Spatial Multiphysics Models of the Radiation Gas Dynamics of Super Orbital Re-Entry Space Vehicles

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Abstract. The multiphysics models of non equilibrium physical and chemical processes that should be considered together with radiative gas dynamic models for a description of the aero physics of super-orbital space vehicles are described. As an example of application of the multiphysics approach a three-dimensional numerical simulation analysis of radiative gas dynamics of Apollo-17 command module is analyzed. The results of calculations are compared with other numerical predictions, analytical correlations, and available experimental data.

1. Introduction

A variety of multiphysics models developed for a description of large amount of related processes have found a wide application in modern computational physics, especially in basic problems of astrophysics [1,2], physical mechanics [3,4], plasma physics [5–7], theory of combustion, flame, and explosion [8, 9], electromagnetics [10] et al.

The classic examples of the multi-physics problems are the relevant tasks arisen in the radiative gas dynamics (RadGD) of re-entry space vehicles. For a reliable description of the processes developed near and inside the streamlined surface at extremely high velocities it is necessary to include in consideration the following branches of science:

- gas dynamics and continuum mechanics of solid materials,
- thermodynamics and statistical physics,
- applied quantum mechanics, quantum chemistry, and quantum statistics,
- physical and chemical kinetics of gases and heat protective materials,
- radiation heat transfer,
- computational fluid dynamics (CFD).

Solution to such a multiphysical problem appears to be very complicated due to the fact that the physical processes under consideration are interdependent and appropriate partial differential equations of mathematical physics turn out to be strongly nonlinear. These are some examples of such an interrelation:

- gas heating in shock layer and attendant chemical kinetics,
- nonequilibrium dissociation and ionization, as well as attendant relaxation processes,
- thermo-chemistry of heat-protection materials and the conditions in gas phase in surrounding boundary layers,
— physical kinetics of the processes of filling and depletion of quantum states in atoms and radiation heat transfer,
— coupling physical-chemical and radiative processes with gas dynamics.

Investigation of various multiphysical problems of radiative gas dynamics is directly connected with creating and developing of new theoretical and computational models. Wide spectrum of physical-chemical, quasi-classical and quantum models are used for a description of nonequilibrium processes, such as:
— quasi-classical theory of velocities of chemical reactions,
— quantum-chemistry models of chemical transformations,
— collisional-radiative (CR) models,
— quantum-kinetic models,
— multi-temperature kinetic models.

As for the interaction between radiation and gas dynamic processes, one can also use various models of such a coupling, for example:
— strong radiative-gas-dynamic interaction,
— weak radiative-gas-dynamic interaction,
— radiative gas dynamics with a strong reabsorption of heat radiation,
— volume emission approximation (RadGD of optically thin gas),
— RadGD of optically dense gas,
— RadGD with weak and strong influence of fine structure of atomic lines.

The principal feature of modern models of radiation gasdynamics is a consideration of the spatial nature of the radiation heat transfer. To take into account this feature, two-dimensional and three-dimensional computer models of computational physics should be used. Non-local nature of the selective heat radiation makes these models extremely labour- and time-consuming.

A general problem of the fundamental aero physics is the reliable computational and theoretical predictions of the aerothermodynamic and electro-physical parameters of compressed layers near the space vehicle surfaces. Up to now this problem has not been solved despite a significant progress made in recent decades.

Depending on flight conditions of spacecrafts, substantially different mechanisms for elementary physical and chemical processes are realized in the heated gas of the shock layer. The diversity of these processes, together with uncertainty in a knowledge of mechanisms of corresponding reactions, often leads to different results of the kinetic modeling not only in the values of reaction rates, but also in their nomenclature.

Another unresolved issue is the need to take into account physical and chemical non-equilibrium behind the shock front due to rarefaction of gas flows. Absence of thermalization of internal degrees of freedom leads to the necessity of using different models of chemical and physical kinetics, among which the models of multimode relaxation are the most applicable. These models are based on the Born-Oppenheimer approximation and on the various kinds of the resonant energy exchange between quantum states.

Differences in translational, vibrational and electronic temperatures require for a modification of the models of chemical kinetics through the use of models of nonequilibrium dissociation. Such models have been developed, however, the lack of reliable criteria for the use of different models leads to the fact that in practice each research has to look for the most suitable model in particular situation.

