂</td>
<td>3.65 × 10⁻¹⁵</td>
<td>-0.35</td>
<td>108000</td>
<td>3.65 × 10⁻⁴</td>
<td>-2.5</td>
<td>0.0</td>
</tr>
<tr>
<td>14</td>
<td>NO + N₂⁺ = NO⁺⁺ + e⁻ + N₂</td>
<td>3.65 × 10⁻¹⁵</td>
<td>-0.35</td>
<td>108000</td>
<td>3.65 × 10⁻⁴</td>
<td>-2.5</td>
<td>0.0</td>
</tr>
<tr>
<td>15</td>
<td>N + NO⁺ = NO⁺ + N⁺⁺</td>
<td>1.66 × 10⁻¹¹</td>
<td>-0.93</td>
<td>61000</td>
<td>7.97 × 10⁻¹⁶</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Coefficient rates for neutral components are provided in Table 3. In the model [38], the temperature controlling reaction is used (it includes electron temperature and translational temperature). This temperature is found as the mean of the electron and transitional temperatures, \(T_e = T_e^\theta T^{1-\theta}\). The value of \(\theta = 0\) is used. The coefficients which are required to assess ionization reactions are reported in Table 5.

Table 5. Kinetic model from [38] for ionization reactions
The diagram of the computational domain is shown in Figure 3. The external boundary of the computational domain is removed from the sphere by 4 mm at the braking point and by 8.65 mm at the top point. The problem is solved in an axisymmetric formulation. At the next step, an axisymmetric formulation is considered and the model is solved for air as a mixture of 23.3% of O, 76.7% of N, and corresponds to a flight speed from 2438.4 to 6705.6 m/s. The freestream is considered as a mixture of 23.3% of O and 76.7% of N. The Knudsen number under the conditions of the problem under consideration is Kn = λ/(2R) = 0.008 m and corresponds to the flow regime of a continuous medium.

### Table 6. Equilibrium constant coefficients for model from [38]

<table>
<thead>
<tr>
<th>No</th>
<th>Reaction</th>
<th>( A_1 )</th>
<th>( A_2 )</th>
<th>( A_3 )</th>
<th>( A_4 )</th>
<th>( A_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>O+e(^-) = O(^+)+e(^-)</td>
<td>0.614</td>
<td>-6.755</td>
<td>-0.774</td>
<td>-16.003</td>
<td>0.006</td>
</tr>
<tr>
<td>3</td>
<td>N+e(^-) = N(^+)+e(^-)</td>
<td>0.201</td>
<td>-3.966</td>
<td>-0.042</td>
<td>-18.063</td>
<td>0.126</td>
</tr>
<tr>
<td>8</td>
<td>O+NO(^+) = NO+O(^+)</td>
<td>0.148</td>
<td>-1.011</td>
<td>-4.121</td>
<td>-0.132</td>
<td>0.006</td>
</tr>
</tbody>
</table>

For reactions 2 and 3, the equilibrium constant is

\[ K_e(T) = \exp \left[ \frac{A_1}{Z} + A_2 + A_3 \ln(Z) + A_4 Z + A_5 Z^2 \right]. \]

For reaction 8 the equilibrium constant is found from the relation

\[ K_e(T) = \exp \left[ A_1 + A_2 \ln(Z) + A_3 Z + A_4 Z^2 + A_5 Z^3 \right]. \]

Here, \( Z = 10000/T \). Table 6 reports the equilibrium constant coefficients.

### 4 Computational domain and mesh

To estimate the used numerical method as applied to the calculations of the gas-dynamic parameters of hypersonic flows around blunt bodies, the flow around a sphere is simulated in a wide range of parameters of the incident flow. The choice of the sphere is due to detailed studies of this body shape in various works [15, 16, 23].

