

# Finite element modeling of thermal stresses in aerospace structures from polymer composite materials

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**Abstract.** The conjugate problem of aerodynamics and heat and mass transfer in heat-shielding structures made of ablating polymer composite materials is considered. To determine the heat fluxes in the shock layer, the chemical composition of the atmosphere is taken into account. A mathematical formulation of the joint problem is formulated and an algorithm for numerical solution is proposed. An example of a numerical solution of the problem for the reentry spacecraft Stardust is presented. It is shown that due to the high temperatures of aerodynamic heating of a structure made of a polymer composite material, an intense internal generation of gas appears in the structure of the material, which can lead to the destruction of the material. **Key words:** polymer composite material, finite element, aerodynamic heating, mathematical formulation.

## 1 Introduction

In the process of entry into the Earth's atmosphere of the returning spacecraft, high heat fluxes are formed in the shock layer and non-equilibrium chemical reactions occur, which leads to high temperatures on the surface of the spacecraft itself, and, as a result, to the need for its thermal protection [1-4]. The most commonly used method of protection is passive, which consists in the use of ablative composite materials. Ablative thermal protection is based on physical and chemical processes occurring in the bulk of the material, with significant energy absorption. The advantages of the passive method of thermal protection include: cost, ease of use, reliability, no restrictions on the maximum heat flow and a large selection of materials due to the development of organic chemistry. In [5-7], a mathematical model of the processes of internal heat and mass transfer in polymeric heat-shielding materials during non-stationary heating was developed, taking into account the processes of thermal destruction, gas formation and filtration of gases in the pores of the material.

Since to determine the thermal loads it is necessary to solve the problem of aerodynamics, the adjoint problem will be two systems of equations:

- the Navier-Stokes equations, supplemented by the equations of chemical kinetics, describing the change in the chemical composition of the gas;

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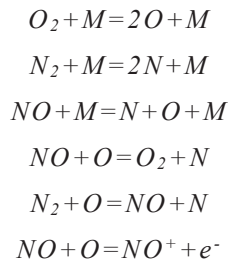
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- equations of internal heat and mass transfer in a heat-shielding structure.

## 2 Mathematical formulation

### 2.1 Navier-Stokes system and equations of chemical kinetics

Let us consider the oncoming flow as a mixture of 23.3% oxygen  $O_2$  and 76.7% nitrogen  $N_2$ . Let us assume that the gas flowing around the body consists of seven components ( $O$ ,  $N$ ,  $NO$ ,  $NO^+$ ,  $O_2$ ,  $N_2$ ,  $e^-$ ), and as possible chemical reactions occurring in the shock layer at high temperatures, we consider the following:



Here  $M$  means any of the 6 considered components that are catalysts,  $e^-$  – electronic component. We will associate the index  $i = \overline{1, 6}$  with components  $O$ ,  $N$ ,  $NO$ ,  $NO^+$ ,  $O_2$ ,  $N_2$  respectively.

Consider the system of equations for a viscous, chemically-reacting heat-conducting gas [8-16]:

$$\left\{ \begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} &= 0, \\ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p \mathbf{E} - \mathbf{T}_v) &= \mathbf{0}, \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot ((\rho \varepsilon + p) \mathbf{v} - \mathbf{T}_v \cdot \mathbf{v} + \mathbf{q}) &= 0, \\ \frac{\partial \rho y_i}{\partial t} + \nabla \cdot \rho y_i \mathbf{v} &= \nabla \cdot (\rho D_i \nabla \cdot y_i) + \dot{\omega}_i, \end{aligned} \right. \quad i = \overline{1, 4}. \quad (1)$$

The following constitutive relations are added to these equations:

$$\mathbf{T}_v = \mu_1 (\nabla \cdot \mathbf{v}) \mathbf{E} + \mu_2 (\nabla \otimes \mathbf{v} + \nabla \otimes \mathbf{v}^T) - \text{viscosity tensor}; \quad (2)$$

$$\mathbf{q} = -\lambda \nabla \theta - \sum_{k=1}^6 \rho D_k \nabla y_k (c_{pk} \theta + e_{vk} + h_k^0) - \text{heat flow}; \quad (3)$$

$$p = \rho \frac{R_0}{M_0} \theta - \text{Mendeleev-Clapeyron ratio.} \quad (4)$$