Prediction of the radiative heating of entering space vehicles and study of coupled radiative gas dynamic processes in shock layers at orbital and especially for the super-orbital conditions of return into Earth atmosphere has revived a new interest due to modern plans for a return from Moon and closest planets of the Solar system. In spite on the fact that radiation heat transfer processes, as applied to the problems of aerothermodynamics of re-entry space vehicles, have been considered more than forty years, unanswered questions still remaining a lot up to now. The scientific tasks followed from these questions have to be resolved to provide reliable aerothermodynamic prediction of creating space vehicles of the new generation.
This paper is dedicated to the analyze of spatial radiative heating of the Apollo command modules. It is well known that significant resources for testing and quantification of the aero thermodynamic characteristics of the re-entering command modules were spent within the framework of the Apollo program [11-13]. An engineering-level predictions of the expected flight heating rates were created on the basis of the ground-based tests in low enthalpy wind tunnels, shock tunnels and the free-flight facilities. Two flight tests of the Apollo command modules were conducted at orbital (Apollo-09,11) and at super-orbital speeds (Apollo–17,20) [13]. Table 1, reproduced from Ref.13, lists the relevant entry conditions for each of the four Apollo test flights. In table 1 $V_{\infty}$ is the entry velocity at atmospheric interface, $\alpha$ is the angle of attack, and $Q_{max}$ is the maximum theoretical heating rate determined by engineering correlations at a spherical stagnation point. Entry trajectories of these flight tests are presented in figure 1.

Table 1. Apollo descent modules entry conditions [13]

| Spacecraft Number | $V_{\infty}$, km/s (nominal) | $\alpha$, deg | $Q_{max}$, W/cm$^2$ |
|-------------------|-----------------------------|---------------|---------------------|
| 009               | 7.67                        | 20            | 186                 |
| 011               | 8.29                        | 18            | 91                  |
| 020               | 10.73                       | 25            | 237                 |
| 017               | 9.60                        | 25            | 488                 |

In the present the numerical investigation bases on some previously published works [14-18]. Detailed analysis of radiative gas dynamics of experimental space vehicles Fire-II and Stardust was presented in [14,15]. Several recent publications were dedicated to studying the real re-entry conditions of super-orbital capsule [16,17]. Some analytical correlations for intensity of convective and radiative heating, based on a large number of numerical simulation results, were recently suggested in [18].

In our previous papers [19-22] we analyzed radiative aero thermodynamics of segmental-conical space vehicle of large size (the Prospective Transport Vehicle – PTV) that is intended for flight of six astronauts. Start of this investigation was made in papers [19, 20], where the radiative aero thermodynamics of the orbital re-entry space vehicles similar to PTV was studied.

Some problems of radiative gas dynamics of re-entry space vehicle of large size and super orbital speed, as well as of coupled radiative gas dynamic interaction and non-equilibrium dissociation for large-scale returned space vehicles were considered in [21, 22].

The paper presents numerical results of the heating prediction for the surface of the Apollo command modules at orbital and super orbital velocities with a use of the author’s computer codes.

Computer platform **NERAT-3D** (Non-Equilibrium Radiation Aero-Thermodynamics) + **ASTEROID** [19–24] together with various models of chemical kinetics of ionized air is used for such numerical study. The computational fluid dynamic code **NERAT-3D** is based on groups of governing equations that reflect multiphysical nature of the problem under consideration. These are: (a) the Navier-Stokes and continuity equations, (b) the equations of mass conservation of separate species, (c) the equation of energy conservation, including total and vibrational energy of molecules N$_2$, O$_2$ and NO, and (d) the equation of radiation heat transfer in the multi-group approximation.

All equations are formulated in curvilinear coordinate system related with the Apollo geometry, which was borrowed from [25] (see figure 2). Calculations were carried out with using a multi block
and multi grid computational technology in three-dimensional geometry. The finite-difference approach was used.

![Graph](image_url)

Figure 1. Trajectories of Apollo command modules.

Three dimensional investigations of radiative gas dynamic processes are extremely time-consuming. Therefore multi-block and multi-grid numerical techniques were used for investigation of the set of governing equations by the time-relaxation method, whereas the multi-group spectral approximation was used for solving the selective radiation heat transfer equation. Computer code NERAT-3D was used together with the following databases of thermodynamic, transport, kinetic and spectral optical properties:

- Database of thermodynamic properties of individual species [26],
- Database of chemical kinetics [27],
- Database of parameters of intermolecular interaction [28],
- Database of physical kinetics [29],
- Database of spectral optical properties is based on the code ASTEROID [30].

