Numerical Study of High Performance Ablative Thermal Protect System by Adding Phase Change Material

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Abstract. Under extreme thermal environment, ablation process of thermal protection system is a key issue in atmospheric re-entry and hypersonic flight vehicles; it displays a strong coupling between ablation mass, velocity and heat transfer. This article presents a method for combining the ablating and melting process, building a right triangle carbon-carbon model for ablation mixed with octadecane phase change material to absorb the heat of combustion delaying the movement of burning interface. For the moving of boundary, it is treated by the modified Stefan model coupled with chemical reaction and thermal radiation at the front leading boundary. The governing equation of heat transfer considering the melting process of phase change material is given by referring the enthalpy method. The effect of volume ratio and aerodynamic heating on the ablation interface and net heat flux on the interface are investigated. Result shows that high volume ratio of the phase change material delays the movement of the interface, and decreases the net heat flux of the interface; on the other hand, high aerodynamic heat accelerates the movement of the interface and increases the interface net heat flux at a given time point. This study can give a rule on how the volume ratio of phase change material influence the ablative process quantitatively.

1. Introduction

With the development of the flight vehicles and spacecraft, the velocity of them has reached hypersonic field. The harsh environment for re-entry into the atmosphere and the high speed bring the severe aerodynamic heat problem. Thus, the effective thermal protection system should be considered. According to the different thermal protection mechanisms, the basic forms of heat protection schemes can be divided into endothermic thermal protection system, mass ejector thermal protection system, radiant heat protection system, mass transfer heat treatment thermal protection system, and integrated thermal protection system (ITPS)[1], among which ablative thermal protection system has been widely adopted in the thermal protect system, because it has the advantage on tuneable density, lower cost and higher heat shock resistance.

For ablative thermal protection system. There are two sides can be considered on the system, new materials and new methods for ablation. For ablative materials, rhenium, molybdenum, and tungsten was considered in early time. Graphite carbon-carbon (C-C) composite material was considered for its high heat capacity and high energy of vaporization [2]. Thus, nowadays C-C composite material is commonly used in ablative thermal protection system (TPS). What’s more, with the development of material science, new composite material has been developed. For the new methods for ablation, during the study of ablation process, the nonlinear phase change problem is the key point: the moving interface at which the phase change occurs. For boundary moving process, Chu and Zhang [3] combined the
moving boundary and finite volume method to calculate the heat exchanger problem, showing that the coupling algorithm is reliable in the heat exchanger modelling with the run time much shorter than only using finite volume method. Ahmed et al.[4] got a new hybrid grid and meshless method for the numerical simulation result of phase change material with moving boundary, and well compared with the analytical solution. Li et al.[5] used the Stefan moving boundary models for simulation the phase change of heat-dissociation hydrate, getting the laws of temperature and the frontier location. Turkylmazoglu et al.[6] analysed the Stefan problems of phase changing bar using single and double phase models, and show a unique observation is that the solid-liquid interface location grows when the slab moves in the direction of melt or freeze. Abhishek et al.[7] describe a Stefan problem with temperature dependent Thermal coefficients and moving phase change material, also consider the convective boundary condition using spectral tau method to approach; and they show the accuracy of the result by comparing the result with analytical solution and get that the solidification process is affected by Peclet number (Pe) and constant γ, and the process becomes fast as the parameters Pe and γ increase. The study of phase change material melting process varies from different scales, for example, Hasadi et al.[8] showed the melting process of nanostructured phase change materials colloidal suspensions, and observed that for the case of diameter of particle equal to 2 nm, as the mass fraction of the particles increases the solid-liquid interface changes from a planar to unstable morphology during melting. Some materials are widely used for the study of phase changing process such as paraffin wax[9], TiO$_2$[10], open-cell metal foams[11], octadecane[12]. We can choose the octadecane for our simulation.

Besides, for hypersonic vehicles subjected to severe aerodynamic heating, carbon composites ablative materials are commonly used in the thermal protection systems (TPS) for the integrity of the structure[13].

