

Modeling the heat and mass transfer in the pores of the thermal protection carbon-carbon frame during the gas-phase deposition of silicon carbide

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Abstract. This paper is dedicated to the numerical simulation of the gas-phase deposition into the porous carbon-carbon frame for the gradient thermal protection of reentry vehicles. The paper presents the specifics of creating the representative volume elements of the porous carbon-carbon frames based on the microstructure data from the computed tomography scanner, electronic scanning microscope and porosimetry results. The finite-element models of the representative volume elements are created in order to obtain the net independent solution, including the special finite elements at the phase interfaces. The finite-element and finite-volume method was used for calculation, implemented in MSC.Digimat and ANSYS software packages. The effect of the reagent parameters on the gas-phase deposition process, uniformity and rate of silicon carbide deposition was simulated parametrically, and the results are presented.

1 Introduction

The rise in the international space programs and the development of new generation reentry space vehicles are calling for the design of heat-resistant thermal protection. The selection of the thermal protection type is affected by the reusability factor, the character and the level of thermal loads. For instance, disposable structures (like reentry vehicles or solid propellant motors) employ ablative thermal protection coating (TPC) from polymer composite materials (CM) [1, 2]. The protective mechanisms in TPC trigger the endothermic reactions of melting, destruction, evaporation, filtration of the destruction products through the porous frame and their injection into the boundary layer, the film of the melted substances flowing over the surface. Moreover, the heat transfer through the coating is reduced by the formation of the porous frame and the increase in the radiative ability of the surface. The drawbacks of the ablative TPC include the physical-chemical transformation in CM resulting in irreversible changes in the aerodynamic and thermal protection properties affecting their reusability.

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Due to technical, technological and economic reasons, reusable large spacecraft do not employ ablative TPC, since they alter their shape, dimensions in the operation process, and lose their heat-insulating ability as a result of physical chemical transformations. The perspective aerospace vehicles require TPC which can withstand fluctuating power loads, high-velocity reactive gas and erosion particles flows. Carbon-ceramic composite materials (CCCM) are very attractive in this respect, having low density, adequate strength and stiffness properties, small thermal coefficient of linear expansion, capable of working at temperatures above 2000 K, at high heating rates [3-5]. The mass of the thermal protection systems can be reduced by using porous CCCM.

The projects in the gradient TPC and materials at NASA Glenn Research Laboratory and NASA [6-8] demonstrated the possibility of manufacturing these materials to enable the required thermal mode of the spacecraft. The TPC in question were based on CCCM or ceramic matrix composite material with the silicon carbide fiber frame, modified with the high-melt zirconium-based carbide systems.

The complexity and time-intensity of the TPC parts fabrication require the mathematical simulation to be used in order to reduce the time and costs when selecting technological parameters. The main operation in the TPC parts fabrication process is the gas-phase deposition of silicon carbide into the porous carbon-carbon frame lasting hundreds of hours and determining the final physical mechanical, thermal physical and optical properties consistent with the operation requirements. Physical mathematical models of this gas-phase deposition process are further complicated by its non-stationary, multidimensional nature, also the chemical kinetics of the hard phase formation from the gaseous monomethylsilane must be taken into account. The analysis of the current research indicated that the majority of the papers focus on the gas deposition process in a simplified setting [9-12]. As a rule, the problems were solved in a one-dimensional or two-dimensional setting, the porous medium was viewed as a set of cylindrical pores, and the radiative heat transfer in the pores was not taken into account.

2 Problem description

This research aims to develop the algorithm predicting on the micro level the process of SiC gas-phase deposition into the porous carbon-carbon (C-C) frame to create the aerospace thermal protection.

The predicting algorithm includes several stages: microstructural investigations with an electronic scanning microscope and CT scanner, as well as a porosimeter; a 3D geometrical model of the pore space based on microstructural CT; a geometric model of the representative volume element for the C-C frame; a geometric model of the C-C frame pores; finite-element models of the representative volume elements to obtain the net-independent solution; specifying the thermal physical and optical properties of the C-C frame from the porous C-C composite material before and after the gas-phase deposition process, of the furnace heating unit, the tooling and the reaction medium; specifying the technological parameters and the gas-phase deposition process modes; specifying the boundary conditions on the monomethylsilane decomposition kinetics.

The reference data on the porous CCCM structure were obtained from the microstructural analysis of the witness specimen on an optical microscope measuring the dimensions of the non-woven strands. The sample was also subjected to the analysis on the Bruker Skyscan 1172 micro-CT scanner, which uses a multitude of X-Ray images at various angles to create a 3D model of the sample. The 3D model analysis enables detailed investigation of the porous CCCM frame microstructure resulting in satisfactory geometric models of the representative volume elements of the C-C frame.

The physical model of the SiC deposition in the CCCM pores takes into account the following specifics: the gas-phase reactor working compartment and the porous CCCM position; vacuuming the gas-phase reactor and heating it up to the required temperature; the reagent (monomethylsilane) injection into the working chamber; transferring the reagent and the partial interaction products in the gas phase to the heated surfaces of the porous CCCM; the gas-phase components diffusion through the CCCM pores; chemical reactions (decomposition) of the reagent onto the heated surfaces of the CCCM pores; SiC matrix formation; the reaction products desorption; transferring the desorbed products from the surface into the reaction chamber and the pumping duct. In this paper, the problem under consideration is solved using the ANSYS CFX software package and the user-specific programming language.