Radiation emission from the shock layer was calculated with the use of vibrational temperatures, therefore their behavior in shock layer is very significant for the surface radiative heating determination, as well as for the radiative signatures of space vehicles prediction. The dominant optically active components in the shock layer are the following: N\textsubscript{2}, O\textsubscript{2}, NO, N, O, N\textsuperscript{+}, O\textsuperscript{+} and N\textsubscript{2}\textsuperscript{+}. General features of these distributions are the following: large mass fractions of molecular N\textsubscript{2} and O\textsubscript{2} and low mass fractions of atomic N and O in the vicinity of the command module surfaces. Such behaviors of mass fractions are in full agreement with a used assumption concerning catalytic properties of the surface. Obtained distributions of translational and vibrational temperatures will be analyzed below. The vibrational temperatures are introduced in the so called multi-temperature models to characterize the energy accumulated in vibrational degree of freedoms of the diatomic molecules. In this case one uses an assumption concerning Boltzmann’s energy distribution inside some separated degrees of freedom. To verify and validate obtained numerical simulation results several well known calculation and experimental data were used (Fire-II and Stardust) [23,24].

Two calculation cases are presented in this paper. In the first case, the non-equilibrium and quasi-equilibrium regimes at maximal velocity of the space vehicle (V\textsubscript{∞} > 9 km/s) were investigated. This case directly corresponds to super-orbital entry.
The second case characterizes the second entry of the command module into atmosphere \((V_\infty < 7\) km/s), and actually corresponds to orbital entry, since the trajectory parameters of the second re-entry actually coincide with corresponding parameters of regular orbital entry.

The calculation data presented in this paper allow to get a full representation concerning specific properties of the flow field and the aerothermodynamics of super-orbital entering of Apollo command modules in the non-equilibrium and quasi-equilibrium regimes. These data include gas dynamic functions of the flow field at the angle of attack \(\alpha = 25^0\), distributions of translational and vibrational temperatures, as well as mass fractions of gas species. Presented data on spectral radiation heat fluxes and corresponding cumulative functions give a representation about most significant radiative processes which form integral radiative heating of the space vehicle.

![Figure 2. Multi-block calculation grid.](image)

Finally, the numerical simulation results obtained within the framework of the three-dimensional approach will be compared with the data of two-dimensional calculations and engineering correlations [18].

2. Computational multiphysical model of radiative gas dynamics of re-entry command module

At every time step the following groups of governing equations are integrated successively:

\[
\frac{\partial W}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 0, \tag{1}
\]

\[
W = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w
\end{bmatrix}, \quad F_x = \begin{bmatrix}
\rho u \\
\rho u^2 + p - \tau_{xx} \\
\rho u v - \tau_{xy} \\
\rho u w - \tau_{xz}
\end{bmatrix}, \quad F_y = \begin{bmatrix}
\rho v \\
\rho u v - \tau_{xy} \\
\rho v^2 + p - \tau_{yy} \\
\rho v w - \tau_{yz}
\end{bmatrix}, \quad F_z = \begin{bmatrix}
\rho w \\
\rho u w - \tau_{xz} \\
\rho v w - \tau_{yz} \\
\rho w^2 + p - \tau_{zz}
\end{bmatrix}, \tag{2}
\]

\[
\rho c_p \frac{\partial T}{\partial t} + \rho c_p V \nabla T = \text{div}(\lambda \nabla T) + \frac{\partial p}{\partial t} + V \nabla p + \Phi + Q_{\text{rad}} - \sum_{i=1}^{N_i} h_i \sigma_i \left( \nabla T \cdot \nabla T \right) + \sum_{i=1}^{N_i} \rho c_{p,i} D_i \left( \nabla Y_i \cdot \nabla T \right), \tag{3}
\]
\[
\frac{\partial \rho_i}{\partial t} + \text{div} \rho_i \mathbf{V} = -\text{div} \mathbf{J}_i + \mathbf{\dot{a}}_i, \quad i = 1,2, \ldots, N_v,
\]

(4)

\[
\frac{\partial \rho_{e,v,m}}{\partial t} + \text{div} \left( \rho_m \mathbf{V}_{e,m} \right) = \dot{e}_{v,m}, \quad m = 1,2, \ldots, N_v,
\]

(5)

\[
\frac{\partial \mathbf{J}_m}{\partial t} + \kappa_m \mathbf{r} \mathbf{J}_m = \mathbf{j}_m \mathbf{r},
\]

(6)

\[
p = \rho \frac{R_0}{M_z} T = \rho R_0 T \sum_{i} \frac{Y_i}{M_i},
\]