From the study above, we can see the advantage of phase change materials, but nowadays we can see there are a lot of ablative TPS studies, but few of them combine the ablative TPS with phase change materials or take the notice on the model building on the leading edge of the hypersonic vehicles. This paper presents a method for combining the ablating and phase change material and the model building on the leading edge, by building a right triangle carbon-carbon model of Stefan problem coupled with chemical reaction and thermal radiation at the front leading boundary mixed with octadecane composite phase change material under the condition of constant aerodynamic heat flux, and the effect of the aerodynamic heat and volume ratio of the phase change material on the ablative process is studied.

2. Description of physical problem and mathematical model

2.1 Physical problem descriptions

For the supersonic and hypersonic vehicles, the wing is very important, always with large sweep angle and thin wing as shown in Figure 1. And for the serious heating condition on leading edge, we should consider the thermal protection on that. The heat energy will get stored with the cruising speed larger than sonic speed, which cause the shape of the leading edge deformed without effective protection, resulting in the changing in aerodynamic force, even causing the aircraft to be unstable and destroyed. So, it is very important for thermal conduction at the leading edge. Some studies have got some other mechanisms: Zhu et al. [14] presented a typical actively-cooled thermal protection system cooling the leading edge by impingement jet of gaseous helium and get effectively decrease the temperature on the leading edge shown in Figure 2. It is an actively-cooled TPS on which the thermal stress cannot decrease significantly, so mostly we use the passive thermal protection by adding the ablative material on the leading edge.
In this paper, the complex leading-edge ablative material was simplified to a right triangle, and the right triangle model is treated as a one dimensional physical model for Stefan problem with chemical reaction at the leading edge ablation leading interface. Heat is only transmitted along the long right side. The degree of small acute angle is set to $\psi = 0.3\text{rad}$. Due to the aerodynamic heat cannot be transmitted from the leading point, the triangle model must remove the point, so $L$ is length of the long right side after removed the point. We suppose that the limited size of ablation model is fixed with the length of long right side $L=0.5$ m. When the point is removed, the physical model is turned into a right trapezoid model. The transmitted model is described in Figure 3. Assuming that the left edge is the boundary of model and length of the left edge is initial thermal conductive area of ablation body. Which the initial area is expressed as $A_0$, setting the initial area $A_0 = 0.01m^2$. Originally, the ablation body stays its initial temperature. Supposing that the ambient temperature. As the time continued, the solid region where the temperature exceeded the temperature of gasification point. Then, the ablation body of front layer is turned into the gas phase and the front layer will gradually move away from its initial position. Meanwhile, the heat dissipates from the left ablation interface to the internal material. Along with the increase of temperature, the whole ablation body will be preheated after a period of time, for there is also phase change material which will begin to change the phase from solid to fluid with the temperature get to its solid-phase temperature, and all phase change material get to fluid entirely when temperature go to fluid-phase temperature.

On the above states of the physical model, the following assumptions could be proposed: (1) Oxygen density at the leading edge during the chemical reaction period is treated as changeless; (2) Convective heat transfer between air and the ablation body on the surface layer is neglected; (3) Effect of the oxygen partial pressure is neglected; (4) Local atmospheric environmental thermal radiation is neglected.

2.2 Mathematical descriptions

Obviously, the calculation area is limited to the problem based on the above physical descriptions and assumptions, and the governing equations of thermal conductive area are presented.
Instantaneous heat conductive area:

\[ A(X) = A_o + A \tan(\psi) S(t) \quad \tau \geq 0 \] (1)

For thermal governing equation, we use the enthalpy method as followed

\[ \rho \frac{\partial \hat{H}}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} \] (2)

\( \hat{H} \) is the total enthalpy as shown in equation (3). This value consists of the sensible enthalpy \( (h') \) and latent enthalpy \( (h) \):

\[ \hat{H} = h + h' = \int c dT + f(T) \cdot h_c \] (3)

Where \( h_c \) is the effective latent heat of phase change material. \( f \) is the fluid phase fraction \([16]\), can be expressed as equation (4):

\[ f(T) = \begin{cases} 
0, & T < T_s \\
\frac{T - T_c}{T_f - T_s}, & T_s \leq T \leq T_f \\
1, & T > T_f 
\end{cases} \] (4)

Then substitute equation (4) into equation (2), and we can get the governing equation of temperature, as shown in equation (5).

\[ \rho c \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} - \rho h_c \frac{d f(T)}{d t} \] (5)

