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A methodology of investigation and results for heat regimes multiplicity in chemically reacting media with diffusion and convection

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ABSTRACT

Authors propose and apply a methodology of investigation of multiplicity of heat regimes in a chemically reacting inhomogeneous medium with convective processes. The methodology consists of several connected steps, which make it possible to simplify the investigation considerably. Multiparameter spaces are explored using singularity theory, realized in a computer software. An actual problem of multiplicity of heat regimes in a shock layer of a space probe in the Martian atmosphere is an example of the methodology application in the article. Heat-physical characteristics of the shock layer vary themselves in domains of their preset indeterminacy while searching and investigating the regimes multiplicity.

1. Introduction

Methodology of investigation of heat regimes multiplicity of chemically reacting multicomponent flowing medium is of significant interest both from the methodical point of view and for many applications. Moreover, there was no such a methodology particularly for chemically reacting gas mixtures or other multicomponent media in strongly inhomogeneous conditions. We study heat regimes in the shock layer (SL) of a space vehicle (SV) descending in the Martian atmosphere as an example to illustrate the approach we propose. Developing of the fail-safe heat shield cover (HSC) is closely connected with modeling of heat and mass transfer processes in SL between the pushing shock wave (SW) and the spacecraft surface [1–4]. The layer is a multicomponent mixture of chemically reacting gases arising of thermal decomposition of the Martian atmosphere and elements of the HSC [5–7]. A sharply inhomogeneous temperature and mass velocity allocations take place in the layer from SW to SV. Moreover, the layer is an open system, so, different heat regimes can occur there. Successful application of the methodology to this case confirms its performance capability.

Searching and investigation of the heat regimes in the example of this work are performed by variation of thermo-physical characteristics via ambiguity of their definition in the study of heat and mass transfer processes for SL of SV in the Martian atmosphere under the given conditions at the SW and SV surfaces. At the same time generally speaking one can vary boundary conditions at the SW and SV surfaces, the width of the shock layer, etc. under specified thermo-physical characteristics of SL media. The purpose of the analysis is to search among the many perhaps physically admissible regimes for the maximum thermal stress regime (with a maximum heat fluxes on the SV surface). Certainly, the possibility of such a regime should be taken into account when designing the thermal protection of SV.

Finding and investigation of multiplicity is a complex problem that demands special methods. Even so it is a mixture of art and science with no guaranty of successful solution, because it is a distributed problem in a multiparameter space. Investigation of both point systems of equations and space distributed systems was performed by means of the software Ariadne (see [8–10] for more explanations) for multiparameter nonlinear analysis based on singularity theory [11].

The procedure of the multiplicity search and investigation consists of several interconnected steps. The equations under investigation are of quite large dimension (300–400) because they are discretized equations with space derivatives. And they need thorough treatment. Application of the above technology is much simplified if initial points in multiparameter spaces are found using some simplified equations that may be out of physical sense. The steps of processing are the following.

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(1) Investigation of simplified systems of equations.
   (a) Regularization of the point system of equations: the system of chemical reactions is vanished but it can be regularized for convenience to keep its dimension for the further investigation.
   (b) Multiparameter investigation of the point systems of equations with special attention to unstable solutions, appropriate eigenvalues and boundary conditions: this leads to further initial points with necessary properties in multidimensional spaces.
   (c) Multiparameter investigation of Turing bifurcations using simple difference schemes. Additional turning points at the branching curves are also in use here. This step is intended for the same purpose as the previous one.
   (d) Homotopy from the equations with Turing bifurcations to the equations being investigated: the initial points in multiparameter spaces are obtained from the points of low dimensional spaces.
(2) Multiparameter investigation of the equations for multiplicity using precise difference schemes: specially degenerated points of the physical system are under investigation at this step that leads to qualitative structure of the space of parameters.
(3) A specific multiparameter investigation of regimes of heat and mass transfer in SL. Calculation of heat and mass transfer characteristics profiles, their stability and dispersion according to the map parameters and the corresponding bifurcation diagrams. This final phase of research is most interesting for applications.

We use point and simplified systems of equations not only to find solutions of the system being investigated, but also to find a vicinity of multiplicity for appropriate parameters and dimensionless diffusion coefficient among them which really exists only in the space distributed equations. Such a technology is applicable for a wide class of equations shaped in the article title. Steps 1 a–c are preliminary, they can be done more or less thoroughly. The items 3, 4 of the article correspond to the steps 1, 2, respectively. Examples that simplify investigation are within the blocks of the methodology explanation and results for the SL example are in the item 5 (step 3).