(7)

where \( p \) and \( \rho \) are the pressure and density; \( \tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \), \( i, j, k = 1,2,3 \) are the viscous components of the total stress tensor \( \Pi_{ij} = -p \delta_{ij} + \tau_{ij} \); \( \delta_{ij} \) is the Kronecker delta symbol; \( u_x, u_y, u_z \to u, v, w \) are the projections of gas velocity \( \mathbf{V} \) on axis of the Cartesian coordinate system; \( t \) is the time; \( T \) is the translational temperature; \( \mu \) and \( \lambda \) are the viscosity and heat conductivity coefficients, \( c_p \) is the specific heat capacity of gas mixture; \( c_p = \sum_{i} Y_i c_{p,i} ; Y_i \) is the mass fraction of species \( i \); \( c_{p,i} \) and \( h_i \) are the specific heat capacity at constant pressure and specific enthalpy of species \( i \); \( \mathbf{\dot{a}}_i \) is the reaction rate for species \( i \); \( D_i \) is the effective diffusion coefficient of species \( i \); \( \rho_i \) and \( \mathbf{J}_i \) are the density and mass diffusion flux for species \( i \); \( \mathbf{J}_i = -D_i \text{grad} Y_i \); \( N_i \) is the number of species; \( e_{v,m} \) is the specific vibrational energy of \( m \)-th mode of species \( i \); \( \rho_{(im)} \) is the density of \( i \)-th species having \( m \)-th mode of vibration; \( \dot{e}_{v,m} = e_{v,m}(T_v = T) \) is the equilibrium specific vibrational energy of \( m \)-th mode of species \( i \); \( R_0 = 8.314 \times 10^7\text{erg/(K-mole)} \) is the universal gas constant; \( T_{V,m} \) is the vibrational temperature defining energy distribution for separate vibrational mode (which is called as the \( m \)-th mode) of \( i \)-th species;

\[
\dot{e}_{v,m} = \rho_{(im)} \frac{e_{v,m}^{(0)} - e_{v,m} \mathbf{\dot{a}}_{(im)}}{\tau_{m}} - e_{v,m} \mathbf{\dot{a}}_{(im)}, \quad e_{v,m} = \frac{R_0 \theta_m}{M_{(im)} \left[ \exp \left( \frac{\theta_m}{T_{V,m}} \right) - 1 \right]},
\]

(8)

\[
\Phi_\mu = \mu \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + 2 \left( \frac{\partial w}{\partial z} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right)^2 + \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right)^2 - 2 \frac{1}{3} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right)^2 \right]
\]

is the dissipative function. Other variables are defined below.

Equation (5) describes vibrational relaxation processes in non-equilibrium gas flows. The term \( Q_{\text{ vib}} \) in Eq.(3) is the energy source due to vibrational relaxation in multi component gas mixture (vibrational source turn); \( N_v \) is the number of vibrational modes (in the case under consideration \( N_v = 3 \): \( m = 1 \) for \( N_2 \) vibration mode, \( m = 2 \) for \( O_2 \) vibration mode, \( m = 3 \) for the NO vibration modes).

In the case under consideration thermodynamic properties of gas mixture cannot be described using a single temperature because there are relaxation zones with non-equilibrium (i.e. non
Boltzmann’s) occupation of internal degrees of freedom of molecules and atoms. The most simple and popular non-equilibrium thermodynamic models are based on introduction of various translational and vibrational temperatures. Such models are often used for a description of relaxation processes behind shock wave fronts formed due to collisional processes and in expansion parts of gas flows. In such cases the Kirchhoff low is applied to averaged vibrational temperature or to separate temperatures.

Using a symbolic notation for the $n$-th chemical reaction

$$\sum_{j=1}^{N_r} a_{j,n} \left[ X_j \right] = \sum_{j=1}^{N_r} b_{j,n} \left[ X_j \right], \quad n = 1, 2, \ldots, N_r,$$

the rate of formation of $i$-th gas species (in mole/cm$^3$·s) can be written for $n$-th chemical reaction as follows:

$$\frac{dX_i}{dt} = k_{f,n} (b_{i,n} - a_{i,n}) \prod_{j=1}^{N_r} X_j^{a_{j,n}} - k_{r,n} (b_{i,n} - a_{i,n}) \prod_{j=1}^{N_r} X_j^{b_{j,n}} = (b_{i,n} - a_{i,n}) (S_{f,i}^{n} - S_{r,i}^{n}), \quad n = 1, 2, \ldots, N_r, \quad (9)$$

where $a_{i,n}, b_{i,n}$ are the stoichiometric coefficients of the $n$-th reaction; $\left[ X_j \right]$ are the chemical symbols of reagents and products of reactions; $N_r$ and $N_r$ are the number of gas species and number of the chemical reactions; $k_{f,n}, k_{r,n}$ are the rate constants of the forward and reverse reactions; $S_{f,i}^{n}, S_{r,i}^{n}$ are the rates of the forward and reverse reactions.