A hypersonic air flows around a sphere with a diameter \( D = 12.7 \) mm. The selected flow quantities correspond to the values in the experiment to determine the departure of the bow shock wave from the sphere when air flows around [15]. The pressure of the freestream is \( p_\infty = 666.61 \) Pa, and the temperature is \( T_\infty = 293 \) K (the density is \( \rho_\infty = 7.9 \cdot 10^{-3} \) kg/m\(^3\), which corresponds to a flight altitude of 41.87 km). The Mach number varies from 7 to 18 and corresponds to a flight speed from 2438.4 to 6705.6 m/s. The freestream is considered as a mixture of 23.3\% of O\(_2\) and 76.7\% of N\(_2\). The Knudsen number under the conditions of the problem under consideration is \( \text{Kn} = \lambda/(2R) = 0.008 \) m and corresponds to the flow regime of a continuous medium.
the inlet boundary, the boundary conditions for supersonic inflow into the computational domain are specified, and at the outlet boundary, the conditions for supersonic outflow are applied. The no-slip boundary conditions are used on the walls. To simplify specification of outlet boundary condition at the sphere edge, a small section of the wall is considered as an inviscid wall, here slip boundary conditions are specified. The surface of sphere is thermally insulated. The computational mesh consists of \(400 \times 400 = 160,000\) hexagonal cells.

In the axisymmetric case, a three-dimensional mesh is built for the sector of several degrees, and the periodic boundary conditions are set on the sector faces. In this case, cells appear with an aspect ratio much larger than unity near the axis of symmetry. When using explicit schemes, paraxial cells introduce a significant limitation on the global time step. For axisymmetric problems, it is proposed to use a system of equations that differs from the system of equations for plane flows only by the presence of a source term. A plane mesh with a thickness of one cell is built and the approach implemented for flat problems is used, and when calculating the values in the center of the cell, a source term is added on the next time layer, which is explicitly approximated.

An explicit 4th order Runge–Kutta scheme is used for time integration. The AUSM+ numerical scheme proposed in [40] is used to calculate convective fluxes. To increase the order of approximation of the scheme in space, interpolation of values to the face from the centers of the cells is used, and the gradient at the centers of the cells is calculated using the least squares method. Gradient stops are used to keep the scheme monotonous. The method for accumulation of errors estimations in CFD simulations is described in [41, 42]. To evaluate the error accumulation along the computational domain for supersonic steady flow the method proposed in [42] is used.

5 Results and discussion

Air compositions predicted with two chemical models at the stagnation point of sphere are not very different (Table 7). However, calculations with the chemical model proposed in [38] allow to reach steady state more quickly in comparison with the simulations based on chemical model proposed in [37].
Table 7. Molar fractions at the stagnation point of sphere

<table>
<thead>
<tr>
<th>Model</th>
<th>$\alpha_{O_2}$</th>
<th>$\alpha_{N_2}$</th>
<th>$\alpha_{O}$</th>
<th>$\alpha_{N}$</th>
<th>$\alpha_{NO}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>[37]</td>
<td>0.0041</td>
<td>0.632</td>
<td>0.346</td>
<td>0.011</td>
<td>0.010</td>
</tr>
<tr>
<td>[38]</td>
<td>0.0034</td>
<td>0.621</td>
<td>0.341</td>
<td>0.012</td>
<td>0.020</td>
</tr>
</tbody>
</table>

The contours of the flow quantities are shown in Figure 4. The results obtained indicate the correct prediction of the shock wave shape and the main flow elements near the frontal surface (the shape of the bow shock wave, the location of the sonic line). The density and temperature distributions are characteristic of supersonic flow, when their maxima are at the stagnation point of the flow, and minima are in the leeward region. Taking into account the real properties of the gas leads to the fact that the temperature at the stagnation point is lower than the temperature calculated using the perfect gas model.

