HIGHTEMP TECHNIQUE OF HIGH TEMPERATURE GAS FLOWS NUMERICAL SIMULATION

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ABSTRACT

A brief description of effective Navier-Stokes (NS) numerical technique for high temperature gas flows simulation (HIGHTEMP) is given. The NS codes have been developed for various gas-phase models from perfect gas to thermally and chemically nonequilibrium multicomponent and multitemperature gas medium. Slip effects, finite rate energy exchanges, surface catalysis and ablation can be taken into account in the wall boundary conditions. The software package HIGHTEMP involves codes for radiative heat transfer (RHT) computations. Several turbulence models for calculation of turbulent flows can be employed. For numerical integration of NS and RHT equations TVD type finite volume schemes are used. The solvers have been adopted for parallel high performance computing systems using MPI-technology. Some numerical results obtained with developed technique are presented.

INTRODUCTION

The development of the robust, efficient and handly numerical technique for gas flow simulation in a wide pressure, temperature and chemical composition range is a challenging task. HIGHTEMP computing system (CS HIGHTEMP) is elaborated in Institute of Mechanics Moscow State University to provide researches of high velocity aerodynamics, heat transfer and supersonic combustion (Gromov V. G., 2002). The HIGHTEMP technique is based on a software package of NS solvers integrated with thermochemical databases. The NS solvers are developed for three levels of the high temperature thermochemical gas-phase models from perfect gas to multitemperature and multicomponent ionized gas medium. Nonequilibrium chemical reactions, ionization, relaxation of internal energy modes can be included in a kinetic model with consideration their coupling. Gas-phase models can be used with various gas-wall interaction models. Slip effects, finite rate energy exchanges, surface catalysis and ablation can be taken into account in formulation of the boundary conditions. The numerical modeling of flows for high Reynolds numbers is carried out in the framework of Favre-averaged Navier-Stokes equations. The Boussinesq approximation for the turbulent fluxes simulation and several turbulence models for calculation of turbulent transport coefficients can be employed.

The NS equations are solved on the multiblock structured mesh through a finite volume approach. The inviscid fluxes across cell faces are calculated from result of the exact Riemann problem solution. The interfacial values are defined by the limited one-dimensional extrapolation of primitive variables from the cell-centers to the cell faces. The numerical viscous fluxes across cell faces are evaluated using the central and one-sided difference formulas of the second order accuracy. Steady-state solution is defined due implicit iterative procedure. On the every iteration the flowfield parameters are computed due Gauss-Seidel line relaxation numerical method. For time-marching integration of time-dependent NS equations the implicit Runge-Kutta scheme of second order accuracy is used. The NS solvers have been adopted for parallel high performance computing systems using MPI-technology.

The software package HIGHTEMP involves codes for radiative heat transfer computations. RHT equations are solved on the same mesh also through finite volume approach. Multigroup optical model is used to calculate absorption and emission coefficients (Surzhikov S.T., 2000).

The some examples of CS HIGHTEMP application to Earth and Mars atmospheres entry and flow in discharge channel of plasmatron are presented.

1. GAS-PHASE MODELS

1.1. Basic Assumptions

The following main thermochemical assumptions are used in the present version of CS HIGHTEMP:
- gas flow is described by a continuum formulation;
- gas medium is considered as an ideal mixture of thermally perfect gases;
- rotational temperature of molecules is equal to gas temperature;
- NS approximation is used for viscous transfer description.

1.2. Three Levels of Gas-Phase Models

In HIGHTEMP technique gas-phase models are divided to three levels. The first level consists of caloric perfect gas models (*PGM*) in which thermal processes are assumed to be in equilibrium or frozen, and chemical composition is constant. Set of primitive variables **Z**

defining gas state in the time-space point $(t, \vec{r})$ involves on this level following parameters: $\mathbf{Z} = \{p, \vec{u}, T\}$ where $\vec{u}$ is a velocity vector; T is a gas temperature. Thermodynamic pressure p and internal energy per unit mass e for these models are given by

$$p = \sum_{m=1}^{\nu} p_m \; ; \; p_m = \rho R_u T \gamma_m \; ; \tag{1}$$

$$e = \sum_{m=1}^{\nu} e_m(T) \gamma_m \; , \tag{2}$$

where ρ is a density; R_u is an universal gas constant; ν is species number; p_m , γ_m and e_m are respectively a partial pressure, a mole-mass fraction and an internal energy per mole of species *m*. Functions $e_m(T)$ are defined either by analytical expressions or by curve fits. For *PGM* models chemical composition is specified and therefore internal energy of gas mixture is function the gas temperature only: $e = e(T)$.

