NUMERICAL MODELING OF CHARRING MATERIAL ABALATION WITH CONSIDERING CHEMICAL REACTION, MASS TRANSFER AND SURFACE HEAT TRANSFER EFFECTS

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Abstract Accurate calculations for measuring the sacrificing rate of various materials in heat shield systems have not been obtained yet. So having a reliable numerical program that calculates the surface recession rate and interior temperature history is necessary. In this study numerical solution of governing equations for charring material ablation are presented. Thermodynamic properties ρ , C_p , k changes relative to the temperature accompany the nonlinear nature of the governing equations. The Newton-Raphson method along with TDMA algorithm is used to solve this nonlinear equation system. Using Newton- Raphson method is one of the advantages of solving method because it is relatively simple and it can be easily generalized to more difficult problems. The obtained results are compared with reliable sources in order to examine the accuracy of compiling code.

Keywords Ablation and surface recession rates; Interior temperature history; Charring material ablation; Newton Raphson; Numerical method

چکیده اطلاعات زیادی در مورد سیستم های سپر حرارتی موجود نمی باشد و اطلاعات موجود در بعضی موارد به صورت دقیق نیست. دلیل اصلی این است که محاسبات دقیقی برای اندازه گیری نرخ از بین رفتن مواد مختلف هنوز بدست نیامده است. بنابراین داشتن برنامه ای کامپیو تری مطمئن که بتواند نرخ از بین رفتن سطحی جسم را محاسبه و گستره درجه حرارت داخلی را بدست آورد لازم می شود. در این کار تحقیقاتی حل عددی معادلات حاکم برای مواد از بین رفتنی ارائه می شود تا بتواند نرخ این از بین رفتن و پاسخ گوئی حرارتی یک سپر حرارتی را پیش گوئی کند. در این کار از روش نیوتن – رفسان همراه با الگوریتم سه قطری در حل سیستم معادلات غیر خطی حاکم بر مساله به کار گرفته می شود. استفاده از روش نیوتن-رفسان که نسبتا خیلی ساده تر است می تواند به سادگی برای مسایل مشکل تعمیم داده شود.

1. INTRODUCTION

One of the first methods to increase efficiency of the missile systems is reducing the weight which causes the increase in missile velocity and its range. In order to satisfy this need, using composite technology has been increased in aerodynamic industry. According to the limitation in functional temperature of these materials, we need to use thermal protective systems which are designed to increase the weight of the structure in optimized conditions. In returned phase to atmosphere a high aerodynamic heating is produced because of the high velocity and compactness of the air molecules in front of the missile and kinetic to thermal energy conversion. This phenomenon is of considerable importance especially around the nose and it can destroy the structure, too. It is clear that no heat insulation can bear this environment unless by special mechanism which reduces the effect of strong heat flux. Some of these kinds of high temperature thermal systems used in these conditions include: heat-sink system, reflex-cooling, leakage cooling and ablative cooling, shown in Figure 1. So they absorb and lose some amount of heat flux when exposed to hot gases. In this manner, ablative insulation sacrifices itself for the main structure and prevents it from damage.

Nomenclature

B'	normalized mass (blowing driving force)	***Subscripts***	
B'_C	normalized ablation rate	ab	ablation
B'_g	normalized pyrolysis gas flux	c	of char
C_p	specific heat	cond	conduction
C_{pg}	specific heat of pyrolysis gas	conv	convective
E	activation energy	cw	cold wal
g_h	heat transfer coefficient	eq	equilibrium
g_m	mass transfer coefficient	er	erosion
h	enthalpy	e	at edge of boundary layer
$\dot{m}$	mass flux	g	pyrolysis gas
P	pressure	gw	value for pyrolysis gas at the wall underside
$\dot{q}$	heat flux	i	grid index
$\dot{q}_{net}$	net heat flux conducted into slab	j	resin component index
S	surface recession	r	recovery
St	Stanton number (sometimes Stanton number is shown as C)		
$\dot{S}$	surface recession rate	ref	reference value
T	temperature	rr	re-radiation
t	time	v	virgin
Z	in- depth distance from surface	w	at the wall
α	thermal diffusivity	o	in the absence of mass injection (“blowing”)
$\Delta h_{pyr(g)}$	heat of pyrolysis per gas produced	∞	final reaction state
ε	emissivity	***Superscripts***	
θ	transformed temperature	n	time index
ρ	density	o	old
σ	Stefan-Boltzmann constant	*	non-dimensionalized quantity
φ_{blow}	blowing correction factor	ˆ	estimate
φ_{HAL}	heating augmentation level	-	average

