A FINITE VOLUME MODEL OF CHARRING AND ABLATION
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ABSTRACT
The one dimensional (axisymmetric) charring ablation problem has been considered. Finite volume is used for spatial discretisation. The time marching is fully implicit. The mesh is stationary for the charring case. The charring front has a discontinuity in the heat flux. During ablation, the cell adjacent to the ablation front undergoes variation in volume. The Sherman-Morrison method is used to obtain the solution using the tridiagonal method, as the matrix is very close to being tridiagonal. This results in an efficient algorithm.

KEYWORDS: charring, ablation, finite volume

1. INTRODUCTION
The problem of charring and ablation has been well analysed. One of the earlier works was by Moyer and Rindal [1]. They developed a one-dimensional code which solved the energy equation with pyrolysis gas effects. The code was implicit in time and took properties at the previous time step. Later, Keyhani, Polehn and Krishnan [2], [3] developed one dimensional finite difference thermal response codes and also investigated the coupling of the thermal energy equation with the gas equation. Their finding was that the coupling does not significantly affect the temperature field. Blackwell [4], Blackwell and Hogan [5] developed a control volume finite element method for solving ablation problems on translating and nodedropping grids with a fully implicit time integrator. A contracting grid scheme for one-dimensional ablation was presented by Hogan et. al [6] in which the relative size of grid cells and the total number of cells is fixed throughout the problem, and each node translates at a fraction of the surface recession rate. Amar et. al. [7] have analysed the problem with a moving mesh, using finite volume. Lin [8] has looked at the quasi steady state solutions. Chen and Milos [9], [10], [11] have done one, two, and three-dimensional ablation studies with applications. The objective of the current work is to model the charring and ablation processes using a fixed mesh control volume and develop an efficient algorithm for the solution of the same. The algorithm is a generic one for moving isothermal heat sink fronts. In the present work, the charring and ablation fronts are assumed to be isothermal and infinitely thin. The flux has a discontinuity across the charring front. The finite volume method is formulated to take care of the discontinuity properly. During ablation, only the cell adjacent to the ablating boundary gets deformed. When the cell becomes sufficiently small, it is merged with the adjacent one. The time integration is fully implicit. The Jacobian is close to tridiagonal. The Sherman-Morrison formula is used to solve the linear system as two tridiagonal ones. The computational model and algorithm are presented in Section 2. The uncharred, charred and the ablating cases are considered. Section 3 deals with the results, while the discussion of results is carried out in
Section 4. The conclusions are given in Section 5.

2. COMPUTATIONAL MODEL AND ALGORITHM

The computational domain is initially divided into \( N \) uniform cells. The initial node is \( x_0 \) and \( x_N \) the last one. The finite volume cell \( i \) is between nodes \( x_{i-1} \) and \( x_i \). Heat flux is applied at \( x_N \). The boundary at \( x_0 \) is assumed to be isothermal, at the initial temperature itself. The integration in time is fully implicit with a constant step size \( \Delta t \).

2.1 Uncharred Case

The conventional energy balance is given as

\[
\frac{V(\rho \overline{c_p} T)^{n+\frac{1}{2}} - (\rho \overline{c_p} T)^{n}}{\Delta t} = \sum A_i q_i^{n+1},
\]

where \( q_i \) is the inward flux and \( A_i \) the corresponding face area. The superscripts \( n \) and \( n+1 \) are used to denote the time steps. The properties have been taken implicitly (at time step \( n+1 \)).

For the cartesian case, the face area \( A \) is unity, while for the axisymmetric case \( A_i = 2\pi x_i \), where \( x_i \) is the co-ordinate of the face. Thus, the same formulation can be used for both Cartesian and axisymmetric cases, with a different expression for the face area.