Here are marked:  $\rho$  – gas density [kg/m<sup>3</sup>];  $\mathbf{V}$  – velocity vector [m/s];  $\mathbf{E}$  – metric tensor;  $\varepsilon = c_v \theta + \frac{\mathbf{V}^2}{2}$  is the total energy mass density [m<sup>2</sup>/s<sup>2</sup>];  $c_v = \sum_{i=1}^6 y_i c_{vi}$ ,  $c_p = \sum_{i=1}^6 y_i c_{pi}$  – specific heat capacities at constant volume and pressure [J/(kg K)];  $\theta$  – temperature [K];  $p$  – mixture pressure [Pa];  $R_0 = 8.31$  – universal gas constant [J/(mol K)];  $\mu_1, \mu_2$  – viscosity coefficients [Pa s];  $\lambda$  – thermal conductivity [W/(m K)];  $\frac{1}{M} = \sum_{i=1}^n \frac{y_i}{M_i}$ ,  $M$  и  $M_i$  – molar masses of the gas mixture and the i-th component of the gas mixture [kg/mol];  $y_i = \frac{\rho_i}{\rho}$  – mass concentration of the i-th component;  $D_i$  – diffusion coefficients [m<sup>2</sup>/s];  $\dot{\omega}_i$  – mass rate of formation of chemical components [kg/(m<sup>3</sup>·s)];  $e_{vk} = \frac{1}{2} \cdot \frac{R_0}{M_k} \cdot \theta$  – vibrational energy of molecules for the Lighthill model [J/kg];  $h_k^0$  – enthalpy of formation of the component [J/kg] (Table 1).

**Table 1.** Enthalpies of formation of components.

Component	O	N	NO	O <sub>2</sub>	N <sub>2</sub>	NO <sup>+</sup>
$h_k^0$ , [J/kg]	$8.79 \cdot 10^5$	$1.92 \cdot 10^6$	$1.71 \cdot 10^5$	0.0	0.0	$4.1 \cdot 10^6$

In this paper, we consider a model of a linearly viscous gas, in which we assume  $\mu_1 = -(2/3)\mu_2$ . The coefficients of viscosity, thermal conductivity and diffusion are calculated according to the molecular theory of gas mixtures.

For the considered chemical reactions, the conditions of conservation of the atomic composition and the condition of quasi-neutrality of the mixture take place:

$$\gamma_4 = 0.21 - 0.5(\gamma_1 + \gamma_3 + \gamma_6),$$

$$\gamma_5 = 0.79 - 0.5(\gamma_2 + \gamma_3 + \gamma_6),$$

$$\gamma_6 = \gamma_7,$$

where  $\gamma_i = \frac{y_i}{M_i}$  – size concentrations [mol/kg].

## 2.2 Equations of internal heat and mass transfer

Next, consider a heat-shielding structure made of a polymer composite material. Under the action of high temperatures, usually above 300 °C, internal physicochemical transformations occur in polymer composite materials - thermal destruction processes that lead to irreversible changes in the structure and loss of mass of the material. The starting material consists of two

phases: a filler (fiber or reinforcing particles) and a polymer matrix. When heated in the process of thermal destruction, the polymer matrix decomposes into two new phases: coke (solid pyrolytic residue) and gas, which is in the pores and is filtered through them to the surface of the material. Thus, the original composite material is considered as a 4-phase structure [5-8].

$$\begin{cases} \rho_b \frac{\partial \varphi_b}{\partial t} = -J, \\ \frac{\partial \rho_g \varphi_g}{\partial t} + \nabla \cdot \rho_g \varphi_g \mathbf{v}_g = J\Gamma, \\ \rho c \frac{\partial \theta}{\partial t} = -\nabla \mathbf{q} - c_g \nabla \theta \cdot \rho_g \varphi_g \mathbf{v}_g - J\Delta e^0, \end{cases} \quad (5)$$

the notation is introduced here:  $\varphi_b, \varphi_g$  – volume concentrations of the polymer and gas phases;  $\rho_b, \rho_g$  – density of the original polymer matrix and gas phase [ $\text{kg}/\text{m}^3$ ];  $c_g$  – heat capacity of a gas at constant volume [ $\text{J}/(\text{kg K})$ ],  $\rho$  and  $c$  – density and heat capacity of the composite,  $\mathbf{q}$  – heat flow vector [ $\text{W}/\text{m}^2$ ],  $\theta$  – composite temperature [ $\text{K}$ ];  $\mathbf{v}_g$  – gas phase velocity [ $\text{m}/\text{s}$ ];  $\Delta e^0$  – specific heat of thermal degradation of the matrix [ $\text{J}/\text{kg}$ ];  $J$  – mass rate of thermal degradation of the matrix [ $\text{kg}/\text{m}^3\text{s}$ ];  $\Gamma$  – matrix gasification coefficient.