Since the chemical reaction rate is primarily determined by the level and distribution of temperature in the reactor chamber, and the thermal field inside the chamber is not known in advance, the problem in this paper is formulated with the account for the conductive, convective and radiative heat transfer. As a result, the mathematical model of the gas-phase deposition for SiC into the porous CCCM part includes the equation of the multi-component flotation (with macro and micro level description of heterogeneous chemical description) and the equation of the conjugate heat transfer reaction in complex geometry systems and in the pore volume. The mathematical model is based on the Navier-Stokes equations for the multi-component reacting gas mixture, as well as on the chemical kinetics equations (in particular, takes into account Arrhenius equation for the reacting surfaces) [13, 14].

The thermal physical characteristics of the reacting medium and the gas-phase reactor consistent with the operation temperature are presented in [15, 16]. The following assumptions are introduced for the mathematical simulation of the deposition process: the reaction medium is optically transparent; the radiative heat transfer surfaces are grey (emissivity unaffected by the wavelength); the surfaces are diffusely radiating and diffusely absorbing; the changes in the thermal physical properties in the representative volume elements of the porous CCCM are not taken into account when the SiC matrix is formed.

3 The results of the heat and mass transfer mathematical simulation in the pore space

The first stage of research was concerned with the conjugate heat transfer during SiC gas-phase deposition in the gas-phase reactor with a CCCM blank, the second stage dealt with the mass transfer in the reaction chamber of the gas-phase reactor, the third stage dealt with the microlevel heat and mass transfer in the pore space. In order to simulate the heat and mass transfer during the gas-phase deposition of SiC in the CCCM pores, geometric models were created, which were divided into hexagonal and prismatic finite elements and volumes, so that a net-independent solution was obtained with acceptable degree of discretization. The total number of elements was 1,200,000 (Fig. 1). The elements in the model were bound by the contact condition of the adjacent surface elements.

The boundary conditions for the monomethylsilane concentration fields, pressure, renewal rate and thermal state in the near-surface layer of the porous CCCM blank were obtained at the second stage of simulation. It is known that the structure, density and the residual porosity of the CCCM are directly affected by the technological parameters of the process (temperature, curing time), while the homogeneity of the ceramic matrix is affected by the physical chemical and thermal physical properties of the precursor. Consequently, this paper included parametric calculation in order to estimate how the uncertainty in the precursor properties influences the technological parameters of CCCM production. The

variable properties are the dynamic viscosity and the thermal conductivity coefficient. These parameters are considered critical for determining the features of heat and mass transfer in the porous medium.

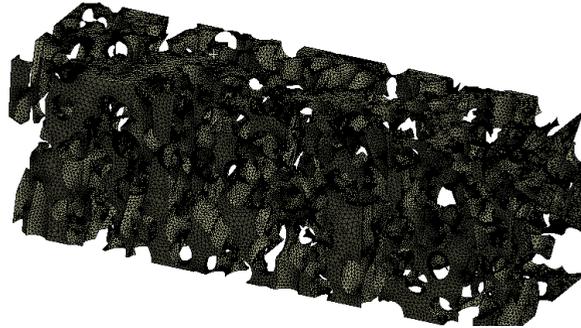


Fig. 1. Finite-element model of the CCCM pore representative volume element.

Below are some of the results of the mass and heat calculation in the CCCM pores during the SiC gas-phase deposition at 880K temperature in the reaction chamber and $0.43 \cdot 10^{-5}$ Pa·s dynamic viscosity. Figs. 2 and 3 show the calculation results for the velocity field and SiC growth rate in the pore space.

As a result of the mass and heat transfer calculation in the CCCM pore space during the SiC gas-phase condensation onto the carbon frame with the varied precursor properties, it was demonstrated that :

- when the dynamic viscosity of monomethylsilane changes from $0.43 \cdot 10^{-5}$ Pa·s to $6.88 \cdot 10^{-5}$ Pa·s, the maximum deposition rate changes by less than 0.5%, but the mass and heat transfer is less intensive and the precursor velocity in the pore space decreases by more than a factor of ten;

- when monomethylsilane heat conductivity coefficient changes from 0.0113 W/(m·K) to 0.1816 W/(m·K), the maximum deposition rate changes by less than 0.5%, which is determined by the precursor flow only slightly influencing the intensity of the heat transfer with the pore surfaces

4 Conclusion

1. As a result of the research, the algorithm for the mathematical simulation of SiC gas-phase deposition into the porous CCM was developed, which enabled:

- parametric modelling of SiC gas-phase deposition into the representative volume elements of the porous CCCM;

- determining that the change in monomethylsilane dynamic viscosity from $0.43 \cdot 10^{-5}$ Pa·s to $6.88 \cdot 10^{-5}$ Pa·s alters the maximum deposition rate by less than 0.5%, but the mass and heat transfer becomes less intensive and the precursor velocity in the pore decreases by more than a factor of ten;

- establishing that the change in monomethylsilane heat conductivity coefficient from 0.0113 W/(m·K) to 0.1816 W/(m·K) alters the maximum deposition rate by less than 0.5%, which is determined by the precursor flow only slightly influencing the intensity of the heat transfer with the pore surfaces.

