International Journal of Heat and Mass Transfer 109 (2017) 725–736

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

A coupled thermal/fluid/chemical/ablation method on surface ablation of charring composites

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ARTICLE INFO

Article history:
Received 11 November 2016
Received in revised form 3 February 2017
Accepted 18 February 2017

Keywords:
Surface ablation
Coupled thermal/fluid/chemical/ablation method
Charring composites
Thermal protection

ABSTRACT

The surface ablation of charring composites is critical for estimating the performance of the thermal protection system of a hypersonic vehicle during reentry. A coupled thermal/fluid/chemical/ablation method is proposed to solve the surface ablation of charring composites with the pyrolysis. Comparing to the previous method, it considers that the chemical reactions between the pyrolysis gases and the oxidative gases in the boundary layer have further influences on the oxidation of surface char in the Park's model. The new mathematical models are discretized by using the center and up-wind formats, and solved by the FORTRAN and MATLAB codes written. The numerical results indicate that the coupled method shows a validation in solving the surface ablation by comparing to the experimental data, and it can more accurately determine the surface recession rate of charring materials. This study will be helpful for the design of the thermal protection systems in hypersonic reentry vehicles.

1. Introduction

Thermal protection system (TPS) is essential for safety of vehicles subjected to severe aerodynamic heating [1]. Reentry vehicles usually take charring materials as TPS materials due to their volume and surface ablation to protect the vehicles from the huge amount of heat generated by the friction of the atmosphere [2–6]. On the one hand, the researchers focused on the volume ablation process of these composites. For instance, the models for the volume ablation often used heat conduction equations considering the pyrolysis of materials to calculate the in-depth materials' thermal performances, such as the reported Li's pyrolysis interface and layer models [7–9], which could estimate the thickness of each layer during the pyrolysis. Also, the heat conduction equation combining with the Arrehinus's law served as a model for obtaining the mass flow rate of pyrolysis gases during heating [10,11]. Furthermore, the mechanisms of pyrolysis gases produced from the pyrolysis in the porous char were deeply studied by many researchers. For example, with the species mass conservation, momentum conservation expressed by Darcy's law and energy conservation for gases and solid equations, the products produced from phenol, the pressure distributions in the materials and temperatures for both pyrolysis gases and solid could be analyzed [12,13]. Then in recent years, the thermodynamics and transport properties were determined by Mutation++ and measured using gas chromatography techniques [14,15]. On the other hand, the surface ablation is worthy for attention. It is the phenomenon that the gases in the boundary layer react with surface char companying with the mass loss and the surface recession. Firstly, the chemical reactions occurring at materials' surface for the oxidation of graphite under reentry conditions were usually (1) $C + O_2 \rightarrow CO + O$; (2) $C + O \rightarrow CO$; (3) $C + O + O \rightarrow C + O_2$ or (1) $C + O_2 \rightarrow CO$; (2) $C + N \rightarrow CN$; (3) $3C \rightarrow C_3$, in which the thermo-chemical and the sublimation reaction rates were based on both the kinetic theory and the experimentally determined reaction probabilities by the Knudsen-Langmuir equation [16–22]. And the well-known slow and fast reaction rates at high temperatures were proposed by Scala after reviewing the kinetic data and reaction-rate expressions by several authors [23]. Also, Maabs concluded the previous researches on the kinetic expressions for estimation of the chemical reaction rates at high temperatures and presented the temperature range of each expression [24]. Secondly, the computer program such as Charring Material Ablation which coupled with a boundary layer solver could obtain the regression of the ablation surface [25]. But this program could not easily obtain the gas generation rate in the fast decomposing materials. And STABII program took temperature dependent materials properties as well as the surface recession into account [26]. Simultaneously, the influences of the chemical

