

## THERMAL ANALYSIS OF CHARRING MATERIALS BASED ON PYROLYSIS INTERFACE MODEL

by

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*Charring thermal protection systems have been used to protect hypersonic vehicles from high heat loads. The pyrolysis of charring materials is a complicated physical and chemical phenomenon. Based on the pyrolysis interface model, a simulating approach for charring ablation has been designed in order to obtain one dimensional transient thermal behavior of homogeneous charring materials in reentry capsules. As the numerical results indicate, the pyrolysis rate and the surface temperature under a given heat flux rise abruptly in the beginning, then reach a plateau, but the temperature at the bottom rises very slowly to prevent the structural materials from being heated seriously. Pyrolysis mechanism can play an important role in thermal protection systems subjected to serious aerodynamic heat.*

Key words: *pyrolysis, pyrolysis interface model, charring materials, thermal protection system*

### Introduction

The performance of the thermal protection system (TPS) is critical, since mass reduction trades directly with increase in science payload for a given reentry mass or reduction in launch vehicle cost by using a lighter entry system and a smaller launch vehicle [1]. Charring materials are used in TPS for reentry vehicles such as Apollo and Orion capsules. TPS can operate by absorbing heat through decomposition and rejecting it via pyrolysis gas injection back into the boundary layer of gas. Traditionally, the design of a TPS has heavily relied on ground test. Ablation and pyrolysis of charring materials were investigated through an ablation test motor [2]. Besides, it is very important to understand the physical and chemical behavior of the TPS subjected to aerodynamic heat [3]. The pyrolysis interface is moving, so this is a moving boundary problem. Some researchers analysed the temperature distribution, the mass loss rate and the surface recession through simulation [4-6]. Huang *et al.* [7] used the central difference scheme to solve moving boundary problem in the one-dimensional thermal response. However, there were a few discussions on the thermal response and the moving rate of pyrolysis interface in charring materials. This study will mainly focus on calculating the thermal response of polyester phenolic composites based on the pyrolysis interface model.

### Pyrolysis interface model and numerical approach

The temperature gradient vertical to the surface is much higher than that in the other orientation, so the 1-D pyrolysis interface model in fig. 1 can be built on the base of the

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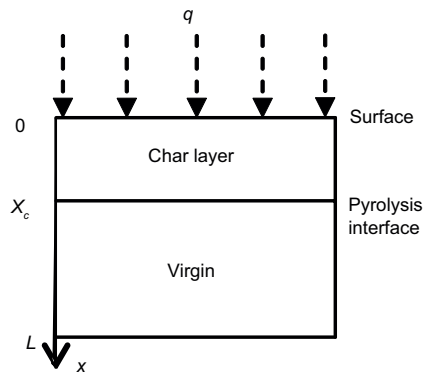


Figure 1. The pyrolysis interface model

layer and a virgin materials layer. Based on the Fourier's law of heat conduction, the heat conduction equations of the two layers are, respectively, deduced as:

$$\rho_1 c_1 \frac{\partial T(x,t)}{\partial t} = k_1 \frac{\partial^2 T(x,t)}{\partial x^2} + \dot{m}_p c_p \frac{\partial T(x,t)}{\partial x} \quad 0 \leq x \leq X_c \quad (1)$$

$$\rho_2 c_2 \frac{\partial T(x,t)}{\partial t} = k_2 \frac{\partial^2 T(x,t)}{\partial x^2} \quad X_c \leq x \leq L \quad (2)$$

The boundary conditions are given in the form:

$$-k_1 \frac{\partial T(x,t)}{\partial x} = q \quad x = 0 \quad (3)$$

$$T(x,t) = T_p \quad x = X_c \quad (4)$$

$$k_2 \frac{\partial T(x,t)}{\partial x} = 0 \quad x = L \quad (5)$$

where  $\rho$ ,  $c$ , and  $k$  are the density, specific heat capacity, and thermal conductivity, respectively, the subscripts 1 and 2 are a char layer and a virgin materials layer, respectively;  $\dot{m}_p$  is the mass flow rate of pyrolysis;  $c_p$  – the specific heat capacity of pyrolysis gas.

Pyrolysis mass rates are determined by the energy balance equation on a pyrolysis interface, which is represented by the relation:

$$-k_1 \frac{\partial T(x,t)}{\partial x} = -k_2 \frac{\partial T(x,t)}{\partial x} + \dot{m}_p h_p \quad x = X_c \quad (6)$$

$$\dot{m}_p = (\rho_2 - \rho_1) \dot{X}_c \quad (7)$$

where  $h_p$  is the latent heat in pyrolysis and  $\dot{X}_c$  is the moving rate of pyrolysis interface.