The second level consists of two classes of one temperature chemically nonequilibrium models: *STN* (Single Temperature Neutral) and *STI* (Single Temperature Ionized). The vector of state on this level is $\mathbf{Z} = \{p_1, ..., p_\nu, \vec{u}, T\}$. Thermal and caloric equations of state are given by Eqs. 1-2. For models *STI* in addition it is assumed that mixture is quasi-neutral

$$\sum_{m=1}^{\nu} z_m p_m = 0 \, , \tag{3}$$

where z_m is the charge number.

The term 'species' can designate the chemical species or some discrete energy state of the chemical species. These models are useable for description of flows when internal energy modes of species are in equilibrium with translational mode or frozen, or for state-to-state description of a population of the some internal energy levels.

The third level of models consists from two classes of multitemperature models *MTN* and *MTI*. The vector of state on this level involves following components: $\mathbf{Z} = \{p_1, ..., p_\nu, \vec{u}, T_1, ..., T_\eta\}$. These models may be used for both modal and state-to-state description of a population of the internal energy levels. The temperature T_n is parameter of partition functions for the n^{th} group of energy modes of one or several chemical species. It is assumed that translational temperature of all heavy particles is $T = T_1$. For model *MTN* thermal equation of state is given by Eq.1. For model *MTI* expression for partial pressure of free electrons is changed to form

$$p_e = \rho R_u T_e \gamma_e \tag{4}$$

where subscript "*e*" denotes free electrons. Caloric equation of state for these models is given by

$$e = \sum_{m=1}^{\nu} e_m(T_1, ..., T_\eta) \gamma_m \, , \tag{5}$$

1.3. Transport Properties

Transport properties are required to describe the viscous fluxes of species mass, momentum, and energy in gas medium. Viscous fluxes for NS approach are linear functions of space derivatives of primitive variables $\mathbf{Z}$ with coefficients as functions of $\mathbf{Z}$ components (Kolesnikov A.F., 2002). Viscous fluxes are defined from linear equations with coefficients as functions of mole weights and transport cross sections of pair collisions (collision integrals). For calculation of collision integrals good results are obtained using spherically symmetric potentials depending only on distance between colliding particles. In the present version of CS HIGHTEMP collision integrals of pair neutral-neutral are calculated on Lennard-Jones potential at low temperature and on exponential repulsive potential at high temperature. Collision integrals for pair neutral – non parent ion are calculated on the polarization potential for low temperature and also on exponential repulsive potential at high temperature. At an evaluation of diffusion type collision integrals for pair neutral - parent ion effect of resonant charge transfer is taken into account. The collision integrals of electron - neutral scattering are calculated using experimental results and estimations. The interactions of charged particles are described on the basis of the screened Coulomb potential. Parameters of potentials for pair of identical particles are taken from published data and are included into database. Parameters of potentials for the particles of different kinds are determined on the combinatorial rules. Obtained data are used in the form of curve fits as temperature functions.

1.4. Kinetic Models

The nonequilibrium chemical reactions and ionization, nonequilibrium excitation of vibrational and electronic energy of species for modal and multi-level descriptions may be included into gas-phase kinetic model (Ed. by Chernyi G.G., 2004). Global, quasi-global and detailed reaction mechanism can be used in the chemical kinetics model. The rate of detailed chemical reactions and ionization is determined by the mass action law with rate constants specified in the generalized Arrhenius form. Vibration excitation mechanism can involve *VT*, *VV*, *VE*, *Ve* and *VC* energy exchanges. Different types of coupling of kinetics processes have been realized in the codes. A convenient form of kinetic data specifications has been developed.

2. GAS-WALL INTERACTION MODELS

2.1. Slip Phenomena

Near wall effects of the gas rarefaction are described in frames of continual approach taking into account slip effects in the boundary conditions on the wall (Gupta R.N., 1986)

2.2. Thermochemical Interaction

Various thermochemical gas-wall interaction models consistent with gas-phase modeling are provided. In these models finite rate of exchange by vibrational and electronic energies, catalytic reactions, chemical reactions between gas and surface material can be taken into account. Nonequilibrium surface catalysis is defined by a set of reactions of physical and chemical adsorption - desorption on active sites and Eley-Rideal or Langmuir-Hinshelwood reactions between gas and adsorbed particles (Afonina N.E., 2001). Thermo-chemical destruction (ablation) of the surface is modeled in quasi-steady approximation by the specified set of heterogeneous reactions (equilibrium, nonequilibrium or given destruction rate as function of wall temperature). It is possible to use unsteady ablation model in coupling with calculation of unsteady 1D heating and destruction of the heat protection covering.