The rate of formation of mole per cm$^3$ for $i$-th gas species is written in the following form:

$$W_i = \sum_{n=1}^{N_r} (b_{i,n} - a_{i,n}) (S_{f,i}^{n} - S_{r,i}^{n}), \quad \text{mol/(cm}^3\text{·s)}, \quad (10)$$

and the mass formation rate of species $i$ can be calculated as follows:

$$\dot{\omega}_i = M_i W_i, \quad \text{g/(cm}^3\text{·s)}. \quad (11)$$

To calculate the rates of formation it is necessary to know the forward and reverse reaction constants for each $n$-th reaction

$$k_{f(r),n} = A_{f(r),n} T^{n f(r),n} \exp\left(-E_{f(r),n}/kT\right), \quad (12)$$

where $A_{f(r),n}, n_{f(r),n}, E_{f(r),n}$ are the approximation coefficients for the forward ($f$) and reverse ($r$) reaction rates. Kinetic model, presented in [27] was applied. Note, that the equilibrium constant for each $n$-th chemical reaction is determined as follows

$$K_n = k_{f,n}/k_{r,n}, \quad (13)$$

that in turn are determined by thermodynamic data [26].

Thermodynamic properties of individual chemical species were calculated by the polynomial approximations [26]. This data base contains tables of the approximation constants for each individual species in the temperature range of 100 – 20 000 K. The Gibbs function can be calculated as follows:

$$\Phi_j = \varphi_{1,j} + \varphi_{2,j} \ln x + \varphi_{3,j} x^{-2} + \varphi_{4,j} x^{-1} + \varphi_{5,j} x + \varphi_{6,j} x^{2} + \varphi_{7,j} x^{3}, \quad (14)$$
\[ \left( \frac{d\Phi}{dx} \right)_j = (\varphi_{2,j} - 2\varphi_{1,j}x^2 - \varphi_{4,j}x^{-1} + \varphi_{5,j} + 2\varphi_{6,j}x^2 + 3\varphi_{7,j}x^{-1}) \frac{1}{x^2}, \]
\[ \left( \frac{d^2\Phi}{dx^2} \right)_j = (-\varphi_{2,j} + 6\varphi_{3,j}x^{-2} + 2\varphi_{4,j}x^{-1} + 2\varphi_{6,j}x^2 + 6\varphi_{7,j}x^{-1}) \frac{1}{x^2}. \]

General properties of thermodynamic potentials allow predict the enthalpy, heat capacity at constant pressure and equilibrium constants as following:

\[ h_j = xT \left( \frac{d\Phi}{dx} \right)_j + \varphi_{6,j} \times 10^3, \text{ J/mole}, \]
\[ c_{p,j} = 2x \left( \frac{d\Phi}{dx} \right)_j + x^2 \left( \frac{d^2\Phi}{dx^2} \right)_j, \text{ J/mole-K}, \]
\[ \ln K_e(p/p_a) = \frac{1}{R_T} \sum_{j=1}^{N_e} \left( a_{j,n} - b_{j,n} \right) \left( -T \Phi_j + \varphi_{6,j} \times 10^3 \right), \quad (15) \]

where \( p_a = 101325 \text{ Pa}; \quad x = T/10000. \)

The radiation heat transfer equation (6) is formulated in a general form. The solution of this equation allows calculate a total radiation heat flux that can be presented in the following form:

\[ q_R = q_{R,\Omega} = \int_4^0 \int \mathcal{J}_\omega (r, \Omega) \omega d\omega = \int \Omega q_{R,\omega} (r) d\omega, \]
\[ q_{R,\omega} (r) = \int \mathcal{J}_\omega (r, \Omega) \omega d\omega, \quad q_R = (q_R \cdot n), \quad (16) \]

where \( \mathcal{J}_\omega (r, \Omega) \) is the spectral intensity of heat radiation; \( \mathcal{\kappa}_\omega (r) \) is the spectral absorption coefficient; \( j_\omega (r) \) is the spectral emission coefficient calculated in the case of local thermodynamic equilibrium (LTE) by the Kirchhoff low

\[ j_\omega (r) = \mathcal{\kappa}_\omega (r) j_{b,\omega} (r), \quad (17) \]

where \( j_{b,\omega} (r) \) is the black body spectral intensity (the Planck function); \( r \) is the coordinate of a point; \( \Omega \) is the directional vector; \( \Delta \omega_{rad} \) is the total spectral range of heat radiation (in the given case \( \Delta \omega_{rad} = 1000 - 200 000 \text{ cm}^{-1} \)).