In addition, there is only a virgin materials layer ( $X_c = 0$ ) before char layer arises. The surface temperature is less than  $T_p$  in this period. The heat conduction equation is:

$$\rho_2 c_2 \frac{\partial T(x,t)}{\partial t} = k_2 \frac{\partial^2 T(x,t)}{\partial x^2} \quad 0 \leq x \leq L \quad (8)$$

following assumptions: (1) pyrolytic reaction only occurs on the pyrolysis interface that the pyrolysis layer between a char layer and a virgin materials layer, and (2) pyrolysis gases do not react chemically with the porous char layer through which it flows.

From the model, we know that the surface temperature rises up to the pyrolysis temperature  $T_p$  during  $0-t_0$  s, and materials start to decompose. Then the pyrolysis interface moves to the interior and a porous char layer appears, while pyrolysis gas flows through the char layer and injects back into the boundary layer of gas. After a char layer comes into being (heating time  $> t_0$  s), the surface temperature is more than  $T_p$  and there are two layers which are a char layer and a virgin materials layer.

The boundary conditions are:

$$-k_2 \frac{\partial T(x,t)}{\partial x} = q \quad x = 0 \quad (9)$$

$$k_2 \frac{\partial T(x,t)}{\partial x} = 0 \quad x = L \quad (10)$$

The initial condition is given by:

$$T(x,0) = T_0 \quad (11)$$

The heat conduction equations are obviously transient so that we have to discrete space domain and time domain, respectively. Here we use the central difference format for space domain and implicit format for time domain as:

$$\frac{\partial T(x,t)}{\partial x} = \frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x} \quad (12)$$

$$\frac{\partial T^2(x,t)}{\partial x^2} = \frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{(\Delta x)^2} \quad (13)$$

$$\frac{\partial T(x,t)}{\partial t} = \frac{T_j^n - T_j^{n-1}}{\Delta t} \quad (14)$$

We put eqs. (12), (13), and (14) into eq. (1) and then let:

$$r = \frac{k_1}{\rho_1 c_1} \frac{\Delta t}{(\Delta x)^2}, \quad z = \frac{\dot{m}_p c_p}{\rho_1 c_1} \frac{\Delta t}{\Delta x}$$

so that the discrete equation can be deduced as:

$$\frac{T_j^n - T_j^{n-1}}{\Delta t} = r \frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{(\Delta x)^2} + z \frac{T_{j+1}^n - T_{j-1}^n}{2\Delta x} \quad (15)$$

Let  $A = 1 + 2r$ ,  $B = r + z$ ,  $C = r - z$ , and  $D = T_j^{n-1}$ , eq. (15) can be written as:

$$T_j^n = \frac{B}{A - CP_{j-1}} T_{j+1}^n + \frac{CQ_{j-1} + D}{A - CP_{j-1}} \quad (16)$$

where

$$P_j = \frac{B}{A - CP_{j-1}}, \quad Q_j = \frac{CQ_{j-1} + D}{A - CP_{j-1}}$$

The pyrolysis interface is moving with the heating. In order to use Thomas algorithm to calculate the discrete equation, we introduce the method which fixes the time step while changing space step to get the moving rate of pyrolysis interface. The energy balance eq. (6) becomes:

$$-k_1 \frac{T_{j+1}^n - T_j^n}{\Delta x} = -k_2 \frac{T_{j+1}^n - T_j^n}{\Delta x} + (\rho_2 - \rho_1) h_p \frac{\Delta X_c}{\Delta t} \quad (17)$$

From eq. (17), we can get the new moving distance  $\Delta X_c$  of a pyrolysis interface with every fixing time step:

$$\Delta X_c = \frac{\left( k_2 \frac{T_{j+1}^n - T_j^n}{\Delta x} - k_1 \frac{T_{j+1}^n - T_j^n}{\Delta x} \right) \Delta t}{(\rho_2 - \rho_1) h_p} \quad (18)$$

Based on the above mathematical models and the iterative approach, we can write a computer code to calculate the thermal response.

## Results

Taking a polyester phenolic composite as an example, we can study one dimensional transient thermal behavior of homogeneous charring materials by means of the written computer codes. The temperature  $T_p$  on the pyrolysis interface is taken as 873 K, the latent

**Table 1. Physical parameters**

	$\rho$ [kgm <sup>-3</sup> ]	$c$ [Jkg <sup>-1</sup> K <sup>-1</sup> ]	$k$ [Wm <sup>-1</sup> K <sup>-1</sup> ]	$L$ [mm]
Char layer	406.3	1588	61.7	
Virgin materials	1300	1507	0.2407	20
Pyrolysis gas		3266		

heat  $h_p$  in the pyrolysis is 231.5 MJ/kg, and the initial temperature  $T_0$  is 300 K. The physical parameters of materials and pyrolysis gas are given in tab. 1.