2.2 Modeling of Charring

It is assumed that the charring front is a line(with zero thickness) and the flux has a jump across the front. The front equation is

\[
\rho h_{ch} v_{ch} = \left[ k \frac{\partial T}{\partial x} \right]_{x = x_{ch}},
\]

where \( v_{ch} \) is the velocity of the charring front and \( h_{ch} \) the heat of charring. The charring front is assumed to be isothermal(at \( T_c \)) and the charring front equation becomes the one for the determination of charring velocity. It is assumed that if any gases are released during the charring process, they have a very low residence time in the solid and thus escape fast. Hence, the gas energy equation is not considered. As shown in figure 1, if the front is in between the cell centres of two cells \( i \) and \( i+1 \), then the discretised fluxes on both sides of the front would be given as

\[
q_{left}^{n+1} = k \frac{T_{ch} - T_i}{x_{ch} - x_i},
\]

\[
q_{right}^{n+1} = k \frac{T_{ch} - T_{i+1}}{x_{ch} - x_{i+1}},
\]

where \( T_{ch} \) is the temperature of the charring front.

The front energy balance then becomes

\[
\rho h_{ch} v_{ch} = q_{left}^{n+1} - q_{right}^{n+1}
\]

At the new time step, the front equation becomes

\[
\rho h_{ch} v_{ch}^{n+1} = q_{left}^{n+1} - q_{right}^{n+1}
\]

Inserting the expression for \( x_{ch}^{n+1} \) as\( x_{ch}^{n+1} = v_{ch}^{n+1} \Delta t \), where \( x_{ch} \) is the front position at the time step \( n \), the expressions for \( q_{left}^{n+1} \) and \( q_{right}^{n+1} \) are

\[
q_{left}^{n+1} = k \frac{T_{ch} - T_{i-1}}{x_{ch} - x_{i-1}},
\]

\[
q_{right}^{n+1} = k \frac{T_{ch} - T_{i+1}}{x_{ch} - x_{i+1}}
\]

The superscript \( n+1 \) has been dropped for \( v_{ch}^{n+1} \).

![Figure 1. Charring Front and Adjacent Cells](image-url)
For the cell energy balance, when the charring front is in the cell or in the neighbouring one, the flux is determined from the temperature gradient applying at the edge of the cell. For example, if the front is in between cells $i$ and $i+1$ and is in cell $i+1$, then the flux transferred from $i$ to $i+1$ would be

$$q_{i,i+1} = k \frac{T_{ch} - T_i}{x_{ch} - x_i}.$$  \hspace{1cm} (9)

As in the case of front equation, the flux at time step $n+1$ is $\frac{x_{ch}^{n+1}}{x_{ch} - x_i}$ as

$$q_{i,i+1}^{n+1} = k \frac{T_{ch} - T_i^{n+1}}{x_{ch} - x_i^{n+1}}.$$  \hspace{1cm} (10)

When the front enters cell $i$, then the flux expression becomes

$$q_{i,i+1} = k \frac{T_{ch} - T_i}{x_{ch} - x_i}.$$  \hspace{1cm} (11)

In addition, the energy absorbed by the charring front will be added as a sink term in the energy equation of the cell containing the charring front. The cell energy equation for that cell becomes

$$\rho_c V \frac{T^{n+1} - T^n}{\delta t} = \sum A_j q_j^{n+1} - \rho v_{ch} A_{ch} h_{ch}.$$  \hspace{1cm} (12)

where $A_{ch}$ is the face area of the charring front. In this case, the additional unknown is the charring velocity $v_{ch}$ and the front energy equation is the additional equation, leading to a $N + 1$ system. The system becomes nonlinear because of the presence of $v_{ch}$ in the face flux in the vicinity of the charring front.

