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Research Paper

A new mechanism of surface ablation of charring materials for a vehicle during reentry

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HIGHLIGHTS

- A novel mechanism of the surface ablation of charring material.
- A coupled thermal/fluid/chemical/ablation model.
- The combustion of pyrolysis gases can protect the surface of charring material.
- Larger activation energy can improve the thermal protection performance of material.
- Smaller frequency factor can improve the thermal protection performance of material.

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ABSTRACT

Coupled thermal/fluid/chemical analysis for the surface ablation of charring materials in a vehicle during hypersonic reentry has been conducted. The pyrolysis layer model is presented to simulate the thermal responses of the material, the relations of the normal shock wave are adopted to obtain the aerodynamic parameters in the boundary layer, and the counterflow diffusion model considering chemical mechanisms of hydrocarbons is proposed to solve the combustion of the pyrolysis gases. Meanwhile, the gas-solid chemical reactions of surface char are coupled with the thermal responses, the aerodynamic parameters and the combustion of the pyrolysis gases. The new equations of surface ablation for the charring materials are discretized by the central and the up-wind difference formats. A coupled mechanism of surface ablation is simulated by using our computer codes. Numerical results indicate that the consumption of oxygen in the combustion of the pyrolysis gases can protect charring materials from the surface ablation in some degree. Furthermore, selecting charring materials with larger activation energy and smaller frequency factor can effectively improve the thermal protection performance of charring materials. This study will be helpful for the design of the thermal protection system in reentry vehicles.

1. Introduction

Thermal protection system (TPS) is essential for safety of vehicles subjected to severe aerodynamic heating. Reentry vehicles usually take charring materials as TPS materials [1]. Owing to the low thermal conductivity and the pyrolysis, charring materials can protect the vehicle from the huge amount of heat generated by the friction of the atmosphere [2–6]. Simultaneously, surface of charring materials ablates because of its oxidation with the boundary-layer gases, along with the combustion of the pyrolysis gases. Generally speaking, the surface ablation mechanism of charring materials is a rather complex and difficult issue.

Researchers kept eyes on the models for the surface ablation of charring materials. Physical and mathematical models were developed to simulate the thermal behavior of the charring materials. For example, a common method was solving the Fourier's equations combining with the Arrhenius equations [4,7,8]. This method paid attention to the pyrolysis of the phenolic resin ignoring the surface ablation, or predicted the surface recession rate by thermal analysis tests, in which the heating rate depended significantly on the experimental conditions which differed from those of the aerodynamic environment. Another two models - the pyrolysis interface model and the pyrolysis layer model - were built in our previous researches to simulate the thermal response and the surface recession rate [9–12]. They could predict roughly the position of the material surface and the mass ablation rate of surface char at any time in the reentry without considering the combustion of the

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Nomenclature

L	thickness of boundary layer [m]
x	spatial coordinate in axial direction [m]
r	spatial coordinate in radial direction [m]
d_0	diameter of single carbon fiber [μm]
G	function of density, radial velocity and radial coordinate [$\mathrm{kg \cdot m^{-3} \cdot s^{-1}}$]
F	function of density and axial velocity [$\mathrm{kg \cdot m^{-2} \cdot s^{-1}}$]
T	gas temperature [K]
Y	mass fraction [–]
ρ	gas density [$\mathrm{kg/m^3}$]
c_p	specific heat at constant pressure [$\mathrm{J \cdot kg^{-1} \cdot K^{-1}}$]
λ	thermal conductivity [$\mathrm{W \cdot m^{-1} \cdot K^{-1}}$]
μ	dynamic viscosity [$\mathrm{kg \cdot m^{-1} \cdot s^{-1}}$]
$\dot{\omega}$	chemical reaction rate [$\mathrm{mol \cdot m^{-3} \cdot s^{-1}}$]
h	specific enthalpy [J/kg]
W	molecular weight [kg/mol]
V	diffusion velocity [m/s]
u	gas velocity in axial direction [m/s]
v	gas velocity in radial direction [m/s]
p	gas pressure [Pa]
C_p	molar heat capacity at constant pressure [$\mathrm{J \cdot mol^{-1} \cdot K^{-1}}$]
X	mole fraction [–]
$\overline{W}$	mean molecular weight [kg/mol]
D_{jk}	multicomponent diffusion coefficients [$\mathrm{m^2/s}$]
D_{km}	mixture averaged diffusion coefficients [$\mathrm{m^2/s}$]
D_k^T	thermal diffusion coefficients [$\mathrm{kg \cdot m^{-1} \cdot s^{-1}}$]
υ'	stoichiometric coefficient of reactant [–]
υ''	stoichiometric coefficient of product [–]
for	forward rate constant
rev	reverse rate constant
$[X]$	molar concentration [$\mathrm{mol/m^3}$]
$\dot{m}$	mass injection rate [$\mathrm{kg \cdot m^{-2} \cdot s^{-1}}$]
κ	the radius of curvature at stagnation point [m]
α_{zl}	mass exchange coefficient [m/s]
k	reaction rate constant [m/s]
k_0	frequency factor [m/s]
c	mass concentration [$\mathrm{kg/m^3}$]
Nu_{zl}	Nusselt number [–]
Ω	diffusion volume [$\mathrm{m^3/mol}$]
Re	Reynolds number [–]
Sc	Schmidt number [–]
E	activation energy [J/mol]
Fb	dimensionless number describing the combustion status [–]
Ma	Mach number [–]