2. The results of the parametric calculations help to select and validate the technological parameters for SiC gas-phase deposition to densify the porous blanks for aerospace thermal protection parts.

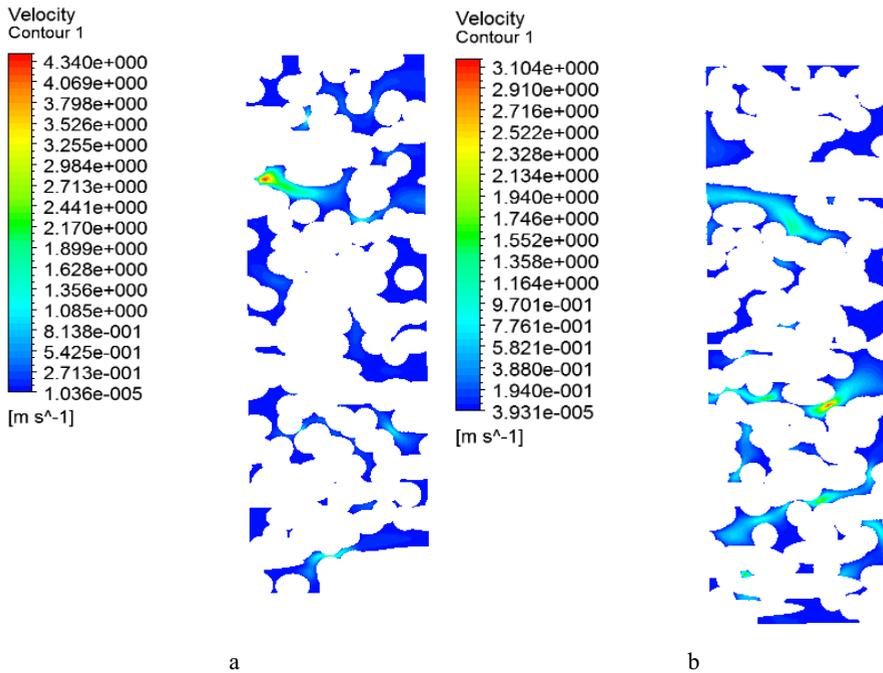


Fig. 2. Velocity fields in the pore space of the CCCM representative volume element during the SiC gas-phase deposition, m/s: a – 10 microns from the end surface; b – 45 microns from the end surface.

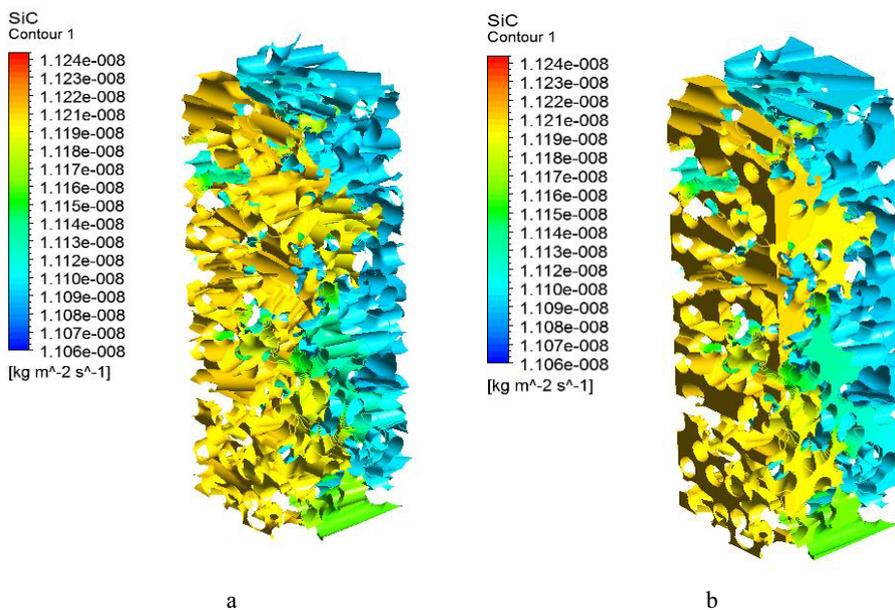


Fig. 3. SiC deposition rate on the reacting surfaces in the CCCM representative volume element, $kg/(m^2 \cdot s)$: a – in the pore zone; b – in the near-surface zone.

Some results of this paper were obtained as part of the grant agreement № 14.577.21.0099 by the Russian Federation Ministry of Education and Science (unique identifier for Applied Scientific Research — RFMEFI57714X0008) in the framework of the priority area “Transport and space systems” of the federal target programme “Research and development in the priority areas of the Russian science and technology development for 2014-2020”.

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