Computational conjugate modeling of aerodynamical flow and thermal stresses in ablative composite structures

Yu I Dimitrienko, M N Koryzkov, Yu I Yurin, A A Zakharov and S V Sborschikov
Bauman Moscow State Technical University, Moscow, 105005, Russia
E-mail: dimit@bmstu.ru

Abstract. The conjugate problem of aerodynamics and thermomechanics for a composite structures made of ablating composite material such as carbon/phenolic or glass/phenolic is considered. The problem includes a three-dimensional Navier-Stokes system of equations - for a high-speed flow around the structure, as well as a system of internal heat and mass transfer in an ablating composite and a three-dimensional theory of elasticity of anisotropic material with variable properties. To solve the conjugate system of equations, a numerical algorithm is developed based on the finite-volume method for solving the Navier-Stokes equations and the finite-element method for solving the equations of heat and mass transfer and thermomechanics. Examples of computations for modeling reentry vehicles are presented. The features of the distribution of heat and mass transfer fields and thermal stresses in the structures caused by the effects of thermal decomposition of the composite during non uniform heating are shown.

1. Introduction

Composite polymer materials, mainly ablative carbon/phenolic and glass/phenolic composites, are still the important types of materials used in heat-shielding systems of re-entry vehicles (RV) moving in dense layers of the Earth’s atmosphere, as well as other planets (Mars, Venus). In [1-3], a mathematical model was developed for the processes of internal heat and mass transfer in ablative polymeric composite materials during non-stationary heating, taking into account the processes of thermal decomposition, gas generation and gas filtration in the pores of the material. Since at different times of the descent of the RV in the atmosphere, varying power and thermal loads act on its ablative structure, in order to set the boundary conditions for the problem of thermomechanics, it is necessary to first solve the problem of aerodynamics. The general formulation of the conjugate problem of aerodynamics and thermomechanics of a ablative heat-shielding structure consists of three systems of equations:
• Navier-Stokes equations for an external high-speed flow;
• equations of internal heat and mass transfer in ablative composite structure;
• equations of thermoelasticity of the ablative heat-shielding structure.

2. The mathematical formulation of the conjugate problem.

Consider the system of equations for a viscous heat-conducting gas (Navier-Stokes equations) [4,5]:
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,
\]
\[
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + \rho \mathbf{E} - \mathbf{T}) = 0,
\]
\[
\frac{\partial \rho c}{\partial t} + \nabla \cdot ((\rho c + p) \mathbf{v} - \mathbf{T} \cdot \mathbf{v} + \mathbf{q}) = 0,
\]
where \( \rho \) is the gas density, \( t \) is time, \( \mathbf{v} \) is velocity vector, \( p \) is pressure, \( \mathbf{E} \) is the unit tensor, \( \varepsilon \) is the density of the total energy of the gas, \( \mathbf{T} \) is the viscous stress tensor and \( \mathbf{q} \) is the heat flux vector, \( \nabla \) - nabla-operator. We add to this system the determining ratios of the perfect gas:

\[
\rho = \frac{R \theta}{M}, \quad \varepsilon = c, \quad \varepsilon = c + |\mathbf{v}|^2 / 2.
\]

\[
\mathbf{T} = \mu_1 (\nabla \cdot \mathbf{v}) \mathbf{E} + \mu_2 (\nabla \otimes \mathbf{v} + \nabla \otimes \mathbf{v}^T),
\]

\[
\mathbf{q} = -\lambda \nabla \theta,
\]

where \( R \) is the universal gas constant, \( M \) is the molecular mass, \( \theta \) is temperature, \( c_v \) is the heat capacity at constant volume, \( \mu_1 \) and \( \mu_2 \) are viscosity coefficients, \( \lambda \) is the gas thermal conductivity. Coefficients of viscosity and thermal conductivity are functions of temperature.

The boundary conditions for the system (1), (2) on the surface of a solid with a gas flow are as follows:

\[
v = 0, \quad \theta = \theta_s,
\]

where \( \theta_s \) is the surface temperature of the structure.

Next, we consider a heat-shielding structure made of a ablative polymer composite material. Under the influence of high temperatures, usually above 300 °C, internal physicochemical transformations — thermal decomposition processes — occur in polymer composite materials. As a result, the composite during heating is a multiphase system; in [1-3], a 4-phase system model was proposed in which the 1st phase is a filler (fibers, reinforcing particles), the 2nd phase is a polymer matrix; The 3rd phase is the solid pyrolytic phase, which is formed from the polymer at high temperatures, the 4th phase is the gas, also formed due to thermal decomposition of the initial phase 2 and located in the pores.

