Numerical simulations of heat and mass transfer at ablating surface in hypersonic flow

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Abstract. The numerical technique was developed to solve heat and mass transfer problem in 3D hypersonic flow taking into account destruction of thermal protection system. Described technique was applied for calculation of heat and mass transfer in sphere-cone shaped body. The data on temperature, heat flux and mass flux were obtained.

1. Introduction
The influence of airflow on a body moving in the atmosphere at a speed of several kilometers per second results in heating of the body up to several thousand degrees, and ablation of thermal protection system (TPS) is a natural way of heat removal. The complexity of ground-based experiments on hypersonic flow dictates the need of development of numerical modeling methods for such flows. This area is being developed continuously from middle of the 20th century to present time. Many papers published during this time prove the relevance of this topic, for example, [1–6].

2. Problem setup and solution technique
The simulation method is based on numerical solution of three-dimensional heat equation (1) within TPS, calculation of heat and mass flux on the flow-wall interface, estimation of the surface recession rate, and re-shaping of both surface and interior:

\[
\rho C_p \frac{\partial T}{\partial t} = \text{div}(\lambda \text{grad}(T)).
\]

(1)

Where \(\rho\)—material density of body and TPS layer, \(C_p\)—heat capacity, \(\lambda\)—heat conduction, \(T\)—temperature, \(t\)—time. The ablating surface is considered as moving, the normal velocity of surface element \(v_n\) is defined with mass flux \(\dot{m}\), i.e. \(v_n = \frac{\dot{m}}{\rho}\). The surface under TPS layer is considered as nondestructive and steady (figure 1).

We use Ansys Fluent for solving the heat problem, which is capable of working on unstructured grids using finite volume method. The link between TPS characteristics and flow parameters (surface model) is realized through a solution of the set of equations for mass- and heat-rate at the surface.
\[ q_w = f(T_w, P_w, q_0, \ldots); \dot{m}_w = f(T_w, P_w, q_0, \ldots). \]  \tag{2}

Here, \( q_0 \) is the heat flux from the flow (it can include the radiation flux as well). In the paper, well known model [7] is applied as an example. In this model mass flux is defined by the following expressions:

\[
\frac{1}{\dot{m}_w} = \frac{1}{\dot{m}_r} + \frac{1}{\dot{m}_s}.
\]

Here, \( \dot{m}_r \)—mass flux of carbon due to the reaction mechanism; \( \dot{m}_s \)—mass flux of carbon due to the diffusive mechanism. Expressions for fluxes:

\[
\dot{m}_r = K_r \exp \left( -\frac{T_r}{T_w} \right) P_{O_2}^{1/2},
\]

where \( K_r = 14800, T_r = 22157. \) \( P_{O_2} \)—partial pressure of oxygen (Pa). In equilibrium we can consider \( P_{O_2} = 0.21P. \)

Next, \( \dot{m}_s = 6.67 W_{cw} \dot{m}_d, \) where

\[
W_{cw} = 0.15 + 5.35 \times 10^9 \exp \left( -\frac{T_s}{T_w} \right),
\]

\[
\dot{m}_d = K_d \left( \frac{P_I}{R_{eff}} \right)^{1/2},
\]

\[
T_s = 61670, K_d = 5.38 \times 10^{-5}.
\]

Here, \( P_I \)—pressure on the outer edge of the boundary layer, \( R_{eff} \)—effective radius of surface curvature.

The dependence of the mass flux on the temperature for free-stream velocity 7000 m/s and air density corresponding to altitude 20 km we used is presented in figure 2.

Other material-specific surface models can be easily implemented to the developed method. Next, a sophisticated procedure has been developed to take accurately into account the changes in surface shape followed by interior grid re-building. It was found that the robust way to solve conjugate heat-transfer problem when using separate solvers for hypersonic flows and for interior is to apply heat transfer coefficient approach to represent the heat flux from the flow, \( q_0. \)

To take into account changes in the body shape in the bulk the law of motion for computational grid nodes is to be defined. Once mass flux is determined from the set (2), recession rate is readily obtained. Next, trans-finite interpolation technique is applied to find the node velocity and node position for every grid node within a TPS bulk. Internal iterations are used at every time step to solve for set of equations including boundary conditions (2) coupled with the law of motion for the grid nodes.

Heat and mass transfer models, boundary conditions and node motion law were implemented to Ansys Fluent as a C++ program.
3. Demonstration problem

For validation of the developed method, several 1D/2D test problems on the conjugate heat transfer and moving boundary surface were solved. Good agreement was obtained with the theoretical results. For example we present comparison of calculation with our technique with analytical solution (see figure 3) presented in [1], p.58 for following problem. We considered a one-dimensional uniform rod with length, density, heat capacity and thermal conductivity are equal to 1, heat of evaporation 2 and thermoisolated side surface. Initial and boundary conditions for temperature $T$ were following: $T(x,0) = 0, T(0,t) = 0, \frac{dT}{dx}(1,t) = \text{const} = -5$ ($x$—coordinate). Evaporation began at temperature was equal to 2. Temperature distribution was needed.

Next, 3D unsteady numerical simulation of thermal state within a sphere-cone shaped body was carried out. The hypersonic flow around the body was preliminarily calculated with
the JIHT RAS PlasmAero code [8] and heat transfer coefficient data in terms of Stanton number was delivered to Ansys Fluent. As a material of TPS, the graphite has been used. Unstructured tetrahedral mesh with about of 100,000 grid cells was used for this test. View of the computational grid is shown in figure 4.

The distributions of temperature, heat flux and ablation rate over the body surface are presented in figures 5–8.

4. Conclusions
The numerical technique was developed to solve conjugate heat- and mass-transfer problems on the surfaces of arbitrary shape. It is primarily intended to estimate thermal state within a bulk of a hypersonic vehicle. The key features of this technique are the possibility of using of standard computational environment (including commercial one), the use of unstructured computational grids, ability to work with arbitrary geometries, and ability to apply any heat- and mass-transfer models coupled with adequate surface/interior grid re-building. The technique was carefully validated on 1D, 2D and 3D problems. Good accuracy and efficiency was established.
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