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Modeling ablative behavior and thermal response of carbon/carbon composites

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1. Introduction

Carbon/carbon composites, due to their excellent thermo-physical properties and low densities, have found extensive applications in rocket nozzles, aero plane braking disks, and thermal protection systems of atmospheric re-entry vehicles [1–3]. Use of such composite components would reduce the structure weight for increased payload and enhance the reliability of the system. However, a challenge arises from the complex thermo-chemical environments in which the structures are working. The hostile thermo-chemical constraints give rise to heterogeneous oxidation reactions between carbon and oxidizing species such as H₂O, CO₂, and O₂ from the hypersonic flow, causing undesirable surface recession [4-8], degradation or micro-damage [9,10] of the materials by chemical erosion or ablation. In addition, the surface and interface defects produced by the chemical reaction may result in mechanical erosion. Existing studies indicate that thermo-chemical ablation is the primary cause for surface recession [11], while the effect of mechanical erosion is secondary for advanced carbon/carbon composites with high-density. Accordingly, understanding the mechanism of thermo-chemical ablation is a key from the view point of structure design.

ABSTRACT

Carbon/carbon composites usually work in complex thermo-chemical environments, surface recession is thus inevitable due to chemical ablation and further affects the system stability and safety. In this paper, a model for chemical ablation of the materials which accounts for the effects of non-uniform temperature and pressure is proposed. As an application, the surface recession of a carbon/carbon composites leading edge structure are simulated in detail. The results show that the non-uniform distributed pressure plays an important role in the final ablation configuration. The effects of altitude and oxidation protection on the chemical ablation are discussed as well.

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Besides the correlation with temperature, the oxidation reactions in the chemical ablation of carbon/carbon composites are also

Great efforts have been made to minimize chemical ablation so as to improve the system stability and safety. In addition to experimental explorations [12], numerical models have also exploited to predict the oxidation erosion of carbon/carbon composite materials and structures. A thorough literature review on numerical characterization of ablative materials used for different military and aerospace applications was given in Ref. [13]. To solve the chemical ablation problem for charring or carbon based materials, several approaches [14–16] were developed to calculate the temperature of body and the surface recession caused by chemical ablation. These studies essentially regarded the oxidation reactions of chemical ablation as equilibrium processes, implying that the oxidation species are consumed completely at the gas-solid surface and thus the reactions are fully controlled by the diffusion rate of the reactants. However, experiments [1,2,17] confirmed that the oxidation reaction of carbon/carbon materials at lower temperatures is a non-equilibrium process with the reaction rate in the Arrhenius form. Only at higher temperatures the oxidation reaction is controlled by the diffusion rate of the reaction species. This fact was simulated by some later researches where the non-equilibrium nature of reaction process was taken into account [18]. In particular, by distinguishing the kinemics and diffusion-controlled regimes, the whole chemical reaction process of carbon/carbon materials was formulated [19].

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dependent on the concentration of reaction gases at the surface, which is related to the local pressure [20–22]. In practical applications, the complex local fluid field near the composite structure leads to non-uniform temperature and gas pressure on the surface, thereby giving rise to non-uniform chemical reaction. Nevertheless, most of the existing models are focused on one-dimensional cases [14–16,19] in which the temperature effect is involved but the pressure is presumed constant. Though these models can provide the thermal and ablation information at some positions such as where being most seriously ablated, they are hard to be used to predict the overall erosion configuration of the structure.

Motivated by the above reasons, a chemical ablation model for carbon/carbon composites is developed in this paper to incorporate both effects of non-uniform temperature and pressure. As the application, the thermal and ablation behaviors of a leading edge structure are simulated. Quantitative evaluation of the structure response at different altitudes is performed, and the influence of a possible oxidation protection is discussed.

2. Model and algorithm

The ablation of carbon/carbon composites is a coupled thermochemical process which involves complex heat and mass transfers. Toward a quantitative modeling, the following aspects will be confronted with. First, a transient thermal analysis is needed to provide the temperature field due to incoming heat flux in any time. Next, a chemical ablation model is required to predict the surface recession rate. Finally, a suitable numerical approach is necessary to tackle the evolution of the moving boundaries.

2.1. Transient thermal analysis

A carbon/carbon composite structure may suffer complicated thermal conditions such as aerodynamic heating and radiation flux. To analyze the chemical ablation, the first step is to obtain the transient temperature field *T*. In the rectangular Cartesian coordinate system (x, y, z), the general form of differential equation governing the transient temperature is given by

$$\rho_{C}C_{p}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left[k_{x}\frac{\partial T}{\partial x}\right] + \frac{\partial}{\partial y}\left[k_{y}\frac{\partial T}{\partial y}\right] + \frac{\partial}{\partial z}\left[k_{z}\frac{\partial T}{\partial z}\right]$$
(1)

where ρ_c is the material density, C_p is the heat capacity, and k_x , k_y , k_z are the heat conductivity components in the global directions.