### 2.3 Ablation

Ablation commences when the boundary temperature exceeds a critical value $T_{ab}$. The volume of the final cell decreases continuously. The energy balance for the ablating cell is

$$\rho c V \frac{T^{n+1} - T^n}{\delta t} = \sum A_i q_i^{n+1} - \rho v_{ab} A_{ab} h_{ab}.$$  \hspace{1cm} (13)

The expression for $I^{n+1}$ is

$$I^{n+1} = I^n - v_{ch} A_{ch} \delta t.$$  \hspace{1cm} (14)

For the ablation front, the energy balance becomes,

$$q_{ln} = \rho v_{ab} + k \frac{\partial T}{\partial x}.$$  \hspace{1cm} (15)

When the volume of the ablating cell becomes less than 30\% of the adjacent one, the two cells are merged. The temperature becomes a weighted average of the two merged cells.

### 2.4 Solution Methodology

The equations are nonlinear due to the variation of properties as well as charring and ablation processes. The equations are re-arranged so that it is in the same order as they occur physically. For example, when the charring front is in between cell-centers $j$ and $j+1$, the following order is adopted. The equation for the first $j$ cells is unaffected. The charring-front equation becomes the $j+1$th equation. Following this, the equation for cell $j+1$ becomes the $j+2$th equation and so on.

The ablation front, being at the end is the $i_{ab}+2$th equation. Here $i_{ab}$ is the index of the last cell. The equations are solved using the Newton method, with an almost exact Jacobian. The only terms omitted in the Jacobian are those corresponding to variation of properties with temperature. That is, the derivative (corresponding to variation of properties) is not included in the Jacobian. The properties are taken as corresponding to the temperatures of the previous iteration. Thus, on convergence, in a particular time step, the properties are also implicit.

It was observed that this almost exact Jacobian is essential for a stable solution. Further approximations resulted in the system not converging at certain time steps. Among the other (unsuccessful) approximations tried was
using the $v_{ch}$ from previous time steps for the cell energy equations and using the front energy equations to calculate $v_{ch}$ and $v_{ab}$ using the known temperature field. The Jacobian thus obtained, is almost tridiagonal. There is only one term in addition to the tridiagonal part. This can be handled using the Sherman-Morrison formula (cf. Press et. al. [12]). The system is split into two tridiagonal systems.

The system is of size $N$ in the uncharred case, becomes $N + 1$ after charring. Once ablation commences, it is of $N + 2$ initially and decreases as the last cell gets merged. The algorithm is of first order in time. The spatial accuracy is of second order initially, but the presence of charring and ablation fronts make it first order later. Thus, the main features of the algorithm are that it uses a finite control volume with a fixed mesh and also allows discontinuity in flux across the front. This leads to a coupled nonlinear system for the cell energy equations and the front energy equations. The Jacobian(for the Newton iterations), being almost tridiagonal can be solved efficiently, using the Sherman-Morrison formula. The time marching is fully implicit.

### 3. PROBLEM DESCRIPTION

The case studied here is an axisymmetric case, with the first node $x_0 = 1$ m and the last node $x_N = 1.025$ m. The thickness taken(25 mm) is very small, because the time period $T$ is 100s. In this time, for the chosen heat flux, the penetration depth is less than 25mm, for the chosen material. Hence, it is better to take a smaller thickness, so that better refinement of the region can be made. Charring starts when the heated wall reaches 850K, while ablation commences at 2200K. The charring front is isothermal at 850K while the ablation front is at 2200k. The initial temperature in the domain is 400K. The left boundary $x_0$ is adiabatic, while the heat flux boundary at $x_N$ is given as $q = 80000t$ if $t <= 56$ $q = 4.5E06$ otherwise. That is, the heat flux is linearly increasing till it reaches the value of 4.5E06 and remains constant after that.

#### 3.1 Property Variation

The properties chosen were corresponding to that of Carbon Phenolic.

The density is taken as $\rho=1000 \frac{kg}{m^3}$. The heat of charring($h_{ch}$) is taken as $1.1E07 \frac{J}{kg}$, while the heat of ablation($h_{ab}$) is taken as $4.5E07 \frac{J}{kg}$.

Unless otherwise indicated, all properties and results are in SI units. The other properties at selected temperatures are given in Table 1.