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2017.02.052
0017-9310/

Nomenclature

L	thickness of boundary layer [m]
y	spatial coordinate along the thickness direction in the inner charring material [m]
x	spatial coordinate in axial direction in the boundary layer [m]
t	time [s]
r	spatial coordinate in radial direction [m]
ρ	gas density [kg/m^3]
u	gas velocity/gas velocity in axial direction [m/s]
p	gas pressure [Pa]
h	specific enthalpy [J/kg]
T	gas temperature [K]
c_p	specific heat at constant pressure [J kg^{-1} K^{-1}]
G	function of density, radial velocity and radial coordinate [kg m^{-3} s^{-1}]
F	function of density and axial velocity [kg m^{-2} s^{-1}]
H	eigenvalue for the radial pressure gradient [Pa/m^2]
μ	dynamic viscosity [kg m^{-1} s^{-1}]
v	gas velocity in radial direction [m/s]
λ	thermal conductivity [W m^{-1} K^{-1}]
Y	mass fraction [–]
V	diffusion velocity [m/s]
$\dot{\omega}$	chemical reaction rate [mol m^{-3} s^{-1}]
W	molecular weight [kg/mol]
$\bar{W}$	mean molecular weight [kg/mol]
C_p	molar heat capacity at constant pressure [J mol^{-1} K^{-1}]
X	mole fraction [–]
$[X]$	molar concentration [mol/m^3]
D_{jk}	multicomponent diffusion coefficients [m^2/s]
D_{km}	mixture averaged diffusion coefficients [m^2/s]
D_k^T	thermal diffusion coefficients [kg m^{-1} s^{-1}]
υ'	stoichiometric coefficient of reactant [–]
υ''	stoichiometric coefficient of product [–]
κ	curvature radius [m]
$\dot{m}$	mass flux rate [kg m^{-2} s^{-1}]
k	reaction rate constant
d	diameter of bore [m]
α	reaction probability [–]
ε	emissivity of the ablation surface [–]
σ	Stefan-Boltzmann constant [W m^{-2} K^{-4}]
q	heat flux [W/m^2]
φ	thermal blockage coefficient [–]
ΔH	heat of combustion [J/kg]
R	gas constant [J mol^{-1} K^{-1}]
Q	ablation heat in per area [J/m^2]
θ	graphite vapor pressure coefficient [–]

Subscripts

C	*char*
w	surface
cold	cold wall
r	recovery
f	the position before detached normal shock wave
b	the position behind detached normal shock wave
k	species index
i	ith reaction
s	oxygen-bearing species on the reactant side of the equation
v	vapor
g	gas

reactions occurring in the char layer, i.e. cracking of gases and gas-olid interactions, on the surface ablation were analyzed using frozen, chemical equilibrium, or finite rate models [27]. Another significant part of numerical tools is a three dimensional Navier-Stokes code Langley Aerothermodynamic Upwind Relaxation Algorithm, which could simulate the hypersonic non-equilibrium flow over blunt bodies in order to obtain the parameters, such as pressure and species, used in the surface ablation mechanisms [28]. Finally, the arc jet test facilities in NASA Ames Research Center were built to simulate the high enthalpy aerodynamic environment and measure the materials' properties in ablation [29]. The facilities included the Aerodynamic Heating Facility (AHF), the Panel Test Facility (PTF), Interaction Heating Facility (IHF), and other support systems. On the basis of these arc jet facilities, the measured recession, thermal responses, and shape change were presented for a phenolic impregnated carbon ablator [30,31]. But the experimental methods were not applicable for the ablation due to that these ground tests were difficult to accurately simulate the actual reentry conditions. Meanwhile, the flight tests were prohibitively expensive.

In the previous researches, the way to obtain the surface recession usually takes the gas-solid interactions, the thermal responses of materials' surface and the aerodynamic properties in the boundary layer into consideration. However, the surface ablation of the charring materials is extremely complex, which relates not only with above elements but also with the chemical performances in the boundary layer, like the kinds of the interactions between the pyrolysis gases which inject to materials' surface with the oxidative gases in the boundary layer, the production and consumption of oxidative gases near the materials' surface, the reaction mechanisms of the hydrocarbons [32,33]. In this respect, a coupled thermal/fluid/chemical/ab-lation method is proposed in this paper to estimate the surface recession more accurately.

2. Model

2.1. Physical model

With the surface of charring materials suffering heating, in the inner ablator, the composite is divided into three layers, namely the virgin layer, the pyrolysis layer and the char layer. In the outer ablator adjacent to the material's surface, there is an ablation layer. The detail physical and chemical phenomena in each layer can be seen in Refs. [7–9]. In the mean time, the pyrolysis gases produced in the pyrolysis layer flow to the materials' surface and inject to the boundary layer. In this boundary layer, the pyrolysis gases which are usually hydrocarbons react with the oxidative gas species in the inflow, which form a counterflow diffusion flame. The reactions of above gases affect the aerodynamic performances near the composite's surface, such as the mole fractions, the species and the molecular weights of gases. Using these chemical performances as well as the aerodynamic parameters, the oxidation of surface char occurs. The physical model coupled with the thermal transport in the inner materials, the gases reactions in the boundary layer and the oxidation of surface char built in this paper can be seen in Fig. 1.

In Fig. 1, 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