From the parameters, we have obtained the thermal response of charring materials under the aerodynamic heat flux  $q = 879200 \text{ W/m}^2$ . Figure 2 indicates the changes in surface temperature with heating time. The surface temperature rises rapidly to the pyrolysis temperature in the preliminary time, and then keeps rising steadily, up to 942.2 K at 1000 s. The interior temperature distributions at 10 s, 200 s, 500 s, and 1000 s is shown in fig. 3. The interior temperature distribution consists of two parts corresponding to the two layers. In initial heating time, the temperature distributions far away from pyrolysis interface in virgin layer are  $T_0$ , comparing to which are of enormous rising gradient adjacent to the pyrolysis interface, which can be viewed on dot line. Heating continues and the char layer expands, while the virgin materials layer diminishes, which can be found in the other curves. The temperature gradient of the virgin is greater than that of the char layer, for the reason that the thermal conductivity of the two layers is 0.2407 W/mK and 61.7 W/mK, respectively.

The moving rate of pyrolysis interface changing with the heating can be seen in fig. 4. In the initial heating time, the rate begins to rise rapidly from the pyrolysis at the beginning 0.45 s to 35.7 s, then keeps rising gradually. The moving linear rate of pyrolysis interface rises only 0.0042 mm/s during 100-1000 s, which is almost a steady state. Figure 5 shows the temperature at the bottom changes with the heating. In the initial heating time, the temperature at the bottom barely rises and stays at the initial temperature 300 K. Then it gradually rises up to 306.5 K when the heating time is 200 s. When it is 1000 s heating on the surface, the temperature at the bottom rises to 584.8 K. The temperature at the bottom rises slowly with the function of pyrolysis to prevent the structural materials from being heated seriously.

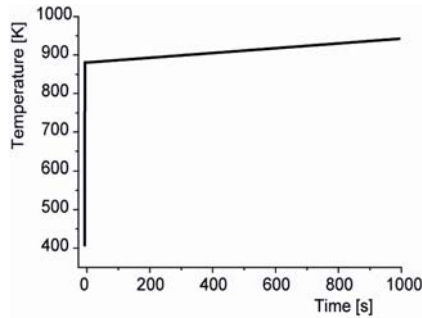


Figure 2. Surface temperatures

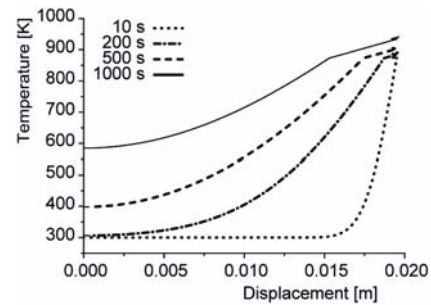


Figure 3. Interior temperature distributions

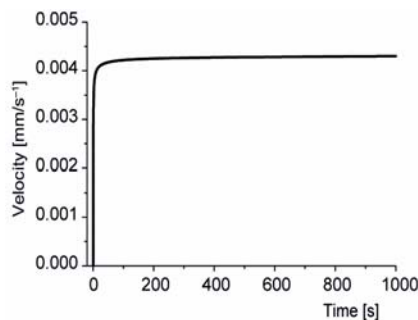


Figure 4. Moving rate of pyrolysis interface

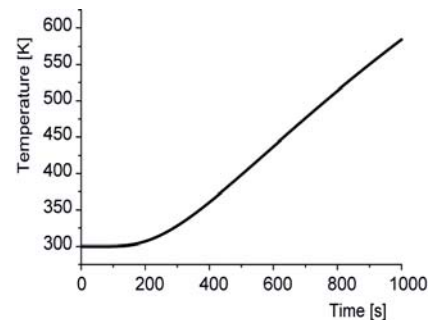


Figure 5. Bottom temperature

## Conclusions

By simulating on the pyrolysis of polyester phenolic composites on the base of the Fourier's law of heat conduction and the pyrolysis mechanism, we have found the thermal response of charring materials under a heat flux. The results show that the moving rate of pyrolysis interface and the surface temperature under a given heat flux rise abruptly in the beginning, then reaches a plateau, but the temperature at the bottom rises very slowly to prevent the structural materials from being heated seriously. With the absorbing heat through decomposition and rejecting it via pyrolysis gas injection back into the boundary layer gas, charring materials can play an important role in thermal protection systems subjected to severe aerodynamic heat.

## Acknowledgment

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## Nomenclature

$c$  – specific heat capacity, [ $\text{Jkg}^{-1}\text{K}^{-1}$ ]  
 $h$  – latent heat, [ $\text{MJkg}^{-1}$ ]  
 $k$  – thermal conductivity, [ $\text{Wm}^{-1}\text{K}^{-1}$ ]  
 $\dot{m}$  – mass flow rate, [ $\text{kgm}^{-2}\text{s}^{-1}$ ]  
 $q$  – heat flux on the surface, [ $\text{Wm}^{-2}$ ]  
 $T$  – temperature, [K]  
 $t$  – heating time, [s]  
 $X_c$  – thickness of char layer, [mm]

## Subscripts

1 – char layer  
 2 – virgin materials  
 $p$  – pyrolysis

## Greeks symbols

$\rho$  – mass density, [ $\text{kgm}^{-3}$ ]

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