3. GOVERNING EQUATIONS

3.1. Navier-Stokes Equations in Integral Form

The integral form of time-dependent Navier-Stokes equations for all considered gas-phase models may be written as

$$\frac{d}{dt}\int_V \mathbf{Q}dV + \int_{\delta V} \vec{n}\cdot\vec{\mathbf{F}}dS = \int_V \boldsymbol{\omega} dV\,, \qquad (6)$$

where V is a fixed control domain; δV is its boundary; $\vec{n}$ is an unit outward normal to δV; $\boldsymbol{Q}$ is a set of the conservative variables per unit volume; $\vec{\mathbf{F}} = \vec{\mathbf{F}}^{inv} + \vec{\mathbf{F}}^{vis}$ represents a sum of inviscid and viscous fluxes of $\boldsymbol{Q}$ through the domain boundary and $\boldsymbol{\omega}$ is a set of the source terms. A composition of the algebraic vectors $\boldsymbol{Q}$, $\vec{\mathbf{F}}^{inv}$, $\vec{\mathbf{F}}^{vis}$, and $\boldsymbol{\omega}$ is defined by used thermochemical model and considered task.

3.2. Radiation Heat Transfer

Radiation heat transfer is described by balance equation written for control domain V with boundary δV in following form

$$\int_{\delta V} \vec{n}\cdot\vec{\Omega} I_\lambda dS = \int_V (j_\lambda - \kappa_\lambda I_\lambda) dV\,, \qquad (7)$$

where $I_\lambda\left(\vec{r},\vec{\Omega}\right)$ is a spectral intensity of the medium, j_λ and κ_λ are spectral emission and spectral absorption coefficients of the medium. These coefficients depend from populations of exited energy levels and optical properties of particles (Surzhikov S.T., 2000).

3.3. Boundary Conditions on the Wall

The boundary conditions on the wall in the general case involve a set of balance relations for mass of species, momentum and considered energy modes. For the 'gray' radiation model of the wall the boundary condition for RHT equation is given by

$$I_{\lambda,w} = \varepsilon_S I_{b,\lambda}(T_s)\,, \qquad (8)$$

where ε_S is a surface emissivity; $I_{b,\lambda}(T_s)$ is a spectral intensity of blackbody radiation at the wall temperature T_s.

4. NUMERICAL METHOD

4.1. Navier-Stokes Solver

The governing equations are solved in curvilinear structured mesh through a finite volume approach. Under this approach the difference equations consist of numerical analogs of the conservation equations for cells covering a computation domain and numerical approximation of the boundary conditions. This method yields an approximate solution $\mathbf{Z}_C$ in the center of each cell and in the center of each cell side lying on the wall. The inviscid numerical fluxes $\mathbf{F}_B^{inv}$ across cell sides are calculated from the result of the exact Riemann problem solution $\mathbf{Z}_B = \Re\left(\mathbf{Z}_B^L, \mathbf{Z}_B^R\right)$ where $\Re$ is the Riemann problem solver. The interfacial values $\mathbf{Z}_B^L$, $\mathbf{Z}_B^R$ are defined by the one-dimensional limited extrapolation of $\mathbf{Z}$ from the cell-centers to the cell sides. The numerical viscous fluxes $\mathbf{F}_B^{vis}$ through cell sides are evaluated using the central and one-sided difference formulas of the second order accuracy.

The steady-state solution is defined due implicit two-layer iterative procedure. Linear implicit operator is similar to quasi-linear form of the governing equations. Operator is solved by the Gauss-Seidel line space-marching method with the *LU*-decomposition of the block-tridiagonal matrices to find solution in every line step. The implicit Runge-Kutta scheme of second order accuracy is used for time-marching integration.

4.2. RHT Solver

The finite volume approach is used to solve *RHT* equations also. Spectral intensity $I_\lambda\left(\vec{r},\vec{\Omega}\right)$ is defined for some discrete intervals of spectra and $\vec{\Omega}$ where spectral intensity is considered as constant. Radiation fluxes across the cell side for discrete values of I_λ are evaluated using known "upwind" approximation. Solution of numerical *RHT* equations is performed by

several walks of cells in different sequence starting from the boundaries.