The shock front surface is sufficiently smooth. The distance between the front of the bow shock wave and the surface of the body is minimal on the stagnation line (a conventional line emerging from the frontal point of the body, collinear to the velocity vector of the unperturbed flow) and monotonically increases with distance from the frontal part of the body along its surface downstream. In some flow regimes, the smoothness of the front and the monotonicity of the distance are violated. At the front, kinks are formed, and some specific formation appears, called a carbuncle [14]. In this case, the flow in the vicinity of the nose becomes substantially different. The carbuncle effect appears only in hypersonic flow regimes. In computer modelling, this effect is revealed both when using a model of an ideal (inviscid and non-thermal) gas, and a model of a gas taking into account its real properties.

The pressure coefficient and the surface friction coefficient are determined by the following relations

$$C_p = \frac{2(p_w - p_\infty)}{\rho_\infty V_\infty^2}, \quad C_f = \frac{2\tau_w}{\rho_\infty V_\infty^2}.$$  

The distributions of pressure and friction coefficients over sphere surface are plotted in Figure 5 for a fixed Mach number. The pressure coefficient takes on a maximum value at the front stagnation point and gradually decreases along sphere surface. Noteworthy is the relatively weak dependence of the pressure distribution on sphere surface on Mach number (for $M > 2$, the regime of hypersonic stabilization practically sets in). CFD results are in a good agreement with the experimental measurements reported in [6]. The distribution of pressure coefficient found from the semi-empirical correlation proposed in [18] (symbols $\bullet$) show a good agreement with CFD results. However, the values of pressure coefficient found from the semi-empirical correlation slightly overestimate those predicted with CFD calculations. The surface friction coefficient has a minimum value at the front critical point, then increases, reaching its maximum value at $\theta = 46^\circ$, and then decreases. The profiles of friction coefficient show a less satisfactory agreement with predictions from semi-empirical correlation (symbols $\circ$).

Useful additional information on the features of the development of a flow near a sphere follows from the distributions of gas-dynamic variables on the axis of symmetry. The numerical simulation results are compared with the previously published data [24] at the Mach number $M = 17.6$ ($V = 5804$ m/s, $p = 57.4$ Pa, $T = 200$ K, $Re = 3.4 \cdot 10^5$). The distribution of pressure on the axis of symmetry in front of the surface of the sphere is shown in Figure 6. There is a fairly good agreement of the calculation results (line 1) with the available data given in the work [24] (line 2). In this case, there is a slight difference in the thickness of
the shock layer. Comparison of the temperature distributions for perfect and chemically reacting gases shows that there are significant (up to 30%) differences in the temperature distribution across the shock layer in the near-wall region, where significant concentrations of chemical components are observed.

While the pressure distributions coincide on the scale of the figure, the temperature values behind the shock wave differ significantly, and the greatest difference occurs at the stagnation point. In the case of an equilibrium chemical reactions, oxygen molecules are absent.
Figure 5. Distributions of pressure coefficient (line 1) and friction coefficient (line 2) on surface of sphere. Symbols • and ○ correspond to semi-empirical correlation [18].

Figure 6. Distribution of pressure coefficient of centreline before sphere.

For a perfect gas, the relative thickness of the shock layer is found from the relation [15]

\[ \frac{\Delta D}{D} = K \varepsilon, \quad \varepsilon = \frac{\gamma - 1}{\gamma + 1} \left( 1 + \frac{2}{\gamma - 1} \frac{1}{M_{\infty}^2} \right), \]

where \( \varepsilon \) is the ratio of the densities in the undisturbed flow and in the shock layer (\( \varepsilon = \rho_{\infty}/\rho_s \)), and \( K = 0.39–0.41 \) is the proportionality coefficient. For low velocities, the flow can be considered frozen, and the differences between the data of the physical and computational experiments are associated with non-equilibrium effects in the gas [15].