The heat and mass transfer equations (5) are closed by the constitutive relations that relate the vector functions and to the temperature and pressure gradients using the Fourier and Darcy laws, as well as the Arrhenius relation for the mass rate of thermal destruction and the Mendeleev-Clapeyron equation (4):

$$\mathbf{q} = -\mathbf{\Lambda} \cdot \nabla \theta \quad \text{- Fourier's law;} \quad (7)$$

$$\rho_g \varphi_g \mathbf{v}_g = -\mathbf{K} \cdot \nabla p_g \quad \text{- Darcy's law;} \quad (8)$$

$$J = J_0 \varphi_b \exp\left(-\frac{E_A}{R\theta}\right) \quad \text{- Arrhenius's law.} \quad (9)$$

where  $J_0$  – pre-exponential factor,  $E_A$  – activation energy of thermal destruction processes,  $\mathbf{\Lambda}$  – thermal conductivity tensor,  $\mathbf{K}$  – gas permeability tensor of the composite.

In addition, for a composite, as for a multiphase system, the mixture ratios and the normalization condition are satisfied (the index refers to the reinforcing filler):

$$\rho c = \rho_f c_f \varphi_f + \rho_b c_b \varphi_b + \rho_p c_p \varphi_p,$$

$$\rho = \rho_f \varphi_f + \rho_b \varphi_b + \rho_p \varphi_p + \rho_g \varphi_g,$$

$$\varphi_f + \varphi_b + \varphi_p + \varphi_g = 1.$$

### 2.3 Boundary conditions for the adjoint problem

Consider the boundary and initial conditions for the adjoint problem (1) – (9). For the system of equations of gas dynamics (1), it is necessary to add boundary conditions:

1) on the surface, where the conditions  $\mathbf{vn} < 0$  and  $|\mathbf{vn}| > a$  (supersonic inlet boundary), free stream parameters are set:

$$\rho = \rho_\infty, \quad \mathbf{v} = \mathbf{v}_\infty, \quad p = p_\infty, \quad y = y_{i\infty}, \quad (10)$$

$y_{i\infty}$  – concentration values of the gas components in the oncoming flow;

2) on the surface, where the conditions  $\mathbf{vn} > 0$  and  $|\mathbf{vn}| > a$  (supersonic exit boundary), boundary conditions are not specified;

3) on the symmetry surface the following conditions are set:

$$\frac{\partial \rho}{\partial \mathbf{n}} = 0, \quad \mathbf{vn} = 0, \quad \frac{\partial v_{\tau_i}}{\partial \mathbf{n}} = 0, \quad \frac{\partial p}{\partial \mathbf{n}} = 0, \quad \frac{\partial y_i}{\partial \mathbf{n}} = 0; \quad (11)$$

4) the initial conditions for system (1) have the form:

$$\begin{aligned} \rho(0, \mathbf{x}) &= \rho_0(\mathbf{x}), & \mathbf{v}(0, \mathbf{x}) &= \mathbf{v}_0(\mathbf{x}), \\ p(0, \mathbf{x}) &= p_0(\mathbf{x}), & y(0, \mathbf{x}) &= y_{i0}(\mathbf{x}). \end{aligned} \quad (12)$$

It is necessary to add the initial and boundary conditions to the system of heat and mass transfer equations (5)-(9):

1) on the inner surface of the composite, we set the adiabaticity and tightness of the gaseous products of thermal destruction:

$$\mathbf{n} \cdot \nabla \theta = 0, \quad \mathbf{n} \cdot \nabla p_g = 0. \quad (13)$$

5) the initial conditions look like:

$$\begin{aligned} \varphi_f(0, \mathbf{x}) &= \varphi_f^0(\mathbf{x}), & \varphi_b(0, \mathbf{x}) &= \varphi_b^0(\mathbf{x}), \\ \rho_g(0, \mathbf{x}) &= \rho_g^0(\mathbf{x}), & \theta(0, \mathbf{x}) &= \theta_0(\mathbf{x}). \end{aligned} \quad (14)$$

To the listed boundary conditions, it is necessary to add the relations on the surface common for the gas and the composite  $\Sigma_w$ , with the help of which the problems of external aerodynamics and internal heat and mass transfer in a composite material are connected. These ratios look like:

- the no-slip condition for the molecules of the incoming gas flow:

$$\mathbf{v} = \mathbf{0}; \quad (15)$$

- boundary condition for the concentration of components (O and N atoms, NO molecules) on the non-catalytic surface of a solid wall

$$\frac{\partial y_i}{\partial \mathbf{n}} = 0; \quad (16)$$

- in relation to the recombination of charged particles, the conditions of an ideal catalytic surface are used

$$y_6 = 0; \quad (17)$$

- heat balance condition

$$-\mathbf{k} \cdot \nabla \theta \cdot \mathbf{n} = q_C - q_{BL} - q_{RW}. \quad (18)$$

