

NUMERICAL ANALYSIS OF ABLATING THERMAL PROTECTION MATERIALS

Daniela V. F. M. Rey Silva
Helcio R. B. Orlande

Universidade Federal do Rio de Janeiro, Departamento/Programa de Engenharia Mecânica, DEM/PEM/EE/COPPE
Cx. Postal 68503 – 21945-970 – Rio de Janeiro, RJ, Brasil
helcio@serv.com.ufrj.br

Abstract. *This paper deals with the numerical solution of the heat transfer problem in materials typically utilized for the thermal protection of space vehicles. The solution methodology implemented is specially important for the design of thermal protection systems for space vehicles subjected to extremely high heat loads, such as those undergoing atmospheric reentry. We solve here the one-dimensional problem in an ablating material. Thermal decomposition of the material is taken into account. The numerical solution for the problem is obtained with the finite-volume method. Results are presented for a thermal protection material with thermophysical properties found in the literature.*

Keywords. *Ablation, Thermal Protection System, Atmospheric Reentry, Enthalpy Formulation, Finite-volume*

1. Introduction

The Brazilian Space Agency (AEB) has been dedicating efforts to build a satellite that will reentry the atmosphere after staying a couple of days in orbit, in a project led by IAE/CTA. The Thermal Sciences and Heat Engines Group (TERMAQ) of PEM/COPPE/UFRJ is involved in the design of the thermal protection system for such satellite, which shall be constituted of ablating and non-ablating materials. Powerful design tools have been developed within the scope of this project, including the use of improved lumped solutions for the analysis of the thermal protection system (Cotta et al, 2001, Cotta and Ruperti Jr., 2002), as well as for the solution of inverse problems for estimating the thermal properties of ablating materials (Rey Silva and Orlande, 2001) and the heat flux at the surface of the thermal protection system (Oliveira and Orlande, 2001, 2002). However, for the mathematical models used in these works we assumed negligible the thermal decomposition of the ablating material.

In this article, we address the numerical solution of the heat transfer problem in thermal protection systems composed of ablating materials, which may undergo thermal decomposition. Ablation is an effective and reliable method, largely used in the aerospace industry, in order to protect the space vehicle and its payload from the high heat fluxes resulting from aerodynamic heating (Swann and Pittman, 1962, Moyer and Rindal, 1967, Torre et al, 1998, Hogger and Gerrenkens, 1982, Leung et al, 1996, 1998.a,b, Chen and Milos, 1999, Kanevec et al, 1999, Loures and Moraes, 2000, 2001, Chen and Milos, 2001, Zapparoli et al, 2001). In the ablation process, the high heat fluxes absorbed by the thermal protection system result on the consumption of the protection material, due to several physical and chemical phenomena taking place. In general words, this process involves phase transitions (melting and vaporization), as well as the thermal decomposition of the virgin material into a charred material.

A one-dimensional formulation is used in this work. The numerical solution for the heat transfer problem in the thermal protection system, involving ablation as well as thermal decomposition of the protection material, is obtained by using the finite-volume method (Maliska, 1995). Properties for nylon phenolic resin (Moyer and Rindal, 1967) are used to obtain the solution of the problem. This solution shows that the temperature increase in the inner regions of the thermal protection system is retarded because of the thermal degradation of the material.

2. Physical problem and Mathematical Formulation

The physical problem under picture in this paper consists of a one-dimensional slab of thickness L , as depicted in Fig. (1). The slab is initially at the uniform temperature T_i , which is lower than the temperature of ablation T_{ab} , and sufficiently low so that thermal decomposition effects are negligible. The surface of the slab at $x = L$ is heated, while the other surface at $x = 0$ is kept insulated. As the slab is heated, thermal decomposition effects, which are strongly temperature-dependent, become significant and the original virgin material degrades into a charred material. Furthermore, eventually the temperature of the heated surface reaches the temperature of ablation; the charred material is then removed and a moving surface problem is established. The time-dependent position of the ablating surface is denoted by $b(t)$.