<table>
<thead>
<tr>
<th>T(K)</th>
<th>$\frac{k (\frac{W}{mK})}{c (M/kgK)}$</th>
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<tr>
<td>300</td>
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</tr>
<tr>
<td>600</td>
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<td>3.460</td>
</tr>
<tr>
<td>2200</td>
<td>3.764</td>
</tr>
</tbody>
</table>

#### 4. RESULTS AND DISCUSSION

The results are presented as temperature history of a particular point and the temperature profile at an end. In addition, the velocity of charring and
ablation fronts, along with the location of these fronts is also presented.

### 4.1 Variation with Grid Size and Time Step

The results are presented for $N = 200$, 400 and 800. The time step $\Delta t$ is also reduced along with $\Delta x$. The value of $\Delta t$ is 0.04s for $N=400$, 0.02 for $N=200$ and 0.01 for $N=400$.

The temperature history at the $0.8N$th cell is presented in figure 2. It can be seen that the profiles become grid independent.

![Figure 2. Temperature History at M = 0.8N](image)

The temperature profile at $t = 100s$ is given in figure 3. The profiles with different $N$ are converging. Similarly, the charring velocity $v_{ch}$ and the charring front position $x_{ch}$ are shown, as a function of time.

![Figure 3. Temperature Profile at t = 100](image)

The charring velocity has oscillatory behaviour for small $N$, but these reduce with increasing $N$. This is probably due to the discontinuity in the heat flux. The charring front position also indicates that there is grid independence and the effect of fluctuations in $v_{ch}$ are not that significant.

![Figure 4. Velocity of Charring Front](image)

![Figure 5. Location of Charring Front](image)

![Figure 6. Velocity of Ablation Front](image)
The behaviour of $v_{ab}$ is also similar. The oscillations are reducing with increasing N. Again, the ablation front $x_{ab}$ shows mesh independence. These oscillations are probably due to the cell merging.

4.2 Comparison with Constant Heat Flux Case

The results are obtained for the case of constant heat flux and compared against the earlier case. The value of the flux is chosen as the average of the ramp case. The average value is 3.234E06 $W/m^2$.

The charring front comparison is given in Figure 8.

As one can see, the charring front advances faster in the constant flux case. At the end, both the fronts are almost in the same location. The behaviour of ablation fronts is similar, as can be seen from Figure 9. The ablation front moves faster for the constant flux case and the two curves converge at the end.

4.3 Computational Cost

The linear solver is tridiagonal, leading to $O(N)$ operations per iteration (in a time step). The number of iterations is invariant with N. Thus, the number of operations per time step is also $O(N)$.

5. CONCLUSIONS

It can be seen that the computational model is reasonably robust and efficient. The use of fixed meshes enable it to be extended easily to 2-dimensions. The results show that the solution obtained is mesh independant. This implies that the numerical scheme is able to capture the flux discontinuity effectively. The scheme is computationally efficient as the number of iterations (per time step) varies very slowly with N. Being a generic one, the algorithm can be applied to other cases with a moving isothermal source. The constant flux and ramp flux cases tend to ‘converge’ at the end, which is as expected. The next step would be to extend the algorithm to two dimensions, include other effects such as energy of released gases and making the charring front a thin layer.
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NOMENCLATURE
A  Face Area of a Cell  
c  Specific Heat  
h_{ab}  Heat of Ablation  
h_{ch}  Heat of Charring  
k  Thermal Conductivity  
N  Number of Cells  
q  Face Heat Flux  
T  Temperature  
T  Time Period  
T_{ab}  Ablation Temperature  
T_{ch}  Charring Temperature  
t  Time  
V  Cell Volume  
v_{ab}  Ablation Front Velocity  
v_{ch}  Charring Front Velocity  
x_{ab}  Charring Front Position  
x_{ch}  Ablation Front Position  
x_{c}  Co-ordinate of cell or face  
x_{f}  Charring Front Position  
\rho  Density  
\Delta t  Time Step  
\Delta x  Mesh Size

REFERENCES