The ablative system deletes the surface temperature of the heat-sink system materials and it prevents the structure overweight. The major aim in studying ablative insulation is calculating the heat distribution in the depth of insulation and the amount of its recession during the missile movement. Figure 1 shows different areas created in a degradable material. The charring layer and the virgin layer have constant density [2]. Historically, the first scientific studies on ablative phenomenon are conducted in late 1960s and early 1970s and they are based on the first study of vonkarman and Liz, [3]. As mentioned earlier, the main aim of predicting ablative insulation behavior is measuring the temperature under the insulation and its recession process when the flying object flies, and as a result designing the optimized insulation. CMA was presented by Aerotherm company in 1968 [4]. This technique solves the energy equilibrium and decomposition equations implicitly along with energy equilibrium conditions of the ablative system. More recently, FIAT is presented in Ames research Center in NASA [5] which is more stable. An ablative program is presented in national laboratories of Sandia that uses the finite volume method along with unstructured mesh [6]. The integral solution (HBI) is one of the engineering solving methods to evaluate complex problems of heat transfer coupled with ablative problems which cause savings in the computer programs running time [7]. This method is considered as the oldest ablative problem-solving in the literature. In this method, Goodman integral method is used to anticipate the charring ablation materials behavior. These pseudo-analytic techniques is invented in late 1950s and early 1960s for some nonlinear problems of heat transfer, and the exponential, polynomial temperature profiles are used in it [8]. The most two recent studies can be mentioned here are quasi-state solutions obtained by Shan Lin [9] and [10]. In the first one, a one-dimensional quasi-state solution for the ablation of charring materials is investigated under the influence of a steady external heat source where the ablation is assumed to proceed at a known fixed constant. In the second one, an analytical modeling of the steady ablation of a 3-dimensional composite is considered.

In this paper, the governing equations are presented in order to anticipate the amounts of recession and the thermal response of charring ablative installations by considering the effect of chemical reactions, mass transfer and heat transfer to the surface (by considering pyrolysis gas effects and fluid-solid interaction). After specifying the boundary conditions, governing equations are solved by using Newton-Raphson method along with TDMA algorithm.

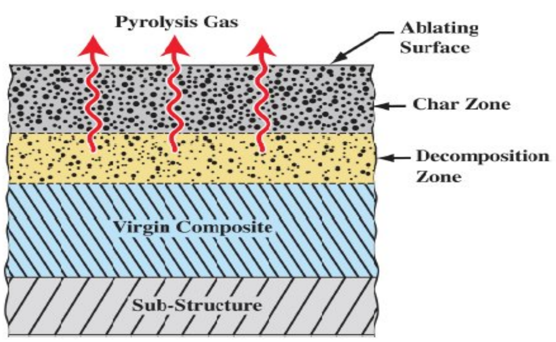

Figure1. A schematic model of the ablative insulation thermo chemical decomposition

2. PROBLEM FORMULATION

As shown in Figure 2, in terms of charring ablative material, it's better for the basic site axis basis to conform the material surface because of the ablative surface recession. In this matter, in contrast with non-charring ablative materials, like graphite and carbon-carbon composites, the mass flux of the pyrolysis gas is not zero. The material density is variable and governing equations are as mentioned in the literature [10]:

Energy equation:

$$\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right)+\dot{S}\frac{\partial}{\partial z}(\rho h)+\Delta h_{pyr(g)}\frac{\partial \rho}{\partial t}+\dot{m}_g C_{pg}\frac{\partial T}{\partial z}=\rho C_p\frac{\partial T}{\partial t} \quad (1)$$

in which, $\Delta h_{pyr(g)}$ is introduced as: $\Delta h_{pyr(g)} = h_g - \bar{h}$

where, $\bar{h} = \dfrac{\rho_v h_v - \rho_c h_c}{\rho_v - \rho_c}$.