$\mathbf{n}$  – surface normal vector;  $q_C$  – density of convective heat flux to the surface;  $q_{BL}$  – heat flux density removed from the surface due to the release of gaseous pyrolysis products from the composite;  $q_{RW}$  – the density of the heat flux removed from the surface due to its own radiation by the heated surface into the environment;

$$q_C = \alpha(\theta_e - \theta_w), \quad q_{BL} = \gamma_{BL} \rho_g \rho_g \mathbf{v}_g \cdot \mathbf{n}(c_p \theta_e - c_g \theta_g),$$

$$q_{RW} = \varepsilon_w \sigma_{SB} \theta_w^4,$$

here  $\theta_w$  – composite surface temperature;  $\varepsilon_w$  – integral emissivity of the composite surface;  $\sigma_{SB}$  – Stefan-Boltzmann constant;  $\alpha$  – heat transfer coefficient between the surface and the external incoming gas flow;  $c_p$ ,  $c_g$  – specific heat capacities of the external gas flow and the gas phase of the composite, respectively;

- temperature continuity condition at the interface  $\Sigma_w$ :

$$[\theta] = \theta_{wg} - \theta_{ws} = 0, \quad (19)$$

where  $\theta_{wg}$  and  $\theta_{ws}$  – composite gas temperature at the surface  $\Sigma_w$  respectively;

- mechanical impact on the composite material from the oncoming gas flow

$$p = p_e; \quad (20)$$

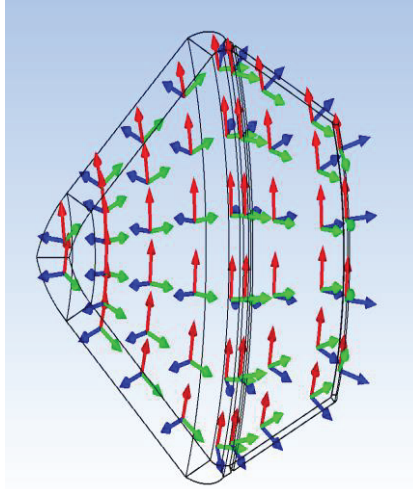
$p_e$  – local pressure of the external gas flow on the surface.

## 2.4 Numerical methods

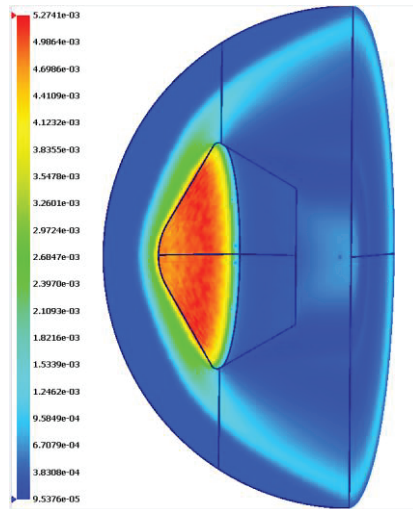
To solve the gas dynamics system the finite volume method is used and for the heat and mass transfer system the finite element method is used [11,13].

## 2.5 Modelling of material properties anisotropy

For thermal protection, consider fabric orthotropic materials. To correctly take into account the properties in different directions, it is necessary to specify the direction of laying the fibers of the fabric. To do this, we introduce a local coordinate system in each finite element (Fig. 1).



**Fig. 1.** Visualization of basis vectors to account for material anisotropy properties.



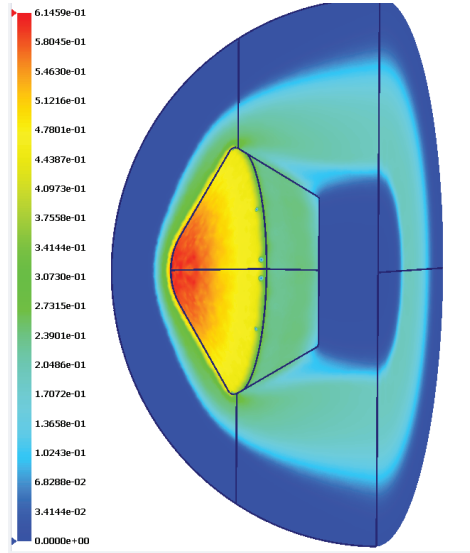
**Fig. 2.** Density distribution in the shock layer,  $\text{kg/m}^3$ .