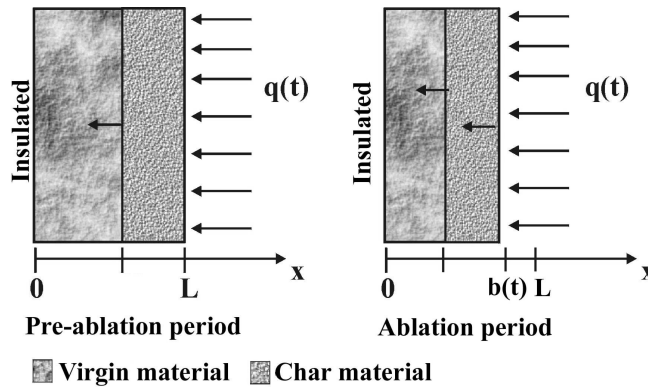


Figure 1. Geometry.

The differential equation governing the conservation of energy in the slab can be written as (Moyer and Rindal, 1967):

$$\frac{\partial}{\partial t}(\rho h) = \frac{\partial}{\partial x} \left(k^* \frac{\partial T}{\partial x} \right) - \frac{\partial}{\partial x} \left(\frac{\dot{m}_g}{A} h_g \right) \quad \text{in} \quad 0 < x < b(t), \quad \text{for} \quad t > 0 \quad (1)$$

where ρ and k^* denote the density and the thermal conductivity of the protection material, respectively; h and h_g are the specific enthalpies of the protection material and of the gases resulting from the thermal decomposition, respectively; \dot{m}_g is the mass flux of gases resulting from the thermal decomposition; and A is the cross section for the gas flow. Note that thermal equilibrium is assumed between the gas and the solid material.

For the numerical solution of the mathematical problem under picture, it is convenient to use a transformation of the independent variables, so that the domain remains fixed. Thus, we define the new independent variables as:

$$X^* = \frac{x}{b(t)}, \quad t^* = t \quad (2.a,b)$$

$$\frac{\partial}{\partial x} = \frac{1}{b(t)} \frac{\partial}{\partial X^*}, \quad \frac{\partial}{\partial t^*} = \frac{\partial}{\partial t} \quad (2.c,d)$$

where $X^* = 0$ for $x = 0$ and $X^* = 1$ for $x = b(t)$.

In terms of the transformed variables, the energy conservation equation given by Eq. (1), becomes

$$\frac{\partial}{\partial t}(\rho h) = \frac{1}{b^2(t)} \frac{\partial}{\partial X^*} \left(k^* \frac{\partial T}{\partial X^*} \right) + \frac{1}{b(t)} \frac{\partial}{\partial X^*} \left(\frac{\dot{m}_g}{A} h_g \right) - X^* \frac{\dot{b}(t)}{b(t)} \frac{\partial}{\partial X^*}(\rho h) \quad (3)$$

where $\dot{b}(t)$ is the velocity of the moving heated boundary.

The density and the specific enthalpy of the slab are volume-averaged, where we introduce in the formulation a local transformation fraction denoted by ε_v . For the virgin material $\varepsilon_v = 1$, while for the charred material $\varepsilon_v = 0$. Therefore, we can write:

$$\rho = \varepsilon_v \rho_v + (1 - \varepsilon_v) \rho_c \quad (4.a)$$

$$\rho h = \varepsilon_v \rho_v h_v + (1 - \varepsilon_v) \rho_c h_c \quad (4.b)$$

where the subscripts v and c refer to the virgin and charred materials, respectively.