2. Problem definition for heat and mass transfer regimes in a chemically reacting inhomogeneous medium with convective processes

Solution of the problem of searching for conditions of multiplicity occurrence proves to be a bulky parametric investigation in arbitrary geometry. We consider a one-dimensional case, but it seems to be no principal obstacles to add more dimensions. We suppose that the following diffusion–reaction-convection vector stationary equation describes mass (diffusion equations) and heat (energy equation) exchange processes in a chemically reacting inhomogeneous flowing medium (compare with (2)–(5))

$$\begin{aligned}&(\mathbf{A}\mathbf{z}')' = -\mathbf{B}\mathbf{z}'f - \mathbf{K};\\&z_i'(0) = 0,\ \ i = 1,\ldots,N-1;\quad z_N(0) = z_N^0;\quad \mathbf{z}(\delta) = \mathbf{z}_\delta.\end{aligned} \tag{1}$$

An equation of motion (see last equation in (2)) is implied to define the flow function f. **A** and **B** in (1) are square matrices defined by heat-physical properties of the medium, moreover, **A** is parabolic (positively definite). **z** – vector of N component concentrations and medium temperature $(c_1,\ldots,c_{N-1},T)^T$, K – vector source, caused by chemical reactions. Concentrations c_i and temperature T are functions in $\eta \in [0,\delta]$, $\mathbf{z}'$ are the derivatives with respect to η (η – Dorodnicyn-Liz dimensionless coordinate of the SL [1]). Boundary conditions close the system. Without loss of generality we pose values of the variables at the right bound and their zero derivatives at the left one, except the temperature which values are given both at the left and at the right (see example below, conditions on SW and SV surface correspondingly).

Example. Let us see the problem for SL heat regimes in a simplified geometry: quasi single dimensional one in the vicinity of the critical front line of the axisymmetric blunt body. The critical front line is the shortest line from the body surface to the pushed shock wave. The SV is an axisymmetric body (sphere) in the simplest case. The flow and the heat-mass transfer picture is time independent near this line [1,2] but flow and transfer are actually nonzero.

It is proposed in this article to consider the heat and mass transfer regimes (heat regimes) in SL paying the main attention to the conditions of their multiplicity. The different heat regimes are characterized by the different sets of profiles of hydrodynamic attributes: temperature, components concentrations and mass velocity which correspond to various heat fluxes at the SV surface and the rate of mass transfer in SL under one and the same boundary conditions at SW surface and one and the same boundary conditions at SV surface (see (4), (5)). In turn different heat flows at the SV surface and different mass exchange velocities in SL correspond to the different degrees of destruction of HSC. To ensure the safety of the SV the greatest interest of HSC design is the heat regime corresponding to the maximum heat current on SV cover (maximum rate of destruction of the HSC).

Let us formulate the problem of heat regimes in the chemically nonequilibrium shock layer using Dorodnicyn-Liz variables (ξ, η) [1] in accordance with this approach. The system of equatios consists of $N-1$ diffusion equations (in the binary diffusion model for simplicity) with sources determined by chemical reactions in the layer. The sources $\{K_i\}$ are algebraic expressions that depend on temperature T and mass concentrations $\{c_a\}$ of the SL gas components. Moreover, the system includes an equation for energy with a source because of chemical reactions too – K_N, which depends on temperature and the concentrations, neglecting viscous dissipation etc. And there is an equation of motion in a flow function f (see [1–4] for details and denotation).

$$\begin{aligned}&(N_1^1 c_1')' = -k_1 c_1' f - K_1\\&\vdots\\&(N_{N-1}^{N-1} c_{N-1}')' = -k_{N-1} c_{N-1}' f - K_{N-1}\\&(\tilde{M} T_*')' = -k_N T_*' f - K_N\\&\textstyle\sum_{i=1}^{N} c_i = 1,\quad 0 < c_i < 1;\quad T_* = T/T_\delta\\&(\tilde{N} f'')' + ff'' + [k - (f')^2]/2 = 0\end{aligned} \tag{2}$$

The simplified system (2) refers to the vicinity of the critical front line. **A** and **B** here are diagonal matrices: $\mathbf{A} = \left\{N_1^1, N_2^2, \ldots, N_{N-1}^{N-1}, \tilde{M}\right\}$, $\mathbf{B} = \{K_1, K_2, \ldots, K_N\}$. Examples of K_i are represented later. It is the system that is investigated numerically here. But generally there can be cross-connection constants in diffusion and energy equations (the multicomponent diffusion model; see [3,4]). The space variable is dimensionless coordinate η. The parameters in (2) depend on heat-physical gas characteristics in SL and are the following ones:

$$\begin{aligned}&\tilde{N} = \frac{\rho\mu}{\rho_\delta \mu_\delta};\quad k = 2\rho_\infty/\rho;\quad k_i = \frac{\mu_\delta}{D_\delta},\quad i = 1,\ldots,N-1;\\&k_N = \frac{\mu_\delta}{\lambda_\delta} c_p T_\delta;\\&\tilde{M} = \frac{\rho\lambda T_\delta}{\rho_\delta \lambda_\delta};\quad N_i^i = \frac{\rho D_i}{\rho_\delta D_\delta}.\end{aligned} \tag{3}$$