Initial condition:

\[ T(X, 0) = T_0, \quad \tau = 0, \quad S(t) = 0 \] (6)

Boundary conditions:

\[ Q_{net} = -\lambda A(X) \frac{\partial T}{\partial x} = Q_{net} - \varepsilon A(X) \sigma (T^4 - T_{amb}^4) + A(X) K_v e^{-\frac{E}{RT}} P_{O_2}^{\frac{1}{2}} h_c X = S(\tau) \] (7)

\[ \frac{\partial T(X, t)}{\partial X} = 0 \quad X = L \] (8)

Net heat flux:

\[ q_{net} = \frac{Q_{net}}{A(X)} \quad 0 \leq X \leq L \] (9)

Some thermal physical properties of graphite are listed in Table 1. Additionally, to calculate the ablation front layer recession, the modified moving boundary controlling equations similar to that in classic Stefan problem are initially given below. Moving boundary controlling equations:

\[ \rho \frac{d S(t)}{d t} = k_v e^{-\frac{E}{RT}} P_{O_2}^{\frac{1}{2}} X = S(t); \quad S(t) = 0 \quad t = 0 \] (10)

equation (10) accounts for the heat balance at the ablation interface. When time \( \delta t \to 0 \), the recession distant is exclusively determined by mass loss of TPS material suffered from chemical ablation. Two dimensionless variables can be introduced in the above equations. Expressing as following:

\[ \eta = \frac{X - S(t)}{L - S(t)} \quad (0 \leq \eta \leq 1); \quad \xi = \frac{S(t)}{L} \quad (0 \leq \xi \leq 1) \] (11)

The \( \eta \) represents the dimensionless moving coordinates, and the \( \xi \) represents the dimensionless coordinate of ablation interface location. Then, plugged the above two dimensionless parameters into the equations in Eqs.(1), (2) and (5)-(11) respectively.
\[ A = A_0 + \tan(\psi) \xi L \]  

Thermal governing equation:
\[
\frac{\partial T}{\partial t} + \frac{\lambda}{L^2 \rho c (1-\xi)^2} \frac{\partial^2 T}{\partial \eta^2} = \frac{\lambda \tan(\psi)}{(1-\eta) L^2 \rho c (1-\xi)^2} + \frac{\lambda \tan(\psi)(A_0 + \tan(\psi) \xi L)}{(1-\eta)L \rho c (1-\xi)^2 (A_0 + \tan(\psi) \xi L)} \frac{\partial T}{\partial \eta} - \frac{h_s}{c} \frac{dt}{dt}
\]

Initial condition:
\[ T(\eta, 0) = T_0 \]

Boundary conditions:
\[
Q_{net} = -\lambda (A_0 + \tan(\psi) \xi L) \frac{1}{L (1-\xi)} \frac{\partial T}{\partial \eta}
\]

\[ = Q_{\text{aero}} - (A_0 + \tan(\psi) \xi L) \cdot \sigma (T^4 - T_{\text{amb}}^4) + (A_0 + \tan(\psi) \xi L) k_e \frac{E}{\Delta t} p_{\Delta t}^{-1} h_e \quad \eta = 0
\]

\[ -\lambda \frac{\partial T(\eta, t)}{\partial \eta} = 0 \quad \eta = 1 \]

Net heat flux:
\[ q_{net} = \frac{Q_{net}}{A_0 + \tan(\psi) \xi L} \quad 0 \leq \xi \leq 1 \]

Moving boundary controlling equations:
\[
\rho_L \frac{d \xi(t)}{d t} = k_e \frac{E}{\Delta t} p_{\Delta t}^{-1} h_e \quad \eta = 0 ; \quad \xi = 0 \quad t = 0
\]

2.3 Discrete process of equation

we use finite difference method (FDM) to discrete the thermal governing equation, for divergence can probably occur when the liquid fraction is directly calculated because of the strong nonlinearity of this problem. Therefore, the modified discretized equation suggested by Voller et al. [17] is adopted as
\[
f_i^{n+1} \left[ T_i^{n+1} - f^{-1}\left( f_i^m \right) \right] = f_i^m + \frac{\frac{d f}{d T}}{c} \left[ T_i^{n+1} - f^{-1}\left( f_i^m \right) \right]
\]