Continuity equation**:**

$$\frac{\partial \dot{m}_g}{\partial z}=\frac{\partial \rho}{\partial t}-\dot{S}\frac{\partial \rho}{\partial z} \quad (2)$$

where, $\dot{S} = \dfrac{\dot{m}_{ab}}{r}$, $S^{n} = S^{n-1} + \dot{S}\,\Delta t$.

Decomposition equation:

$$\frac{\partial \rho}{\partial t}-\dot{S}\frac{\partial \rho}{\partial z}=-r_v\left(\frac{r-r_c}{r_v-r_c}\right)^m\sum A_j\, exp\left\{-B_j/(T-T_{ref})\right\} \quad (3)$$

EST and ACE computer codes calculate the ablation rate using the thermodynamic properties of the materials in JANAF tables. The input to these functions are the surface temperature (T_w), the surface pressure ($p_w = p_e$) and the normalized mass flux of pyrolysis gas. The outputs of these functions are in mass flux of surface ablation, and gas enthalpy at the wall. The mass transfer coefficient is calculated from ablative mass flux as following functions which have been introduced in Ref. [10]. In these relations B'_C and B'_g are calculated from the following equations:

$$B'_g = \dot{m}_g / g_h\ ,\ B'_c = \dot{m}_c / g_h\ ,\ \dot{m}_w = \dot{m}_g + \dot{m}_C\ ,\ g_m = g_h = r_e u_e St \quad (4)$$

$$g_h = g_{h0}\,\phi_{blow} \quad (5)$$

$$\varphi_{blow} = \frac{ln(1+a\,B')}{a\,B'} = \frac{a\,B'_0}{exp(a\,B'_0)-1} \quad (6)$$

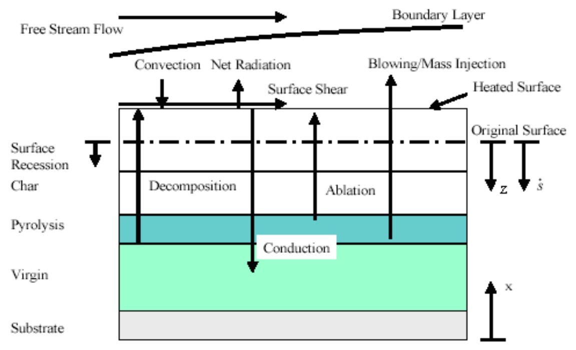

Figure 2. Thermo chemical decomposition presentation of charring ablative material

After obtaining mass transfer constant from the above equations by the standard assumption of "Lewis number = L_e =1", heat transfer coefficient is obtained.

If, $B'_g = 0$, the above equations can be used for carbon-carbon ablative material. Usually, the heat transfer is obtained in the absence of mass injection. Here, the subscript 0 is related to the area without ablation and pyrolysis gas mass flux.

ϕ_{blow} is related to the blowing resulted from the gas entering the boundary layer and it is calculated as:

$$B' = \dot{m}_w \big/ g_h \,,\, B'_0 = \dot{m}_w \big/ g_{h0} \,,\, B' = B'_0 / \varphi_{blow} \tag{7}$$

in which,

$$\hat{\varphi}_{blow} = a\,\hat{B}'_0 \big/ (exp(a\,\hat{B}'_0) - 1)\,, \tag{8}$$

$$\hat{B}'_0 = (\dot{m}^o_{ab} + \dot{m}^o_{gw}) \big/ g_{h0} \,,\; \hat{B}'_g = \dot{m}_{gw} \big/ (g_{h0}\hat{\varphi}_{blow})$$