The specific enthalpies for the virgin and charred materials are respectively obtained from:

$$h_v = h_v^0 + \int_0^{T_{ref}} c_{Pv} dt \quad (5.a)$$

$$h_c = h_c^0 + \int_0^{T_{ref}} c_{Pc} dt \quad (5.b)$$

By differentiating Eq. (4.a) with respect to time we can write:

$$\frac{\partial \varepsilon_v}{\partial t} = \frac{1}{\rho_v - \rho_c} \frac{\partial \rho}{\partial t} \quad (6.a)$$

By differentiating Eq. (4.b) with respect to time and using Eqs. (4.a), (5.a) and (5.b), we can write:

$$\frac{\partial}{\partial t}(\rho h) = \bar{h} \left(\frac{\partial \rho}{\partial t} \right) + \rho c_p \left(\frac{\partial T}{\partial t} \right) \quad (6.b)$$

where

$$\rho c_p = \rho_v \varepsilon_v c_{p_v} + (1 - \varepsilon_v) \rho_c c_{p_c} \quad (6.c)$$

and

$$\bar{h} = \frac{\rho_v h_v - \rho_c h_c}{\rho_v - \rho_c} \quad (6.d)$$

The substitution of Eq. (6.b) into Eq. (3) yields the following expression for the energy conservation in the slab, written in conservative form and in terms of temperature and density change rates:

$$\rho c_p \left(\frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial X^*} \left(\frac{k^*}{b^2(t)} \frac{\partial T}{\partial X^*} - \frac{1}{b(t)} \frac{\dot{m}_g}{A} h_g + X^* \frac{\dot{b}(t)}{b(t)} \rho h \right) - \bar{h} \left(\frac{\partial \rho}{\partial t} \right) - \frac{\dot{b}(t)}{b(t)} (\rho h) \quad (7)$$

After deriving the energy conservation equation in the form given by Eq. (7), we can write the following two problems for the pre-ablation and ablation periods, respectively:

Pre-Ablation Period ($0 < t \leq t_{ab}$):

$$\rho c_p \left(\frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial X^*} \left(\frac{k^*}{b^2(t)} \frac{\partial T}{\partial X^*} - \frac{1}{b(t)} \frac{\dot{m}_g}{A} h_g \right) - \bar{h} \left(\frac{\partial \rho}{\partial t} \right) \quad \text{in } 0 < X^* < 1, \quad \text{for } 0 < t \leq t_{ab} \quad (8.a)$$

$$\frac{\partial T}{\partial X^*} = 0 \quad \text{at } X^* = 0, \quad \text{for } 0 < t \leq t_{ab} \quad (8.b)$$

$$\frac{k^*}{b(t)} \frac{\partial T}{\partial X^*} = q(t) \quad \text{at } X^* = 1, \quad \text{for } 0 < t \leq t_{ab} \quad (8.c)$$

$$T = T_i \quad \text{for } t = 0, \quad \text{in } 0 < X^* < 1 \quad (8.d)$$

where t_{ab} is the time required for the temperature of the heated surface at $X^* = 1$ to reach the temperature of ablation T_{ab} . We note that $b(t) = L$ and $\dot{b} = 0$ for $0 < t \leq t_{ab}$.

Ablation Period ($t > t_{ab}$)

$$\rho c_p \left(\frac{\partial T}{\partial t} \right) = \frac{\partial}{\partial X^*} \left(\frac{k^*}{b^2(t)} \frac{\partial T}{\partial X^*} - \frac{1}{b(t)} \frac{\dot{m}_g}{A} h_g + X^* \frac{\dot{b}(t)}{b(t)} \rho h \right) - \bar{h} \left(\frac{\partial \rho}{\partial t} \right) - \frac{\dot{b}(t)}{b(t)} (\rho h) \quad \text{in } 0 < X^* < 1, \quad \text{for } t > t_{ab} \quad (9.a)$$

$$\frac{\partial T}{\partial X^*} = 0 \quad \text{at } X^* = 0, \quad \text{for } t > t_{ab} \quad (9.b)$$

$$T = T_{ab} \quad \text{at } X^* = 1, \quad \text{for } t > t_{ab} \quad (9.c)$$

$$T = T_i(X^*) \quad \text{for } t = t_{ab}, \quad \text{in } 0 < X^* < 1 \quad (9.d)$$

The heated surface position and velocity, $b(t)$ and $\dot{b}(t)$, respectively, are obtained from the energy balance at the heated surface, that is,

$$\rho H_{ab} \frac{db(t)}{dt} = -q(t) + \frac{k^*}{b(t)} \frac{\partial T(b(t), t)}{\partial X^*} \quad \text{for} \quad t > t_{ab} \quad (9.e)$$

with

$$b(t_{ab}) = L \quad (9.f)$$

where H_{ab} is the heat of ablation.