In equation (19) \( T_i^n \) means the temperature of the \( mth \) iteration at the \( nth \) time level for the \( i \) node, and we can use \( T_i^n \) to replace the convergence result of the \( nth \) time level for the \( i \) node. This equation is used to weaken the nonlinearity. When the second term on the right part of equation (19) is equal to 0, the calculation is converged. Then governing equation can change to:
\[
\frac{T_i^{n+1} - T_i^{n}}{\Delta t} = G \frac{T_i^{n+1} - 2T_i^{n+1} + T_i^{n+1}}{\Delta \eta^2} - F \frac{T_i^{n+1} - T_i^{n+1}}{2\Delta \eta} - \frac{he}{c\Delta\eta} \left[ f_i^{n+1} + \frac{d f}{d T} \left( T_i^{n+1} - f^{-1}\left( f_i^m \right) \right) \right]
\]

\[ G = \frac{\lambda}{\rho c L^2 (1-\xi)^2} \quad F = \frac{\lambda}{\rho c} \left( \frac{1}{(1-\eta)L (1-\xi)^2} + \frac{\tan(\psi)}{(1-\eta) L (1-\xi)^2 (A_0 + \tan(\psi) \xi L)} \right) \]

Boundary conditions:
\[ BT_{i+1}^{n} = CT_{i+1}^{n} + D \eta = 0 \quad B = C = (A_{y} + \tan(\psi)\xi L) - \frac{\lambda}{\Delta \eta(1 - \xi)} \]  
(22)

\[ D = Q_{\text{max}} - (A_{y} + \tan(\psi)\xi L)\sigma \left[ \left( T_{i+1}^{n} \right)^{4} - \left( T_{\text{max}} \right)^{4} \right] + (A_{y} + \tan(\psi)\xi L)k_{p}e^{-\frac{E}{RT_{i+1}^{n}}} \rho_{0}^{2}h_{i} \]  
(23)

\[ -\lambda_{c} \frac{T_{M1}^{n+1} - T_{M2}^{n+1}}{\Delta \eta} = 0 \quad \eta = 1 \]  
(24)

Net heat flux:

\[ q_{\text{net}} = \frac{Q_{\text{net}}}{(A_{y} + \tan(\psi)\xi L)} \]  
(25)

Moving boundary controlling equations:

\[ \frac{\xi_{i+1}^{n+1} - \xi_{i}^{n}}{\Delta \tau} = \frac{1}{\rho L} k_{0} e^{-\frac{E}{RT_{i}^{n+1}}} \frac{1}{\rho_{0}^{2}} \]  
(26)

2.4 Numerical method

The specific calculation steps are specifically listed as follows:

1. Using the initial temperature and dimensionless ablation front interface location distribution \( T_{0}^{0}, \xi_{0}^{0} \) respectively, update the temperature distribution \( T_{1}^{1} \) by TDMA algorithm. The superscript and subscript letter represent time layer and number of the inner iteration at specific time.

2. Using the updated the value of temperature, calculate the interface \( \xi_{1}^{1} \) via equation (26).

3. Finding the maximum value relative error, \( \Delta T_{i}^{n} = \left| T_{i}^{n} - T_{o} \right| \), \( \Delta \xi_{i}^{n} = \left| \xi_{i}^{n} - \xi_{0} \right| \). If \( \Delta T_{i}^{n} \leq \varepsilon_{i} \) and \( \Delta \xi_{i}^{n} \leq \varepsilon_{i} \), \( \varepsilon_{i} = \xi_{i} = 5 \times 10^{-4} \), then the present values are considered convergent and go to Step 1. If either of the judgmental condition fails, repeat step 1 until satisfied.