5. GENERAL STRUCTURE AND OPERATION OF CS HIGHTEMP

The CS HIGHTEMP consists of following main parts:

- database of molecular, thermochemical and transport properties of individual gases;
- databases of transport properties for the some sets of species;
- kinetic databases for the some sets of chemical and thermal processes;
- codes for calculation and fitting of thermodynamic properties for individual species;
- codes for calculations of transport properties of gas mixtures;
- codes for generation of thermochemical models (generators of models);
- NS and RHT solvers for different classes of models;
- BATCH COMMAND codes for control of EXECUTE codes compilation.

The CS HIGHTEMP can be associated with other database or CS, for example optical database and grid generation CS.

The generation of EXECUTE code is performed in two steps. On the first step information about model, containing in the databases and additional files, converts by the codes-generators to a set of INCLUDE files used for compilation EXECUTE codes, and DATA files used for codes execution. On the second step the compilation of EXECUTE code for specific task is performed under control of special BATCH COMMAND codes. On this step additional information about geometry, grid, and the like is used also.

6. APPLICATIONS

6.1. Martian Atmosphere Entry Computations

The axisymmetric flow over spherically blunted 60-deg half-angle cone with cylindrical afterbody is considered (Gromov V. G., 2002). The shape and sizes of the body are presented on Fig. 1.

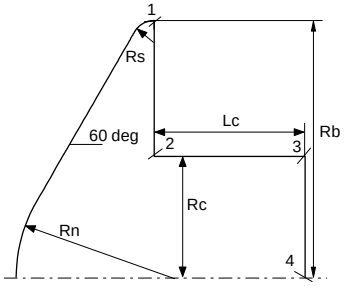

Figure 1. Shape and sizes of the body. Rn=1.0m, Rs=0.15m, Rb=1.7m, Rc=0.8m, Lc=1.0m

For detailed flowfield and surface heating calculations both one-temperature *STN* and five-temperature *MTN* gas-phase models were employed.

STN model contains 11 species: O, C, N, Ar, O_2, N_2, CO, C_2, CN, NO, CO_2. For this gas-phase model four gas-wall interaction models were considered: fully neutral to all chemical processes wall (*NCT*), fully catalytic to recombination of CO_2 and O_2 and neutral to other reactions wall (*FCT*), partially catalytic wall (*PCT*) and chemically equilibrium wall (*EQW*). The partially and fully catalytic models are based on a mechanism of heterogeneous recombination of O_2 and CO_2 involving reactions of chemical adsorption-desorption of atoms O and Eley-Rideal reactions recombination O_2 and CO_2.

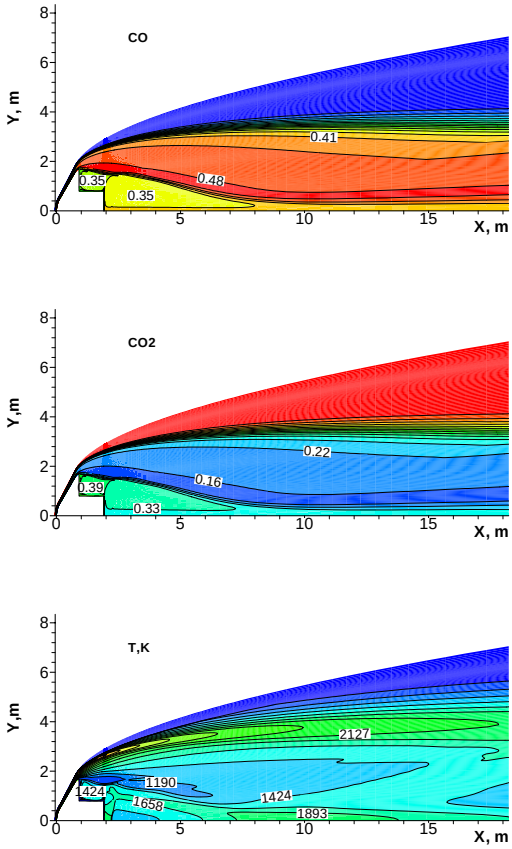

Figure 2. Distributions of CO and CO_2 mole fractions, and gas temperature T,K. Model STN-FCT

Fig.2 shows predicted distribution of CO, CO_2 mole fractions and gas temperature *T* in computation domain for $\rho_\infty = 2.93 \cdot 10^{-4}$ kg/m^3, $V_\infty = 5223$ m/s. Fig.3 demonstrates effect of the wall catalysis on the forebody and afterbody surfaces heating for the same free conditions.