The flow rate of gases resulting from the thermal decomposition, \dot{m}_g , can be obtained by taking into account mass conservation for the problem, that is,

$$\left(\frac{\partial \dot{m}_g}{\partial x} \right) = A \left(\frac{\partial \rho}{\partial t} \right) \quad (10)$$

where A is the cross section for the gas flow.

The gas flow rate resulting from the thermal decomposition at the position x in the slab is obtained as

$$\frac{\dot{m}_g}{A} = \int_{x'=0}^x \left(\frac{\partial \rho}{\partial t} \right) dx' \quad (11)$$

or, in terms of the transformed independent variable, we obtain,

$$\frac{\dot{m}_g}{A} = \int_{X'=0}^{X^*} \frac{1}{b(t)} \left(\frac{\partial \rho}{\partial t} \right) dX' \quad (12)$$

The material density ρ and the density change rate $\partial \rho / \partial t$ (this one required for the calculation of the gas flow rate with Eq. (12)) can be obtained by taking into account the virgin material constituents. The virgin material is considered in this paper to be composed of three constituents, named generally as A, B and C. Materials A and B are supposed to be the constituents of the virgin material matrix, while material C is supposed to be the reinforcement (dispersed medium). Therefore, the density of the composite is given by:

$$\rho = \Gamma(\rho_A + \rho_B) + (1 - \Gamma)\rho_C \quad (13.a)$$

where the subscripts A, B and C refer to materials A, B and C, respectively, $(\rho_A + \rho_B)$ is the density of the matrix, ρ_C is the density of the reinforcement, and Γ is the volume fraction of the matrix in the virgin material. Thermal conductivity and specific heat are computed as:

$$k^* = \varepsilon_v k_v^* + (1 - \varepsilon_v) k_c^* \quad (13.b)$$

$$c_p = \varepsilon_v c_{p_v} + (1 - \varepsilon_v) c_{p_c} \quad (13.c)$$

The rate of change of density, resulting from the thermal decomposition, is therefore given by:

$$\left(\frac{\partial \rho}{\partial t} \right) = \Gamma \left(\frac{\partial \rho_A}{\partial t} + \frac{\partial \rho_B}{\partial t} \right) + (1 - \Gamma) \left(\frac{\partial \rho_C}{\partial t} \right) \quad (14)$$

The rate of decomposition of each constituent is assumed here to be given by an Arrhenius equation in the form:

$$\left(\frac{\partial \rho_i}{\partial t} \right) = -\kappa_i \exp\left(\frac{-E_i}{RT}\right) \rho_{0i} \left(\frac{\rho_i - \rho_{ri}}{\rho_{0i}} \right)^{m_i} \quad \text{for} \quad i = A, B \text{ or } C \quad (15)$$

In Eq. (15), ρ_{ri} denotes the residual density of material i , when the thermal decomposition is complete.

We note that Eqs. (14) and (15) also need to be written in terms of the transformed independent variables, that is, the density rate of change is given by:

$$\left(\frac{\partial \rho}{\partial t}\right) = \left(\frac{\partial \rho}{\partial t}\right) + X^* \frac{\dot{b}(t)}{b(t)} \left(\frac{\partial \rho}{\partial X^*}\right) \quad (16)$$

3. Method of Solution

In this work, the problems given by Eqs. (8) and (9) were numerically solved with the finite-volume method (Maliska, 1995) for the pre-ablation and ablation periods, respectively. A fully implicit discretization was used to advance the solution in time and the WUDS interpolation function was used in the spatial discretization. However, note the non-linear character of the problem, which involves temperature- and phase-dependent properties, as well as a moving boundary. Such a non-linear character requires an iterative procedure for the solution of each problem, as described next.