4. Saving the convergent values and apply them as the initial conditions of the next time layer, repeat Step 1.

### Table 1. Some thermal physical properties of C-C material

| Parameters                      | C-C               | Octadecane[15] |
|---------------------------------|-------------------|-----------------|
| Oxidation rate of graphite, \( k_{0} \) /kg·m\(^{-2}\)·s\(^{-1}\) | 3.28×10\(^{9}\)  | 3.28×10\(^{9}\) |
| Thermal conductivity, \( \lambda_{c} \) /W·m\(^{-1}\)·K\(^{-1}\) | 200              | 0.23            |
| Activation energy, \( E \) /cal·mol\(^{-1}\) | 9.66×10\(^{4}\)  | 9.66×10\(^{4}\) |
| Heat value of combustion, \( h_{i} \) /J·kg\(^{-1}\) | 3.28×10\(^{7}\)  | 4.75×10\(^{7}\) |
| Density, \( \rho \) /kg·m\(^{-3}\) | 2000             | 600             |
| Capacity, \( c \) /J·kg\(^{-1}\)·K\(^{-1}\) | 806              | 1850            |

3. Results and discussion

3.1 The grid independence check

In the course of the simulation, the discrete equations are solved numerically by TDMA algorithm. The grid independence is checked as shown in Figure 4. It can be seen that with increase of grid number, the temperature trends a constant value. The final adopted grid number is chosen as 101.
3.2 Effect of volume ratio of phase change material on ablation interface location and net heat flux of ablation front layer

From Figure 5 we can see that with the volume ratio of phase change material increasing, the moving speed of ablation interface recession location will go down. From the volume ratio of phase change material going up from 0 to 0.01, the moving speed of ablation interface location has dropped by 50 percent. And when the volume ratio of phase change material goes up to 0.05, the ablation interface location almost keeps constant. This appearance is caused from the volume ratio changing, for the volume ratio of the phase change material will affect the thermal properties: with the phase change material mixed some heat can be absorbed by the phase changing, so the moving of the interface will be slowed down.

As shown in Figure 6, it presents the effects of different volume ratio of phase change material on the performance of net heat flux on ablation front layer nodes. We can see that the net heat flux decreasing trend is similar with volume ratio varying. But with the volume ratio going up, the decreasing speed of the heat flux will significantly go down. This trend can be discussed for the interface moving, for energy will be released by radiation and materials absorbing, and the releasing speed has relationship with the boundary moving. What’s more, the boundary moving speed means the ablative TPS material consumption rate. Slowing down the rate cases the net heat flux decreasing slowly.

3.3 Effect of aerodynamic heat on ablation interface location and net heat flux of ablation front layer

Figure 7 presents the effects of different aerodynamic heat on the location distribution of ablation front layer on different times. There is no matter for a given condition the trend of the interface moving will not change, and under a high aerodynamic heat condition, the moving of the interface of the ablation
will be quicker. That is because the much heat means more temperature and the high speed of the ablation reaction. We can consider under the high speed, the higher aerodynamic heat, the leading edge of the aircraft will get easily ablative deformation.

From Figure 8 we can get that with the aerodynamic heat changing, the heat flux distribution on the interface of the ablative process. The trend of the heat flux with time is the same as shown in Figure 6: with time flowing, the interface will radiate energy to the surrounding environment, and with temperature rising more, the radiate energy will increase sharply. Thus, the heat flux of the interface will go down. Furthermore, with the aerodynamic heat increasing, we can see the heat flux increase firstly, which is because the input energy is larger, and in a short time the energy output is with no big difference. Then with time goes to 200s, the condition begins to show a opposite trend for larger aero heat get a less heat flux. The reason for this condition is that under the high aerodynamic heat, the moving of the interface will be accelerated and temperature of that will be a higher, so it will get more energy radiated. In other word it also can be expressed as: more aero heat will accelerate the entire process, which means the speed of going down will also be accelerated. That is why after around 200s the higher aero heat will result in a lower heat flux.

4. Conclusions
In this paper, a modified Stefan model is proposed, considering the chemical reaction of ablation showing the movement of the ablating interface, phase change absorbing the burning heat with fluid phase fraction changing, and heated boundary radiation for temperature rising too high. Considering the effect of volume ratio of phase change material and aerodynamic heat to the physical and chemical properties, we use TDMA method to present the temperature distributions and simulate how the burning interface move. From what we get we can derive the heat flux, movement of the interface with considering on the influence of volume fraction and aero heat. We can see the influence of the aerodynamic heat and volume ratio of the phase change material is very significant: high volume ratio of the phase change material delays the movement of the interface, and decreases the net heat flux of the interface; on the other hand, high aerodynamic heat accelerates the movement of the interface and increases the interface net heat flux at a given time point. So the effective phase change material can offset the effects of high aerodynamic heat and is necessary for future application on ablative and phase change TPS.

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