To take into account the high-temperature effects on stand-off distance, the average density distribution reported in [43] is used. In particular, to simplify the calculations it is assumed that the density distribution between the fronts of the bow shock and sphere surface
satisfies to a linear dependence [44]. According to [44], the stand-off distance is inversely proportional to the average density behind the shock

$$\frac{\Delta}{D} = 0.25 \frac{\rho_{\infty}}{\rho}.$$  

This ratio ignores the influence of chemical reactions and leads to rather large errors at high Mach numbers [10]. To take into account chemical reactions, the magnitude of the constant factor changes, and the relationship for the stand-off distance takes the form [44]

$$\frac{\Delta}{D} = 0.41 \frac{\rho_{\infty}}{\rho}.$$  

However, this approach is rather approximate, and finding the average density in the shock layer requires rather laborious calculations [46].

The model proposed in [45] takes into account the geometry of the aircraft head and flow quantities. The approach proposed in [47] allows one to obtain a relation for the stand-off distance, the parameters of which are the Mach number and density. The approach is developed in [10], which gives the shock layer thickness as a function of the Mach number and flight altitude, which varies from 25 to 55 km. The high-temperature air model takes into account 9 components (N₂, O₂, NO, O, N, O⁺, N⁺, NO⁺, e⁻). One of the interesting effects observed in the calculations is the presence of a turning point on the distribution of the shock layer thickness depending on the Mach number. The minimum point corresponds to Mach numbers from 27 to 31, depending on the flight altitude. This phenomenon is explained by the different growth rates of pressure and temperature behind the shock front with an increase in the Mach number, as well as the complex dependence of the transfer coefficients on temperature. The average density in the shock layer has the same behavior.

The comparison carried out in [10] shows that the [44] model, which does not take into account the presence of chemical reactions, and the [44] model, which takes into account chemical reactions in high-temperature air, lead to errors of the order of 11.94% and 8.22% relative to the results of numerical simulation. At the same time, the [10] model gives an average error of about 1.27%, which decreases with increasing Mach number.

The dependence of the dimensionless thickness of the shock layer on the Mach number is shown in Figure 7. Line 1 corresponds to the dependence of the dimensionless distance to the shock wave on the Mach number when using the assumption of fully equilibrium chemical reactions (Kraiko’s model). Line 2 shows interpolated experimental data from [15] with corresponding estimates of measurement errors. Line 3 corresponds to the calculation results using the model of a non-reactive perfect gas with a constant adiabatic exponent (γ = 1.4). Line 4 was obtained on the basis of calculations using the Park model. At M = 14, the equilibrium calculation curve (line 1) comes closest to the experimental data (line 2) and approaches them at higher freestream Mach numbers.

Standoff distance as a function of Mach number number and hight of flight is shown in Figure 8. Standard atmospheric parameters are used in CFD calculations. The standoff distance decreases with a decrease Mach number. Height of flight has a significant effect on stand off distance. The results computed are in qualitative agreement with the data obtained from the semi-empirical correlation proposed in [10].

In a strong shock wave that arises in front of the blunt heat, the kinetic energy of the incident flow is converted into the internal degrees of freedom of air molecules (rotational and vibrational), which leads to a noticeable decrease in temperature in the compressed layer and a decrease in the departure of the shock wave front from the surface.
6 Conclusion

An approach to modelling the flow of a viscous multi-component chemically reacting gas mixture around blunt bodies is developed taking into account the influence of non-equilibrium chemical reactions. A comparative analysis of the calculation results obtained using the developed numerical method with the data available in the literature is carried out. Qualitative and quantitative agreement of the parameters of non-equilibrium flows makes it possible to
judge the correctness of the calculation of chemical concentrations in the shock layer. Quantitative differences are due to different models of chemical reactions of the compared methods, including the rate constants of chemical reactions and boundary conditions.

Different chemical models used in CFD calculations predict different air compositions in the flowfield. However, use of different chemical models lead to slightly different compositions of air on the sphere surface. The chemical models did not significantly affect the friction coefficient, but they produce locally strong effects affecting the stand-off distance.

The calculation procedure for accounting for physical and chemical processes in high-temperature air is implemented as a module that allows connection to commercial packages (for example, Ansys Fluent/CFX) and open source packages (for example, OpenFOAM).

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**References**