For the solution of the problem for the pre-ablation period, given by Eqs. (8.a-d), Eq. (15) for $i = A, B$ and C needs to be solved in order to compute the density change rate for each of the material constituents. This equation is integrated for each finite-volume, by using the temperature of the previous time-step as a first approximation, with the subroutine IVPAG of the IMSL. With the density change rate for each constituent, the density change rate for the material can be computed with Eqs. (14) and (16). Thus, the mass flow of thermal decomposition gases can be computed with Eq. (12) and the transformation fraction with the integration of Eq. (6.a). The physical properties are computed with Eqs. (5) and (13.b,c), by also using the temperature of the previous time-step as a first approximation and the transformation fraction just calculated. All quantities required to advance the solution of Eqs. (8) in time with the discretized equations of the finite-volume method are now available. The temperature values computed with the finite-volume method for all volumes, as described above, are compared with those initially used to compute the physical properties and density change rates. If convergence is not observed, a new iteration is performed because of the non-linear character of the problem.

The solution of the problem for the ablation period, given by Eqs. (9.a-d) is obtained with a procedure similar to the one described above, but it also requires the integration of Eq. (9.e). The integration of this equation is also performed with the subroutine IVPAG of the IMSL, by using the quantities computed for that iteration.

4. Results

Before proceeding to the analysis of cases involving ablation of materials with significant thermal decomposition, let us examine first, as a reference-case, one involving a material with negligible thermal decomposition. We examine here the solution for teflon, for which thermal decomposition is considered negligible (Blackwell, 1988), because we have results obtained with another computer code that does not take into account the thermal decomposition of the material (Rey Silva and Orlande, 2001). The thermophysical properties used for teflon are presented in Tab. (1) (Blackwell, 1988). In order to simulate a material with negligible thermal decomposition by using the computer code developed in this work, we used in Eq. (15) a very large value for the activation energy E_i and considered identical the properties of all three constituents.

Figures (2) to (4) present a comparison of the results obtained with the computer code developed in this work (solid lines) with those obtained with the computer code developed by Rey Silva and Orlande (2001) (symbols), for a slab with thickness $L = 0.01$ m. Both solutions were obtained by using 60 control volumes to discretize the transformed region and a time-step of 0.002 s to advance the solution in time. The results shown in Figs. 2 to 4 were obtained for constant applied heat flux at the surface $X^* = 1$ of $q(t) = 10.00$ kW/m², $q(t) = 20.01$ kW/m² and $q(t) = 29.42$ kW/m², respectively. We can notice in Figs. 2 to 4 an excellent agreement of the results obtained here with those obtained with the negligible thermal decomposition model of Rey Silva and Orlande (2001), for all three different magnitudes of applied heat flux.

Table 1. Thermal properties for Teflon (Blackwell, 1988).

Properties	Symbol	Value	Unit (S.I.)
Specific heat	c_p	1256	J/kg °C
Thermal conductivity	k^*	0.22	W/m °C
Density	ρ	1922	kg/m ³
Temperature of ablation	T_{ab}	560	°C
Heat of ablation	H_{ab}	2.326×10^6	J/kg

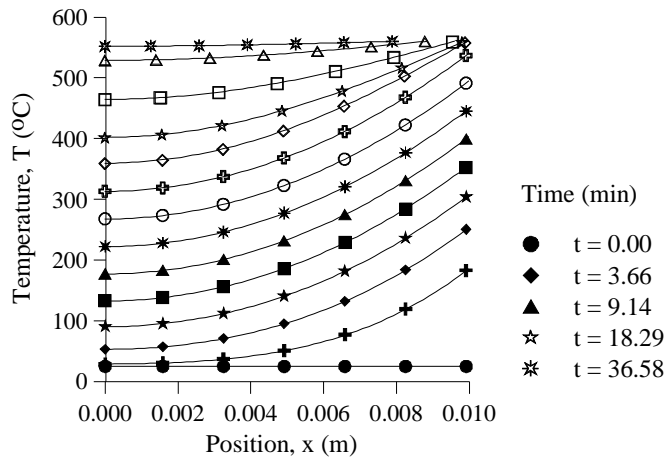


Figure 2. Temperature field with heat flux $q(t) = 10.00 \text{ kW/m}^2$.