Viscosity and heat conductivity of gas mixtures are calculated by the following formulas [31]

\[ \mu = \frac{1}{N_n} \sum_{i=1}^{N_n} \left( Y_i / \mu_i \right), \quad \lambda = \frac{1}{2} \sum_{i=1}^{N_n} x_i \lambda_i + 1 \left[ \sum_{i=1}^{N_n} x_i / \lambda_i \right], \quad (18) \]
\[ \mu_i = 2.67 \times 10^{-5} \sqrt{\frac{M_i T}{\sigma_i \Omega_i^{2.22}}} \text{ g/cm-s}, \quad \lambda_i = 8330 \sqrt{\frac{T}{M_i}} \frac{1}{\sigma_i \Omega_i^{2.22}}, \text{ erg/cm-K}, \quad (19) \]

where \( \sigma_i \) is the effective collision diameter, \( A; \quad \Omega_i^{2.22} = f(T_i) \) is the collision integral;
\[ T_i = kT / \epsilon_i. \]
The effective diffusivity \( D_i \) for species \( i \) is calculated by the Wilke formula [32].

\[
D_i = \frac{1 - x_i}{\sum_{j \neq i} (x_j / D_j)}, \quad \text{cm}^2/\text{s}, \quad D_{i,j} = 1.858 \times 10^{-3} \sqrt{\frac{T^3}{M_i + M_j}} \frac{1}{p \sigma_{i,j}^2 \Omega_{i,j}^{(2,1)}}. \tag{20}
\]

The collision integrals are calculated by the Anfimov approximation

\[
\Omega_{i,j}^{(2,1)*} = 1.157 T_i^{-0.1472}, \quad \Omega_{i,j}^{(1,1)*} = 1.074 T_i^{-0.1604}, \tag{21}
\]

where [27]

\[
T_{i,j} = \frac{kT_i}{e_{i,j}}, \quad \varepsilon_{i,j} = \sqrt{\varepsilon_i \varepsilon_j}, \quad \sigma_{i,j} = \frac{1}{2} (\sigma_i + \sigma_j). \tag{22}
\]

Boundary conditions for pseudo-catalytic surface are used in the following form:

\[
(Y_{i,j})_w = Y_{i,\infty}, \quad i = 1, 2, 3, ..., N_e, \tag{23}
\]

where \( Y_{i,\infty} \) are the mass fractions in the oncoming gas flow.

The surface temperature is calculated using the following assumption:

\[
\varepsilon \sigma T_w^4 = q_w, \tag{24}
\]

where \( \varepsilon \) is the surface emissivity factor; \( \sigma = 5.67 \times 10^{-12} \text{W/(cm}^2\text{K}^4) \) is the Stephan-Boltzmann constant; \( q_w \) is the total heating of the surface (the sum of the convective and radiation heat fluxes).

The ray tracing method was used for calculation of radiation heat fluxes to the surface of Apollo command module. To calculate radiation heat flux to any element of the space vehicle surface, it is necessary to introduce a local spherical coordinate system with an origin at this point and the \( z \)-axis of which is directed along a local normal to the surface, and next to integrate the radiation heat transfer equation along each ray emitted from the chosen point.

In this local coordinate system each ray \( \Omega \) is defined by two angular coordinates, namely, the latitude angle \( \theta \in [0, \pi/2] \) and the azimuth angle \( \phi \in [0, 2\pi] \).

The spectral radiation heat flux is defined by the following formula:

\[
q_{R,w}(\mathbf{r}_j) = \int_0^{\pi/2} d\theta \int_0^{\pi/2} J_{w} (\mathbf{r}_j, \Omega) \cos \theta \sin \theta d\theta, \tag{25}
\]

where \( \mathbf{r}_j \) is the radius-vector of \( j \)-th point on the surface in the laboratory frame of reference; \( J_{w}(\mathbf{r}_j, \Omega) \) is the spectral radiation intensity at the point \( \mathbf{r}_j \) corresponding to a direction of the unit vector \( \Omega \).

Introduction of finite-difference mesh of angular directions allows to integrate equation (6) over angular variables and to calculate the spectral radiation flux:

\[
W_{w}(\mathbf{R}_j) = \sum_{m=1}^{N_{\theta}-1} (\theta_{m+1} - \theta_m) \sum_{n=1}^{N_{\phi}-1} J_w(\Omega_{m,n}) \times \frac{1}{2} \left( \sin \theta_{m+1} \cos \theta_{n+1} \cos \theta_{n} \sin \theta_{m} \sin \theta_{m+1} \cos \theta_{n+1} \cos \theta_{n} \sin \theta_{m} \right) (\theta_{m+1} - \theta_m) =
\]

\[
= \sum_{m=1}^{N_{\theta}-1} (\theta_{m+1} - \theta_m) \sum_{n=1}^{N_{\phi}-1} J_w(\Omega_{m,n}) \left( \frac{\cos^2 \theta_{m+1} - \cos^2 \theta_{n+1} \cos^2 \theta_{n}}{2} \right). \tag{26}
\]
where \( N_\phi \) is the number of rays emitted in the azimuthal direction; \( N_\theta \) is the number of rays emitted in the latitude direction.