If the $L_e = 1$, the value of the constant "a" for carbon-carbon and for carbon- phenolic is 1.5 and 1.3, respectively. In the compiling code, the total time of movement is divided according to the determined time pace. In every moment, the ablative mass flux of the previous moment is shown by $\dot{m}^{\circ}_{ab}$ and the mass flux of pyrolysis gas is shown as: $\dot{m}^o_{gw}$. In every moment, g^o_h and p_w values are conjectural. For correcting blowing constant, the following estimations are proposed:

$$B'_{eq} = B'_{c,eq} + \hat{B}'_g \tag{9}$$

Now, we can specify $B'_{c,eq}, h_{w,eq}$ using the above equations at T_w, p_w and $\hat{B}'_g$ then the following quantities are specified:

$$\begin{aligned}
&\varphi_{blow,eq} = ln(1 + a\,B'_{eq}) / (a\,B'_{eq}) \\
&\dot{m}_{eq} = g_{h0}\,\varphi_{blow,eq}\,B'_{c,eq}\,,\; \dot{m}_{ab} = \dot{m}_{eq}\,f_{tr} \\
&f_{tr} = 1 \Big/ \sqrt{1 + (\dot{m}_{eq} / \dot{m}_R)^2} \\
&\dot{m}_R = a_R (X_{O_2}\,p^*)^{0.5}\,exp\{-E_R/(R\,T_w)\} \\
&h_w = f_{tr}\,h_{w,eq} + (1 - f_{tr})\,h_{w0} \\
&a_R = 4.71 \times 10^6\ Kg/m^2 s \\
&X_{O_2} = 0.21 \\
&E_R = 44 \times 10^3\ K\,cal/K\,mol \\
&R = 1.989\ kcal\,/\,kmol.0k \\
&h_{w0} = \int_{T_{ref}}^{T_w} C_{p0}\,dT \\
&C_{p0} = C_0 + D_0 T \\
&C_0 = 979\ \ J/Kg^o k \\
&D_0 = 0.15\ \ J/Kg^o k^2
\end{aligned} \tag{10}$$

Now, the correction of blowing constant and the mass flux of ablation can be calculated according to $\dot{m}_{ab}$.

$$B'_0 = (\dot{m}_{ab} + \dot{m}^o_{gw}) \big/ g_{h0} \tag{11}$$

$$\varphi_{blow} = a\,B'_0 \big/ (exp(a\,B'_0) - 1) \tag{12}$$

2.1. Boundary conditions In Figure 3, a general ablative material is shown schematically. As it can been seen, we have to model the radiation and conduction, heat production or absorption related to chemical reactions. So, conservation of energy equation in ablative material surface is as follows.

$$\dot{q}_{net} = -\dot{q}_{rr} - \dot{m}_{ab}(h_w - h_u) - \dot{m}_{gw}(h_w - h_{gw}) \tag{13}$$

In order to determine the boundary conditions of the first node ($-k\,\partial T/\partial z|_{z=1} = \dot{q}_{net}$), energy and mass equilibrium in the surface are used. The mass flux pyrolysis gas is not zero like carbon-carbon composite and graphite. There is also density variation as well. So we have [10],

$$\dot{q}_{net} = \dot{q}_{cw}(1 - h_w / h_r)\varphi_{HAL}\,\varphi_{blow} - \varepsilon\,\sigma\,(T_w^4 - T_{ref}^4)$$
$$- \dot{m}_{ab}(h_w - h_u) + \dot{m}_{gw}(h_w - h_{gw}) \quad (14)$$

in which, $\dot{q}_{cw}$ is the heat flux of the cold wall and h_r is the recovery enthalpy calculated by aerodynamic relations. The term ϕ_{Blow} relates to blow resulted from the gas entering the boundary layer and it is calculated by the following equation [10],

$$\varphi_{Blow} = \frac{ln(1 + a_1 B')}{a_1 B'}, \qquad B' = B'_g + B'_C \quad (15)$$