Subscripts

s	surface
f	the position before detached normal shock wave
b	the position behind detached normal shock wave
k	species index
i	ith reaction
g	gas
j	space point in the x direction

pyrolysis gases. Comfortingly, many references were also published about the surface ablation mechanisms of the charring materials. On the one hand, the influence of mass ablation rate on the heat transfer coefficient was presented by the graphite ablation for perfect gas flow [13,14]. The gases and surface interactions such as $O + C(s) \rightarrow CO$, $O + O \rightarrow O_2$, $N + C(s) \rightarrow CN$ and $N + N \rightarrow N_2$ were validated for describing the mass ablation rate of the carbonaceous surface by Park [15]. And the oxidation reactions - $C(s) + O_2 \rightarrow CO + O$ and $C(s) + O \rightarrow CO$ - were proposed to take into account the process of thermo-chemical ablation [16]. Meanwhile, the mass per unit area per second of each gas species on the material surface could be calculated by the Knudsen-Langmuir equation [17]. However, the researchers have not still noticed the combustion of the pyrolysis gases in the boundary layer. On the other hand, the widest way of evaluating the recession rate of charring materials subjected to a hyperthermal environment was based on the ablation tests [18–21].

Actually, surface ablation is related with the reaction mechanism of char and oxygen, the temperature fields, the materials' properties at high temperature, and even the combustion of pyrolysis gases with air in the boundary layer [22,23]. The surface ablation mechanism of charring materials remains longstanding challenge. Toward this objective, a novel thermal/fluid/chemical/ablation coupled mechanism is proposed on the basis of multidisciplinary theory. Furthermore, the effects of four factors (the diameter of the single carbon fiber, the activation energy, frequency factor and components of the pyrolysis gases) on the surface ablation are analyzed.

2. Models

2.1. Physical model

During the reentry, the surface of the charring ablator in a vehicle suffers severe aerodynamic heating. The charring ablator is divided into four layers, namely the virgin layer, the pyrolysis layer, the char layer and the ablation layer (see Fig. 1(a)), whose detail physical and chemical phenomena can be seen in Refs. [9–12].

The pyrolysis gases are generated in the pyrolysis layer, flow to the material surface and inject to the high temperature boundary layer. The pyrolysis gases combust with air in the boundary layer forming a counterflow diffusion flame. In this process, there is a starting reaction interface, where the mole fraction of oxygen just shifts from a positive value to zero. If the starting reaction interface stays outside the material surface, combustion of pyrolysis gases completely protects the material surface, because there is no oxygen reacting with the char. Otherwise, the combustion of pyrolysis gases partly protects the material from surface ablation. By the way, we define the velocity of pyrolysis gases when the starting reaction interface just reaches the material surface as the 'critical velocity'. In the stagnation region, the combustion of the pyrolysis gases and air may be described by the counterflow diffusion flame model, in which the material surface is seen as the fuel nozzle, the detached normal shock wave can be seen as the oxidizer nozzle, and the region of the boundary layer can be seen as the range of diffusion combustion. Fig. 1(b) illustrates this counterflow diffusion flame.

If the starting reaction interface could reach the material surface, the char on the material surface can react with the residual oxygen from the counterflow diffusion flame (see Fig. 1(c)).

In Fig. 1, the bold dashed line represents the starting reaction interface, L represents the thickness of the boundary layer. If x and r denote the independent spatial coordinates in the axial and the radial directions, respectively, the material surface is located at $x = 0$ and the detached normal shock wave is located at $x = L$. At $x = 0$, the pyrolysis gases flow toward the positive x direction. At $x = L$, the oxygen flows toward the negative x direction. In Fig. 1(c), the double-circles and each circular represent the oxygen and the single carbon fiber whose diameter is d_0 reaching micro order at the material surface.