The directing cosines

\[
\Omega_{m,n} = (\omega_x)_{m,n} \mathbf{i} + (\omega_y)_{m,n} \mathbf{j} + (\omega_z)_{m,n} \mathbf{k}
\]

are calculated by the following formulas:

\[
(\omega_x)_{m,n} = \sin \theta \cos \varphi \\
(\omega_y)_{m,n} = \sin \theta \sin \varphi \\
(\omega_z)_{m,n} = \cos \theta.
\]

To calculate spectral radiation intensity the radiation heat transfer equation should be integrated over an inhomogeneous optical path. For this purpose the following solution to the radiation heat transfer equation can be used

\[
J(\tau_v) = \int_0^{\tau_v} B_v(\tau_v') \exp\left[-(\tau_v - \tau_v')\right] d\tau_v',
\]

where \( \tau_v = \int_0^s \kappa_c \text{d}s' \) is the optical depth; \( B_v(T) = \frac{2h\nu^3}{c^2} \left[ \exp(h\nu/kT) - 1 \right]^{-1} \) is the black body radiation intensity; \( s \) is the coordinate along the ray, \( s = 0, \quad s = L \) are the initial (on the surface) and final (on the outer surface of the calculation range or on the space vehicle conjugate surface) coordinates of the segment with directing vector \( \Omega_{m,n} \). The finite-difference scheme for spatial variables \( s \) is formulated for each ray \( \Omega_{m,n} \).

Numerical integration in equation (29) is realized as follows:

\[
J(\tau_{NS}, \Omega_{m,n}) = \exp\left(-\tau_{NS}\right) \left\{ \sum_{k=1}^{NS-1} \hat{B}_k \exp\left(\tau_k\right) \left[ \exp\left(\tau_{k+1} - \tau_k\right) - 1 \right] \right\},
\]

where \( \hat{B}_k = \frac{(B_k + B_{k+1})}{2}, \quad \tau_j = \sum_{i=1}^{j-1} \left( \kappa_i + \kappa_{i+1} \right) (s_{i+1} - s_i), \quad i = 1, ..., NS. \)

The set of governing equations was integrated up to convergence of the velocity projections, temperature, pressure, density, and chemical species concentrations with relative error of about \( 10^{-3} - 10^{-5} \). The gas dynamic equations were integrated separately from other equations with the second order of accuracy in space without the use of additional numerical limits and of smoothing operators [33].

The energy conservation equation was integrated by the implicit finite-different method of the second order in space and time. Continuity equations for chemical species were integrated also by an implicit method of the second order of accuracy.

As was mentioned above, the spectral and group optical properties of gases of complex chemical composition were on-line calculated by the author’s code ASTEROID.

3. Spatial radiative gas dynamics of super-orbital Apollo command module

The aerothermodynamics of Apollo command module was numerically investigated for four trajectory points shown in table 2. In present paper we will analyze in detail the calculated data for the first point. This trajectory point corresponds to extremely nonequilibrium RadGD regime of super-orbital. It should be taken into account that in these cases the incoming gas is very rare. This means that the using of the continuum model of flow field can give rise doubts concerning its justification. Nevertheless, large dimension of the command module and the acceptable correspondence to
experimental and flight data demonstrated in previous works under similar conditions, actually justify the use of this model.

Two-dimensional images of the three dimensional gas dynamic fields around Apollo command module at the angle of attack of $\alpha=25^0$ are shown in figures 3 and 4. Figures and 4 show, correspondingly, the pressure, longitudinal velocity and Mach number, the translational temperature of all heavy particles and vibrational temperatures of N$_2$, O$_2$, and nitrogen oxide.

**Table 2.** Trajectory parameters used as initial data for calculations

| # | $t$, s | $H$, km | $V_\infty$, km/s | $p_\infty$, erg/cm$^3$ | $\rho_\infty$, g/cm$^3$ | Particles concentration, 1/cm$^3$ | Mean free pass, L, cm |
|---|---|---|---|---|---|---|---|
| 1 | 40 | 76.2 | 10.7 | 19.5 | 0.330\cdot10^{-07} | 0.687\cdot10^{-15} | 0.246 |
| 2 | 53 | 67.3 | 10.5 | 78.0 | 0.120\cdot10^{-06} | 0.249\cdot10^{-16} | 0.068 |
| 3 | 220 | 73.2 | 6.5 | 31.8 | 0.523\cdot10^{-07} | 0.109\cdot10^{-16} | 0.156 |
| 4 | 390 | 61.0 | 5.9 | 192. | 0.273\cdot10^{-06} | 0.568\cdot10^{-16} | 0.029 |

**Figure 3.** Pressure $\text{Pres}=p/p_0$ (a), where $p_0$ is the brake pressure in erg/cm$^3$, longitudinal velocity $V_\infty=\hat{u}V_\infty$ (b), and Mach number (c) for the 1st trajectory point.
The functions of a flow field presented in figure 3 show general peculiarities of hypersonic flows around entering command module. These are: an emergence of high pressure shock layer above aerodynamic front shield and domains of subsonic flow in shock layer and above back side surface where a vortex gas movement of large scale is observed. High temperature shock layer and total asymmetry of the flow field due to the angle of attack are also clearly seen there. The flow field in a wake is characterized by higher vibrational temperatures as compared to translational ones.