In the above equation, the amount of a_1 for carbon-phenolic equals 1.3, $\phi_{HALL} \geq 1$, is the abrasion coefficient. It states that, there isn't any abrasion. It equals unity. Also emission coefficient ε equals 0.9. The h_u is determined as follows [10],

$$h_u = \int_{Tref}^{T_w} C_p\, dT = C_{¥}(\sqrt{T_w^2 + D^2} - \sqrt{T_{ref}^2 + D^2}) \quad (16)$$

In the above equation, $C_\infty = 2300 J/kg.0k$, $D = 800^o k$, $T_{ref} = 300^o k$. The determination steps of, $\dot{m}_{ab}$, h_w and h_r was specified in the last section.

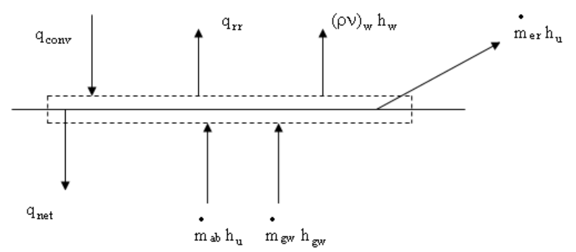

Figure 3. The terms relates to the energy input and output in ablative material surface

3. NUMERICAL SOLUTION

For solving Equation 1, the partial differential terms are substituted by finite difference approximation. Then, according to the non-linear nature of the governing equations, Newton-Raphson method is used with the TDMA algorithm in order to solve the algebraic system of the equations.

4. PRESENTATION OF RESULTS

In order to study the accuracy of Newton-Raphson method in solving the governing equations, first one dimensional non-linear heat transfer equation is solved. The condition is that the material properties are a function of temperature and the results are generalized to more complex problems. In analyzing this problem the specific heat capacity of material and heat conductivity coefficient are considered constant which are assumed as a function of temperature; but, material density is constant. For this problem, heat equation, initial and boundary conditions are considered. Variation of heat conductivity coefficient and specific heat capacity is assumed linear according to temperature and is expressed with the following equations:

$$k(T) = k_1 + \frac{k_2 - k_1}{T_2 - T_1}(T - T_1),$$
$$C_p(T) = C_{p,1} + \frac{C_{p,2} - C_{p,1}}{T_2 - T_1}(T - T_1), \quad (17)$$
$$\alpha = k/(\rho C_p) = k_1/(\rho C_{p,1}) = k_2/(\rho C_{p,2})$$

The analytical solution of this problem is performed using the transformations in [10]. By transferring the energy equation, boundary and initial conditions, similar solution as constant material properties are obtained:

$$\frac{T(z,t) - T_0}{\dot{q}'' L/k} = \frac{\alpha t}{L^2} + \frac{1}{3} - \frac{z}{L} + (\frac{z}{L})^2 -$$
$$\frac{2}{\Pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} exp(-n^2\Pi^2\frac{\alpha t}{L^2}) cos(n\Pi\frac{z}{L}) \quad (18)$$

The parameters used in the solution of the problem are as follows:

$$T_0 = 300k,\ \dot{q}'' = 7.5 \times 10^5\ w/m^2,\ L = 0.01\,m,$$
$$\rho = 8000\,kg/m^3,\ \alpha = k/(\rho C_p) = 2.5 \times 10^{-6}\ m^2/s$$

along with the variations of conductivity coefficient and specific heat capacity in terms of the temperature. In Figure 4, the results obtained with our code are compared with the results of analytical solution at times, t=4s and t=40s. As it can be seen, there is suitable conformity between these two results which is emphasis on the accuracy of Newton-Raphson method in solving non-linear equations. In order to become certain about the program accuracy, the obtained results are compared with the results of Ref. [11]. The considered problem in this reference is a missile that enters to atmosphere from 90km altitude, but the trajectory data are not specified. The cold wall heat flux, the recovery enthalpy and the pressure on ablative material in a specific location of the missile are as below:

$q_{cw,ref} = 1.136J / cm^2 s$, $h_{r,ref} = 2326J / g$,
$p_{ref} = 101325N / m^2 = 1atm$.