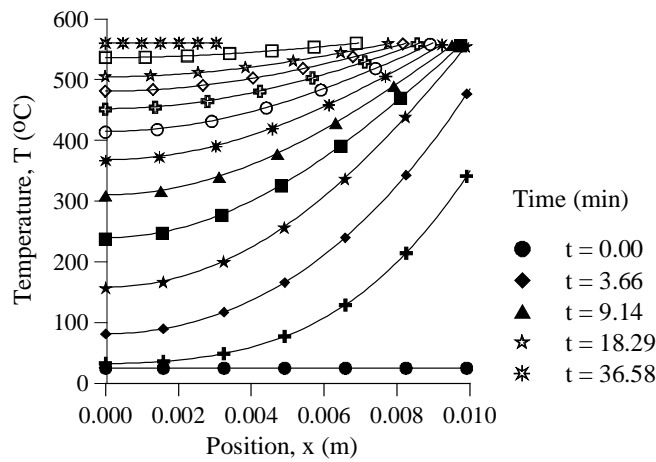


Figure 3. Temperature field with heat flux $q(t) = 20.01 \text{ kW/m}^2$.

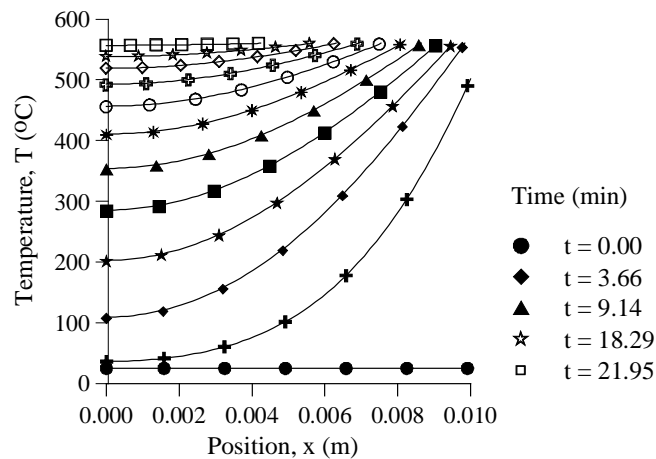


Figure 4. Temperature field with heat flux $q(t) = 29.42 \text{ kW/m}^2$.

After validating the computer code developed in this work by using a limiting case where thermal decomposition effects are negligible, as described above, let us now consider a case involving the heating of a low-density nylon phenolic resin, for which thermal properties were found in the literature (Moyer and Rindal, 1967). Tables (2) to (6) summarize the thermal properties used in this work. In addition, the volume fraction of the matrix in the virgin material is considered to be 0.5, the heat and the temperature of ablation are taken as $H_{ab} = 2.326 \times 10^6 \text{ J/kg}$ (TPSX Material Information) and $T_{ab} = 2505 \text{ }^\circ\text{C}$ (Moyer and Rindal, 1967).

The initial thickness of the thermal protection material is supposed to be $L = 0.005 \text{ m}$. The slab is considered to be initially at the uniform temperature $T_i = 25 \text{ }^\circ\text{C}$ and the applied heat flux is taken as $q(t) = 1 \times 10^5 \text{ W/m}^2$.

For the numerical solution of the problem under picture, the transformed spatial domain was discretized with 1000 volumes and a time-step of 0.005 s was used to advance the solution in time. Such number of volumes and time-step were chosen by using a grid-convergence analysis.

Table 2. Nylon phenolic resin – decomposition kinetic data (Moyer and Rindal, 1967).