Mass fractions of atoms N and O and charged particles are presented in figures 5, 6. These figures give general representation concerning a degree of dissociation of diatomic molecules calculated with applying the models of non-equilibrium dissociation [7].

The distributions of ionized atoms and electrons presented in figures 7 show that under the considered conditions the general sources of electrons are the collisions of nitrogen atoms and electrons. The nitrogen oxide generally appear in the domain of shock wave front.

Distributions of pressure (figure 3), mass fractions of atomic nitrogen and oxygen (figure 5), as well as molecular and ionized species allow understand general peculiarities in formation of the radiation heat fluxes to surface.

General results of numerical simulations are presented in figure 7, where distributions of convective heat fluxes, as well as the integral radiation heat fluxes along the surface in meridional cross sections are shown. In the first case, the radiation heat flux exceeds the convective heat flux on the front shield surface, especially in the domain of leeward part.

Figure 4. Translational (a) and vibrational temperatures (in K) of (b) molecular nitrogen (TvN2), (c) molecular oxygen (TvO2), and (d) nitride oxide (TvNO) for the 1st trajectory point.
In addition to distributions of convective and integral radiation heat fluxes along a surface, the spectral group radiation heat fluxes at six points on the surface in the meridional plane are presented in
Coordinates of these points can be calculated from relations presented in these figures, where $s_1, s_2, \ldots$ are the longitudinal coordinates along the surface measured from the point #1 in figure 8, and $S_{surf}$ is the total length. From these figures one can see that the radiative heating of the front shield significantly exceeds radiative heating for back surface.

As mentioned above, the investigated calculation cases correspond to a rare gas flow. This immediately follows that significant part of ultraviolet (UV) radiation (for wavenumbers of heat radiation of $\omega>50$ 000 cm$^{-1}$) achieves a surface.

Finally we compare the numerical simulation results obtained in present work with available data on preliminary prediction [12,34,35] and analytical correlations [18]. This comparison (figure 9) demonstrates acceptable agreement with previous investigations.

**Figure 7.** Distribution of the convective (1) heat flux ($Q_{w,con}=Q_{w,con} + Q_{w,diff}$, $Q_{w,con}$ is the conductive part of the convective heat flux, $Q_{w,diff}$ is the diffusive part) and integral radiation (2) heat fluxes on the front shield with catalytic surface. Trajectory point #1 (a) and #3 (b).

**Figure 8.** Radiation heat fluxes at six points on the surface in meridional plane of the Apollo-17 for the 1st trajectory points (left picture). Grid for prediction of radiation heat fluxes on the surface. Order of the points specifies the order of bypass the surface (right picture).
4. Conclusion
The examination of urgent multiphysics problems that should be considered for reliable prediction of aerothermodynamics of super-orbital space vehicles has been presented.

Numerical analysis of three-dimensional radiative aerothermodynamics of super-orbital Apollo command module based on the numerical simulation data obtained with using the author computer codes, has been presented. Distinguishing feature of presented data is a comparison of convective and radiative heating of the landing module surfaces, as well as a comparison of obtained calculation data on convective heating with correlation data for heating of front aerodynamic shield.

The author’s three dimensional computational fluid dynamic code NERAT(3D)+ASTEROID has been used for investigation of radiative gas dynamics of super-orbital landing module at entering Earth atmosphere under angles of attack. Three dimensional calculations of convective and radiative heating have been performed. It has been shown that for some trajectory points the radiative heating exceeds the convective heating.

![Graph](image)

**Figure 9.** Data on convective and radiative heating of stagnation point of Apollo-17 along trajectory, which were measured in flight [12], and were predicted in given work and with different methods [18,34,35]:

1 – convective heat flux [18], 2 – integral radiative heat flux [18], 3,6 – prediction of the total heat flux [12], 4 – calorimeter flight data [12], 5 – prediction of the integral radiation heat fluxes [34,35], 6 – convective heat flux (two-dimensional calculations) [36], 8 – total heat flux with radiation heat flux including UV region, 9 – total heat flux without radiation heat flux in UV region, 10 – radiation heat flux including UV region, 11 – radiation heat flux without UV region.
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