The associated boundary conditions for (1) can be specified according to energy balance on the structure surface. Fig. 1 illustrates the current configuration of the receding surface of the structure during ablation, where the dashed line stands for a control volume of infinitesimal thickness [7,23]. The energy fluxes leaving the control volume include the conduction q_N into the materials and the radiation $q_{rad-out}$ away from the surface. The latter takes away by the ablation mass ejector heat flux $\dot{m}_w h_w$, with \dot{m}_w being the materials oxidation rate and h_w the gases enthalpy of reaction product. The inputting energy fluxes involve the conduction q_w from the gas boundary layer, the radiation q_{rad-in} from the



Fig. 1. Energy fluxes over the ablation interface layer.

gas boundary layer, and the enthalpy flux $\dot{m}_w h_{cs}$ absorbed by oxidation reaction. Here h_{cs} is the reaction enthalpy. Therefore, the conduction energy fluxes q_N which provides the link to the in-depth heat transfer equation can be written as

$$-k\frac{\partial T}{\partial s} = q_N = q_w - [\dot{m}_w h_w - \dot{m}_w h_{cs}] + q_{rad-in} - q_{rad-out}$$
(2)

where the term in the square bracket means energy variation caused by the chemical reaction and the values of h_w and h_{cs} can be gathered from literature [23]. In most cases the influence of the radiations q_{rad-in} and $q_{rad-out}$ on the ablation process is not significant and thus is neglected. In contrast, the conduction q_w is a vital parameter which varies with the wall temperature and can be expressed by [20].

$$q_{\rm w} = C_h (T_r - T_w) \tag{3}$$

Here, C_h is the convective heat transfer coefficient, T_r is adiabatic wall temperature, and T_w is the solid wall temperature. The value of C_h and T_r can be obtained from the flow field analysis with the help of computational fluid mechanics software (FLUENT). Consequently, q_w can be updated dynamically with the wall temperature in the heating and ablation process.

2.2. Model of oxidation ablation

Following Refs. [1,19], the oxidation reaction is controlled at low temperatures by reaction kinematics rate, while at higher temperatures by the diffusion rate of gaseous oxygen. Thus, the chemical ablation of carbon/carbon composite should be divided into two regimes [19], reaction kinemics rate controlled and diffusion rate controlled regime.

In the kinemics rate controlled regime, the oxidation reaction rate is determined by

$$\dot{m}_{C,ch} = 12 \times A \times \exp\left(-\frac{E_a}{RT_w}\right) \times C_{O_2} \tag{4}$$

where A is a constant, T_w is the solid wall temperature, C_{0_2} is the concentration of oxygen, E_a is the activation energy, which changes depending on the level of oxidation protection. In the diffusion rate controlled regime, the oxidation rate is determined by the diffusion rate of gas species as [19],

$$\dot{m}_{C,d} = 12 \left(\frac{2\varphi + 1}{\varphi + 1}\right) N \tag{5}$$

in which φ is the ratio of produced CO and CO₂ and N is the diffusion rate of oxygen through boundary layer. The expressions of φ and N are given by

$$\varphi = \frac{\sqrt{1 + 0.3215 \exp(868/T_w)} - 1/0.7656 \exp(868/T_w)}}{0.21 - \sqrt{1 + 0.3215 \exp(868/T_w)} - 1/0.7656 \exp(868/T_w)}}$$
(6)

$$N = 2.07 \times 10^{-6} \frac{P}{P_i} \frac{P_{og}}{R} \frac{T_w^{0.8}}{d} \left[\frac{2422.77(\rho du)^{0.7}}{T_w^{0.55}} + 3.95 \right]$$
(7)

where *P* is the total pressure, P_{og} is the pressure of oxygen in the bulk air, P_i is the logarithmic pressure of inert, *R* is universal gas constant, *d* is characteristic dimension, *u* is flow velocity of air around the body, and ρ is the density of air. Some of the parameters are functions of altitude.

In the whole ablation process, the lower one of the reaction kinemics rate and the diffusion rate plays the dominating role and is used as the oxidation rate. Depicted in Fig. 2 is the variation of the oxidation rate with temperature at P = 1 atm. It is clear that the critical temperature appears at about 1150 K, implying that the

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