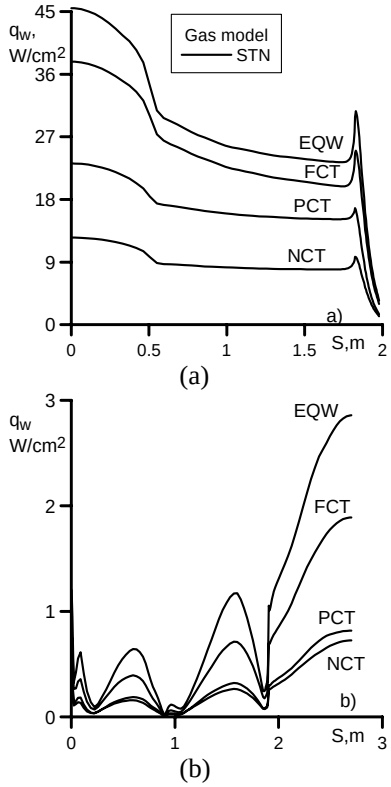

Figure 3. Effect of the wall catalysis on the forebody (a) and afterbody (b) surface heating

The five-temperature *MTN* model involves 21 species: O, C, N, Ar, O_2, N_2, $N_2(A^3\Sigma)$, $N_2(B^3\Pi)$, CO, $CO(A^1\Pi)$, $CO(B^1\Sigma)$, $CO(b^3\Sigma)$, $CO(a^3\Pi)$, C_2, $C_2(d^3\Pi)$, CN, $CN(A^2\Pi)$, $CN(B^2\Sigma)$, NO, $NO(A^2\Sigma)$, CO_2. The non-equilibrium excitation of three vibrational modes of CO_2 and vibration of N_2 are taken into account. A dissociation-vibration coupling was included in description of molecules CO_2 and N_2 dissociation. Model *MTN* is used for calculations of nonequilibrium forebody radiation.

Four radiation models were used for calculation of radiative heating rate (Gromov V.G., 2002):

1. Q-branch model with nonequilibrium population of excited electronic levels and Boltzmann population of vibrational levels at $T_V = T$ (with *MTN* model);
2. Q-branch model with Boltzmann population of excited electronic and vibrational levels of molecules at $T_E = T_V = T$ (with *MTN* model);
3. The multigroup LTE model taking into account only the CO emission in wavelength interval 0.1-0.2 μm (with *STN* model);
4. The multigroup LTE model taking into account the CO emission in wavelength interval 0.1-0.2 μm. and the CO and CO_2 emission induced by vibrational-rotational transitions in wavelength interval 2-10μm (with *STN* model).

Comparison of predicted results is shown on Fig.4. Curve number on Figure is number of radiation model.

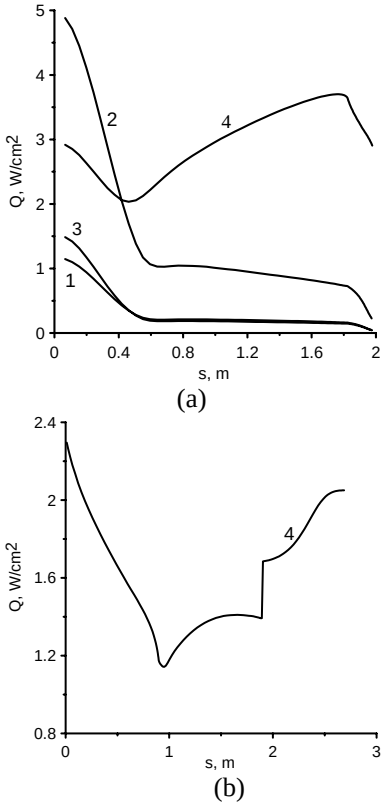

Figure 4. Radiative heat flux distribution along forebody (a) and afterbody (b) surface predicted by various radiation models

6.2. Numerical Simulation of Hypersonic Non-equilibrium Air Flow past Reusable Launch Vehicle

HIGHTEMP technique was applied for modeling of aerodynamics and heat transfer over nose-blunted 3D airplane-type configuration. Conditions used for the calculation represent the point trajectory corresponding to the flight parameters at the altitude of 80 km in the Earth atmosphere (angle of attack is 15^0; velocity is 6788 m/s; free stream pressure is 1.05 Pa; free stream temperature is 198.6 K; surface temperature T_W is 300K). The calculations were performed using *STN* model involving 5 species (O, N, O_2, N_2, and NO) for non-catalytic surface. Total cells number in computational region over nose-blunted 3D airplane-type configuration is about 1.5 millions points compressed over the body surface. It was generated by professor Y.D.Shevelev's group (ICAD RAS) and was kindly given to us.