The mathematical model of internal heat and mass transfer in a thermal decomposition composite consists of a system of equations for changing the mass of the polymer phase, the equation for filtering gaseous products in the pores of the material, and the heat conduction equation

\[
\rho_b \frac{\partial \phi_b}{\partial t} = -J; \quad \frac{\partial \rho_g \phi_g}{\partial t} + \nabla \cdot \rho_g \phi_g \mathbf{v}_g = J \Gamma; \quad \rho_c \frac{\partial \phi}{\partial t} = -\nabla \cdot \mathbf{q} - c_v \nabla \theta - \rho_g \phi_g \mathbf{v}_g - J \Delta e^\theta;
\]

The notation is introduced here: \( \phi_b, \phi_g \) — volumetric concentrations of the polymer and gas phases; \( \rho_b \) is the density of the initial polymer matrix; \( \rho_g \) is the density of the gas phase; \( c_v \) is the heat capacity of the gas at a constant volume; \( \rho \) and \( c \) are the density and heat capacity of the composite, \( \mathbf{q} \) is the heat flux vector, \( \theta \) is the temperature of the composite; \( \mathbf{v}_g \) - is the gas phase velocity; \( \Delta e^\theta \) - is the specific heat of thermal decomposition of the matrix; \( J \) - is the mass rate of thermal decomposition of the matrix; \( G \) is the coefficient of gasification of the matrix.

The heat and mass transfer equations are closed by the defining relations that relate the vector functions \( \mathbf{q}, \mathbf{v}_g \) to the temperature and pressure gradients \( \nabla \theta, \nabla p \), using the Fourier and Darcy laws, as well as the Arrhenius relation for the mass rate of thermal decomposition:

\[
\mathbf{q} = -\Lambda \cdot \nabla \theta, \quad \rho_g \phi_g \mathbf{v}_g = -\mathbf{K} \cdot \nabla \rho_g \Gamma, \quad J = J_0 \phi_b \exp \left( \frac{E_A}{R \theta_0} \right) \cdot \rho_g \frac{\rho_g R \theta_0}{M_g},
\]

where \( J_0 \) is the preexponential factor, \( E_A \) is the activation energy of thermal decomposition processes, \( M_g \) is the molecular mass of the gas, \( \Lambda \) is the thermal conductivity tensor, and \( \mathbf{K} \) is the composite gas permeability tensor.

The boundary conditions for equations (1) - (3) on the heated surface are as follows:
where \( p, \theta \) is the pressure and temperature of the gas flow on the surface of the body, \( \theta_{\text{max}} \) is the temperature of the gas flow on the surface, \( \varepsilon_g \) and \( \varepsilon_s \) are the emission coefficients of the gas and solid, \( \sigma_{SB} \) is the Stefan-Boltzmann constant.

On the inner side of the heat-shielding material, the conditions of tightness and thermal insulation are set:
\[ n \cdot p = 0, \quad n \cdot A \cdot \nabla \theta = 0. \]

To calculate the thermal stresses in the heat-shielding structure, we use the statement of the mechanics of elastic composite media with the presence of thermal decomposition of the matrix [1-3]. These equations consist of equilibrium equations, defining relations, Cauchy relations
\[ \nabla \cdot \sigma - \nabla (\varphi \cdot p) = 0, \]
\[ \sigma = C \cdot (\varepsilon - \varepsilon^0), \quad \varepsilon = a (\theta - \theta_0) - \beta \]

Here are designated: \( \sigma \) - stress tensor, \( \varepsilon \) - small strain tensor, \( \mathbf{u} \) - displacement vector, \( C \) - elastic modulus tensor, depending on temperature and the local anisotropy basis, \( \varepsilon \) - thermal strain tensor, \( a \) - thermal expansion tensor, \( \beta \) - chemical shrink tensor. At high temperatures, the elastic modulus tensor substantially depends on temperature and duration of heating. Various modules for taking into account the effect of temperature on the properties of polymer composites were proposed in 7-11 and others. In this article, we used a model developed in [1-3].

Boundary conditions on the heated surface of the structure
\[ n \cdot \sigma = -(p - \varphi \cdot p) n \]

Boundary conditions on the remaining parts of the surface - free surface or hard termination
\[ n \cdot \sigma = n(\varphi \cdot p) = 0 \quad \text{or} \quad \mathbf{u} = 0 \]

### 3. Numerical methods for solving the conjugate problem.

To solve the aerodynamics problem (1) - (3), a finite-volume second-order approximation method with TVD reconstruction is used [6].