## 3 Results and discussion

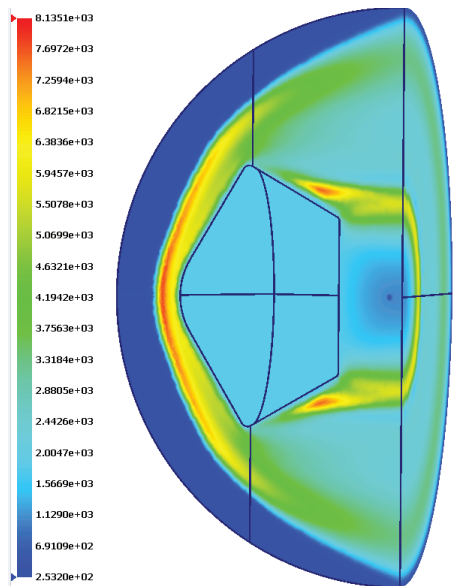
The numerical solution of the problem was carried out for the reentry spacecraft Sturdust [4]. The results were obtained for an altitude of 60 km. and speed of movement 5000 m/s. On figures 2–4 show the density distribution fields, the concentration of atomic nitrogen, and the temperature distribution in the shock layer. It can be seen that the temperature in the shock layer exceeds 8000 K. When using the perfect gas model, the temperature value is 1.5–2

times higher. Therefore, taking into account the chemical composition of the atmosphere under such conditions is necessary.

The design of the spacecraft was supposed to be two-layer. Phenolic fiberglass (outer area) and epoxy fiberglass (inner area) were chosen as heat-shielding materials. On figures 5 and 6 show the distribution of temperature and volume concentration of the gas phase in the heat-shielding layer for a heating time of 210 sec. The most heat-loaded region is the critical bluntness, where the temperature reached 1946 K. It can be seen that the phenolic matrix decomposes under the influence of high temperatures, while the epoxy matrix remains in the low temperature region.



**Fig. 3.** Distribution of atomic nitrogen concentrations in the shock layer.



**Fig. 4.** Temperature distribution in the shock layer, K.



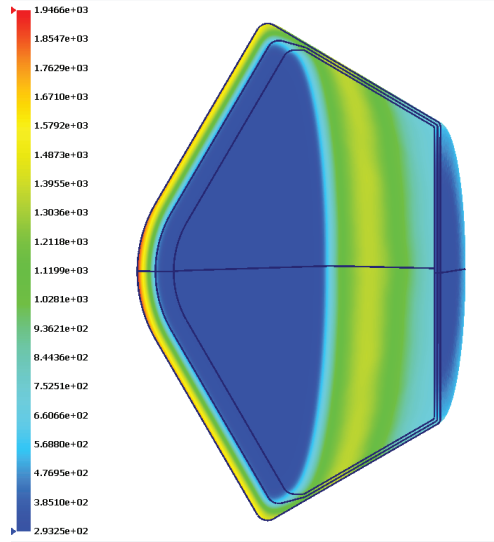


Fig. 5. Temperature distribution in the heat-protective layer, K.

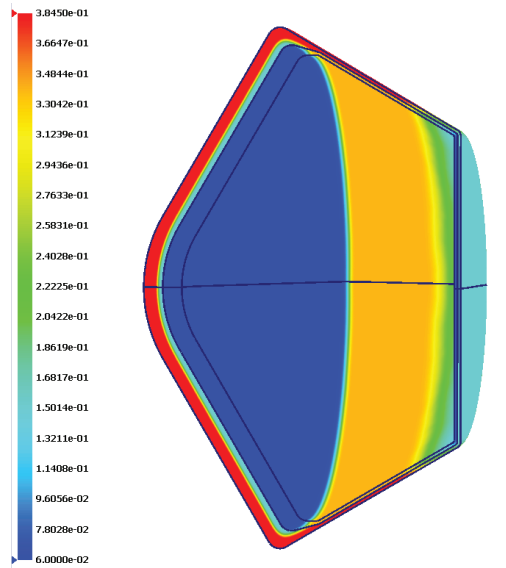


Fig. 6. Distribution of the volume concentration of the gas phase.

## 4 Conclusion

A mathematical formulation of the conjugate problem of high-velocity aerothermodynamics of a chemically reacting gas flow and internal heat and mass transfer in the heat-shielding structure of the reentry spacecraft from ablation composites is considered. Numerical finite-volume and finite-element methods for solving the joint problem is proposed. An example of numerical simulation of the aerothermodynamics of a gas flow is given, taking into account chemical reactions and internal heat and mass transfer for the return space apparatus Stardust. The importance of the chemical composition is shown atmosphere to determine the thermal effects on the surface apparatus design.

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