The NS codes adopted for parallel high performance computing systems have been used for calculations.

Fig. 5 demonstrates the Mach number distribution in shock layer in symmetry plane at leeward and windward sides and in the base region.

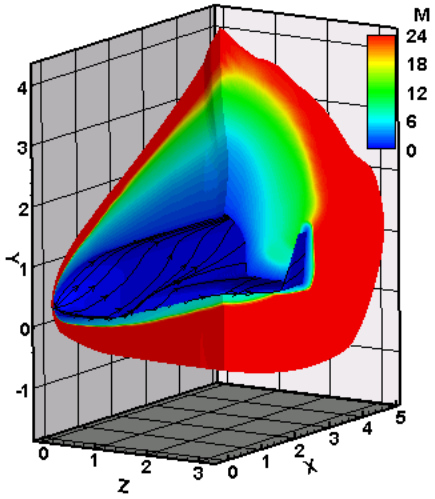

Figure 5. Mach contours in shock layer

6.3. CFD Modelling of Thermally and Chemically Nonequilibrium Flows in Inductive Plasmatron

The thermally and chemically nonequilibrium flows in discharge channel of inductive plasmatron IPG-4 (IPM RAS) and in under-expanded air jets over a butt-end model are studied on base CS HIGHTEMP (Sakharov V.I., 2003). The main IPG-4 parameters in the tests are the following: the anode power supply N_{ap}=45,3 kW (the corresponding power input in plasma N_{pl} =29 kW), the generator frequency f = 1.76 MHz, the air mass flow rate G = 2.4 g/s, the angle of the flow swirl is 45^0, the discharge channel diameter D_C= 80 mm and the length L_C = 40 mm. A conical sonic nozzle with exit diameter D_S = 40 mm and the semi-angle 24^0 is located at the channel upper interface. The ground pressure in the test chamber was sustained at constant level p_∞ = 8.3 hPa. The water-cooled copper model of 20 mm in diameter with flat face was used in the experiment.

The gas mixture consists of 11 species: O, N, O_2, N_2, NO, O^+, N^+, O_2^+, N_2^+, NO^+, e.

Three thermochemical models have been used in CFD modelling:

- one-temperature *STI* model;
- two-temperature *MTI* model with common temperature of the free electrons T_e and vibrational temperatures of O_2, and N_2;
- three-temperature *MTI* model with common vibrational temperatures T_V for molecules O_2, N_2 and individual temperature T_e of free electrons.

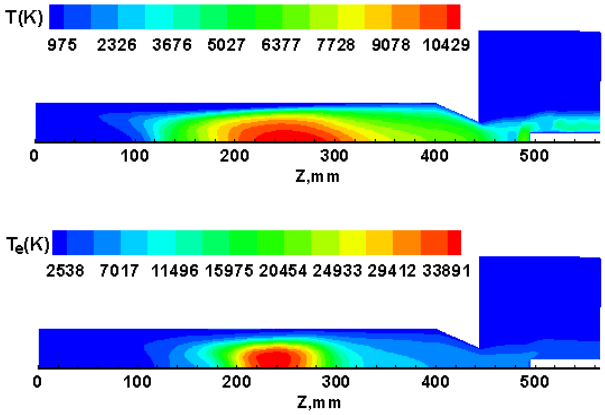

Figure 6. Translational and electron temperature contours in the discharge channel of plasmatron

Distributions of gas and electron temperatures in the discharge channel of plasmatron predicted for three-temperature model are shown on Fig.6.

CONCLUSION

Effective computing system for high temperature gas flows simulation has been developed. The system is based on the package of NS and RHT solvers integrated with thermochemical databases. Presented examples of calculations demonstrate wide possibility of the system for study problem of hypersonic and plasma aerodynamics for aerospace applications.

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