To solve the problem of internal heat and mass transfer (4) - (7), we write the variational statement of the problem
\[
\int \rho c \frac{\partial \varphi_\rho}{\partial t} dV = -\int \delta \varphi_\rho \cdot \rho c \mathrm{d}V,
\]
\[
\int \delta p \frac{M_s}{R \theta} \frac{\partial \varphi_{\rho_s}}{\partial t} dV - \int \delta p \frac{p M_s}{R \theta^2} \frac{\partial \varphi_{\rho_s}}{\partial t} dV = -\int \nabla p \cdot K \cdot \nabla \delta \rho dV + \int \delta \rho \cdot J \Delta \rho dV,
\]
where the variations of unknown functions are indicated through: \( \delta \varphi_\rho, \delta p, \delta \theta \) - the concentration of the polymer phase, pressure and temperature. According to the finite element method, we divide the computational domain into tetrahedra, introduce barycentric coordinates in each element (which coincide with the shape functions in the case of a linear approximation) and represent unknown functions in the following form:
\[
\varphi = [\Phi]^T \{ u \}, \quad p = [\Phi]^T \{ y \}, \quad \theta = [\Phi]^T \{ \vartheta \},
\]
where \( u, y, \theta \) - the values of the corresponding functions at the nodes of the finite element, and \( \{\Phi\}^T = (L_1, L_2, L_3, L_4) \) - is the string of form functions. Then from the variational formulation, we can obtain a local system of equations for each tetrahedron in the form:

\[
[M] \frac{\partial[u]}{\partial t} + [R] [u] = 0,

[M_p] \frac{\partial y}{\partial t} - [S] \frac{\partial [\theta]}{\partial t} + [K_p] [\theta] - [R_p] [u] = 0,

[M_p] \frac{\partial [\theta]}{\partial t} + [K_p] [\theta] - [R_p] = 0, \tag{13}
\]

designations are introduced here for the following matrices:

\[
[M_p] = \int \{\Phi\} \otimes \{\Phi\} \frac{M}{R_0^2} dV, \quad [M_p] = \int \{\Phi\} \otimes \{\Phi\} \rho c dV, \quad [M] = \rho \int \{\Phi\} \otimes \{\Phi\}^T dV,

[S] = \int \{\Phi\} \otimes \{\Phi\} \frac{PM}{R_0^2} dV, \quad [K_p] = \int \{B\}^T \cdot \{K\} \cdot \{B\} dV, \quad [K] = \int \{B\}^T \cdot \{A\} \cdot \{B\} dV,

[R] = J_0 \int \exp \left(- \frac{E}{R_0}\right) \{\Phi\} \otimes \{\Phi\}^T dV, \quad [R_p] = \Gamma J_0 \int \exp \left(- \frac{E}{R_0}\right) \{\Phi\} \otimes \{\Phi\}^T dV, \tag{14}

[q_c] [\Phi] dS - \int \{\Phi\} \psi dV, \quad \{B\} = [L] \otimes [\Phi]^T, \quad [L] = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right),

\psi = c_s \nabla \cdot [\Phi] \cdot \nabla p - J \Delta e^o = c_s \{\theta\} \cdot [B]^T \cdot [K] \cdot [B] \cdot [\theta] - J \Delta e^o.
\]

Collecting system (13) for all finite elements and applying the Runge-Kutta method to solve it, we obtain a linear system of equations with a sparse, asymmetric matrix. To solve it, a numerical bi-conjugate gradient method is used.

To solve the problem of the theory of elasticity (8) - (9), the finite element method is also used.

**Figure 1.** Temperature distribution in the nose cone of modeling RV, K

### 4. Results of computational simulation

A numerical solution of the problem was carried out for a model RV moving at a speed of \( M = 6 \). The design of the model RV consisted of two materials: phenolic fiberglass (critical blunting area), and epoxy fiberglass (shell). In fig. 1 shows the temperature distribution over the thickness of the structure of RV. The most heat-loaded region is critical blunting, where the temperature reached 1400 K. Under the influence of high temperatures, the phenolic matrix of the composite began to decompose, resulting in the formation of a large amount of gas in the pores of the composite. In fig. 2 shows the distribution of pore pressure. The maximum values were achieved in the material with an epoxy matrix, despite the fact that in this region the temperature is lower than in the region of blunting. This effect is explained by the presence of higher
primary porosity in the phenolic matrix, compared with epoxy. In fig. 3. The transverse stresses in the RV structure are presented. Their maximum value is achieved in the region of blunting at a certain depth from the heated surface.

![Figure 2.](image1.png)

**Figure 2.** Pore pressure distribution in the nose cone of modeling RV, Pa.

![Figure 3.](image2.png)

**Figure 3.** Transverse normal stress distribution in the nose cone of modeling RV, GPa.

5. Conclusions

The formulation of the conjugate problem of aerodynamics and thermomechanics of an ablative structure made of thermally destructive composites is considered. Numerical finite-volume finite-element methods for solving this problem are developed. An example of computational simulation for the modeling RV is given. Some effects of the stress state of structures due to thermal decomposition of the composite at high temperatures have been established.

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