The virgin composites density is $1450kg / m^3$ and the charring composites density is $1190kg / m^3$. Its pyrolysis heat is $21630J / gr$ and the heat capacity of pyrolysis gas is $C_{Pg} = 1.6746J / gr.K$. The rate of change of density is calculated by Arrhenius equation (Equation 6) in which, m=2 is considered and the constants A_i and B_i are:

$A_1 = 1.68 \times 10^{-5}$, $A_2 = 2.82$, $A_3 = 3.336 \times 10^4$ [1/ sec],
$B1 = 338$, $B2 = 7049$, $B3 = 15.677$

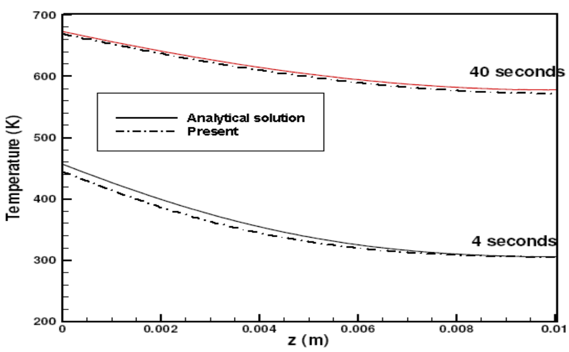

Figure 4. A comparison of temperature distribution with Ref. [10] at t=4s and t=40s

The thermal properties of carbon- phenolic composite can be obtained from handbooks. Comparison of surface temperature profile from Ref. [11] is shown in Figure 5. As it can be seen from the figure, the surface temperature obtained using the method in our paper gives results which are in better agreements with all other previously used methods in average.

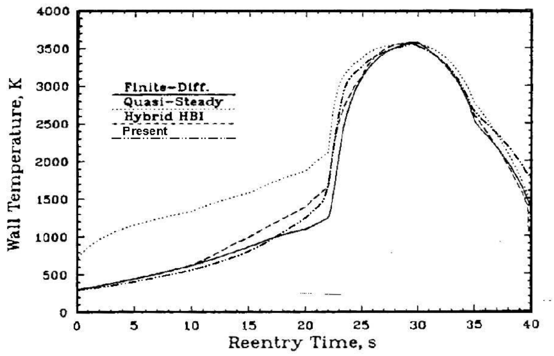

Figure 5. A comparison of the surface temperature profile of carbon-phenolic composite with Ref. [11]

According to Figure 6, the amount of recession in composite surface equals to 3.5 ml. The results from the present code have some differences in this comparison which are because of the nature of the numerical methods used (difference in discretization of the equations, differences in solution methods and the cut-off error in differentiation).

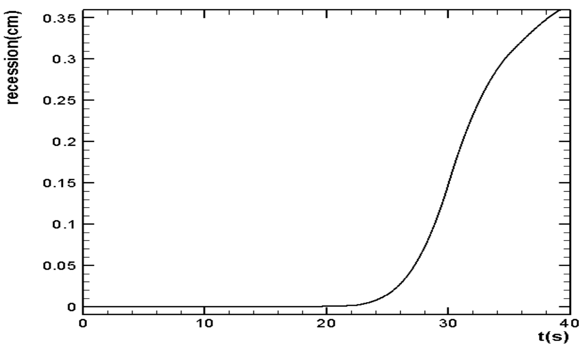

Figure 6. Presenting the profile of the surface recession of carbon- phenolic composite

5. CONCLUSIONS

Using Newton-Raphson method in solving the governing equations is one of the advantages of the presented code. Because this method is easy to understand and can be easily generalized to more complex problems. Besides, this method has a suitable accuracy in solving nonlinear equations because despite the dispersion and low amount of input data, there's a good conformity between the presented results and the results from other references.

6. ACKNOWLEGMENT

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