Component	ρ_{0i} (kg/m ³)	ρ_{ri} (kg/m ³)	κ_i (s ⁻¹)	E_{a_i}/R (°C)	m_i
A	85.271	0.000	1.40×10^4	8556	3
B	255.162	243.185	4.48×10^9	20222	3
C	924.310	0.000	1.85×10^{13}	26500	1

Table 3. Nylon phenolic resin – enthalpies of formation (reference temperature 24.4 °C) (Moyer and Rindal, 1967).

Material	h^o (J/kg)
Virgin material	0
Char material	0
Pyrolysis gas	-2598142

Table 4. Nylon phenolic resin – virgin material thermal properties (Moyer and Rindal, 1967).

T (°C)	c_p (J/kg °C)	k (W/m °C)
-17.59	1214.11	7.85×10^{-2}
93.52	1842.10	8.35×10^{-2}
149.07	2093.30	8.54×10^{-2}
204.63	2260.76	8.72×10^{-2}
260.18	2302.63	8.85×10^{-2}
426.85	2302.63	9.66×10^{-2}
3060.18	2302.63	9.66×10^{-2}

Table 5. Nylon phenolic resin – charred material thermal properties (Moyer and Rindal, 1967).

T (°C)	c_p (J/kg °C)	k (W/m °C)
4.63	418.66	6.23×10^{-2}
537.96	1632.77	1.12
815.74	2051.43	1.53
1093.52	2093.30	1.81
1649.07	2093.30	2.49
2204.63	2093.30	3.49
2371.29	2093.30	3.99
2782.41	2093.30	4.67

Table 6. Nylon phenolic resin – enthalpy of the gas resulting from the thermal decomposition (Moyer and Rindal, 1967).

T (°C)	h (J/kg)
226.85	-5131156
726.85	-1986404
1115.74	1067634
1226.85	2374846
1393.52	4575242
1726.85	6412782
2226.85	8934166
2726.85	13607100

The temperature profiles in the slab are shown in Fig. (5), for different times, up to a moment next to the beginning of ablation. It can be noticed in this figure the thermal decomposition front moving into the slab up to about 7.0 s. Note that the increase of the temperature for the inner regions of the slab is retarded because of the thermal decomposition,

which absorbs energy in order to degrade the original virgin material into a charred material and gases. The convection of the gases generated by the thermal decomposition through the solid matrix also helps to retard the temperature increase in the slab. After the thermal degradation is complete, the temperature in the slab increases very fast. The temperature of the surface reaches the temperature of ablation around 78.0 s. The material is then removed and a moving boundary is established, as described above in this paper.

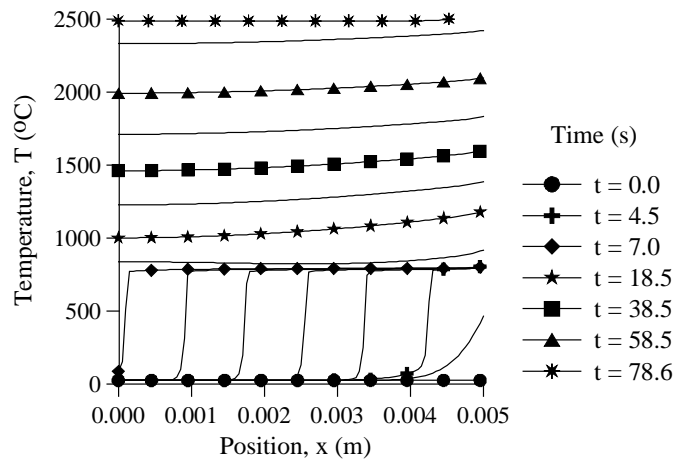


Figure 5. Temperature profiles in the slab for different times.

Figure (6) illustrates the density variation in the slab for different positions. Note that, for the heated surface at $x = 0.005$ m, thermal decomposition effects become significant around 3 s, when the density starts to change from the value of the original virgin material to that of the charred material. The thermal decomposition is complete at this position at about 4.2 s. It is interesting to note that, for the other inner positions shown in Fig. (6), the thermal decomposition takes place almost instantaneously. Such a behavior can also be noticed in Fig. (5), which shows the thermal decomposition front moving towards the inner regions of the slab.

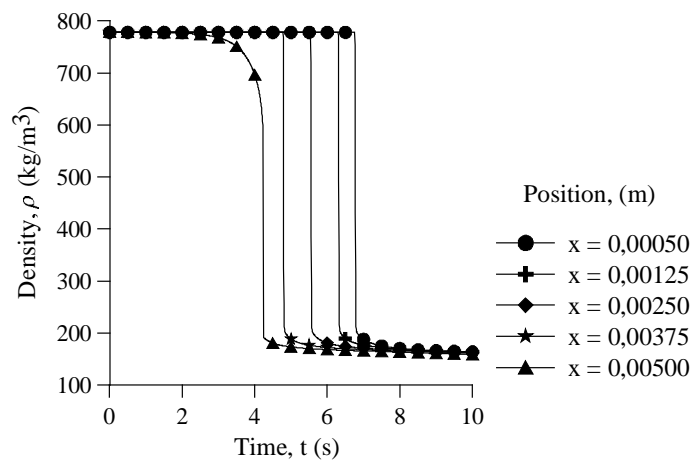


Figure 6. Density variation for different positions.

Figure (7) presents the variation of the mass flow rate of gas per unit area at different positions inside the slab. Notice the sudden increase in such a rate around 4.0 s at the position 0.005 m, which corresponds to the heated surface of the slab. Such an increase is the result of the beginning of the thermal decomposition in the slab, as observed above in Figs. 5 and 6. The mass flow rate at inner positions undergoes a similar increase for later times, when the thermal decomposition front passes through the specific position. It is interesting to note in Fig. (7) that the mass flow rate becomes null around 7.0 s, when the thermal decomposition of the slab is complete.

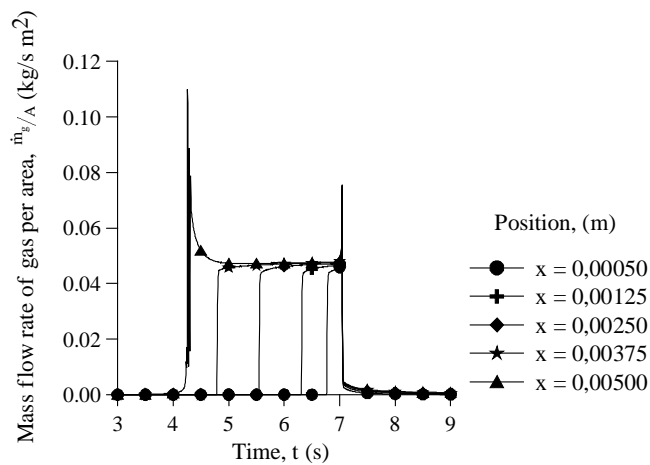


Figure 8. Mass flow rate of gas per unit area

5. Conclusions

In this paper we presented the numerical solution for the one-dimensional ablation problem in materials that undergo significant thermal decomposition. The computer code developed was validated by using a limiting case, involving ablation of teflon, with negligible thermal decomposition.

Numerical results were obtained for a material typical of thermal protection systems of space vehicles undergoing atmospheric reentry, involving a low-density nylon phenolic resin, with significant thermal decomposition effects, for which thermophysical properties were found in the literature. The results obtained show that the increase of temperature in the inner regions of the thermal protection system is retarded because of the thermal degradation of the material.

6. Acknowledgements

This work was sponsored by AEB (Brazilian Space Agency). Partial support provided by CNPq, CAPES, PRONEX and FAPERJ is also greatly appreciated. The authors would like to acknowledge useful discussions with Prof. Renato M. Cotta (PEM/COPPE/UFRJ) as well as with Dr. Luis Loures and Dr. José Bezerra (IAE/CTA).

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