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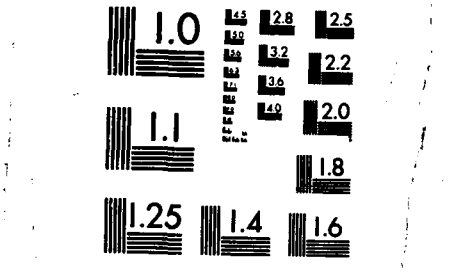

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MELBOURNE, VICTORIA

REPORT

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ABSTRACT

A reactive multi-material, first order numerical model (known as HEAT) for heat conduction in cylindrical coordinates has been developed and tested. The model allows the inclusion of a maximum of three separate materials.

A second order Taylor series expansion was employed in the development of the finite difference scheme within each single material layer. Matching conditons on the interfaces are determined to first order.

The model employs a zero order Arrhenius burn function to describe the heat generated by the thermal decomposition of the reactive components. It also takes into account the latent heat of fusion for each material.

External heat is introduced via a constant temperature boundary condition or a time dependent boundary condition. The model will permit restarts, although only in the cases were total decomposition of the reactive fraction has not occurred.

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C O N T E N T S

A REACTIVE MULTI-MATERIAL FIRST ORDER NUMERICAL MODEL FOR HEAT CONDUCTION IN CYLINDRICAL COORDINATES

1. INTRODUCTION

There are a number of occasions during either storage or service life, when the transient heating of a munition may occur for any one of a number of reasons. These reasons include an external fire, thermal conduction of heat from a hot gun barrel into a loaded round, or even frictional heat generated as air flows past a missile moving at supersonic speeds.

For this report the heating of a shell, trapped within a hot gun barrel was investigated. As the heat flows from the environment into the shell, the temperature rises and the confined explosive will decompose more rapidly producing further heat. If the heat produced by this chemical decomposition cannot be transferred to the surroundings as rapidly as it is produced, thereby stabilising the temperature at an elevated value, the mass of explosive will self-ignite.

The above may occur if the gun barrel temperature is very high. The temperature of the explosive above which a thermal explosion is produced, is known as the critical temperature. Given the chemical and physical parameters of a particular system the critical temperature may be exceeded.

A reactive multi-material, first order numerical model (called HEAT), has been developed to solve the two dimensional heat conduction problem for a cylindrical geometry. This model employs a second order Taylor series expansion of the transient heat equation within each single material layer. Continuity across material interfaces is achieved using a first order approximation. HEAT may be employed to determine whether a particular event should be deemed critical or under control.

In what follows, the model used for the calculations is formulated. This is followed by a description of how the HEAT code was validated. Further improvements, the results obtained and a discussion of them are then given.

2. THE MODEL

HEAT was developed to study the transient heating from a hot gun barrel into a failed to fire shell although many problems of similar geometry may also be studied. It employs the cylindrical geometry of a shell, but neglects the heat sink action of any attached fuze or warhead. The longitudinal axis of the shell is taken as the axis of symmetry, or z-axis, while the radial direction is denoted as the r-axis. The metal and liner thicknesses (materials 1 and 2, respectively, of Fig. 1) need not be uniform, although the high explosive must have a constant radius. These assumptions were considered acceptable for the problem at hand.

In Fig 1, an illustration of the model in its most general form is provided, i.e. a cross section through the cylinder with the axis of symmetry being the left hand boundary. A maximum of three distinct material layers has been incorporated into this model, although this can easily be increased by modifying the code.

The partial differential equation describing unsteady thermal conduction with an internal heat source is as follows:

$$\rho \frac{C_p}{\lambda} \frac{\partial u}{\partial t} = \nabla^2 u + S \qquad (1)$$

where,

ρ = density of the material
u = absolute temperature
C_p = specific heat
λ = thermal conductivity

and where S is the source term described by the Arrhenius burn function [1]:

$$S = \rho Q (1 - \epsilon)^n Z e^{-E/Ru} \text{ , for r,z within explosive}$$

$$= 0 \qquad \text{otherwise}$$

where
n = the order of reaction
ϵ = the fraction of explosive decomposed.
Q = heat of reaction
Z = collision number
E = activation energy
R = gas constant

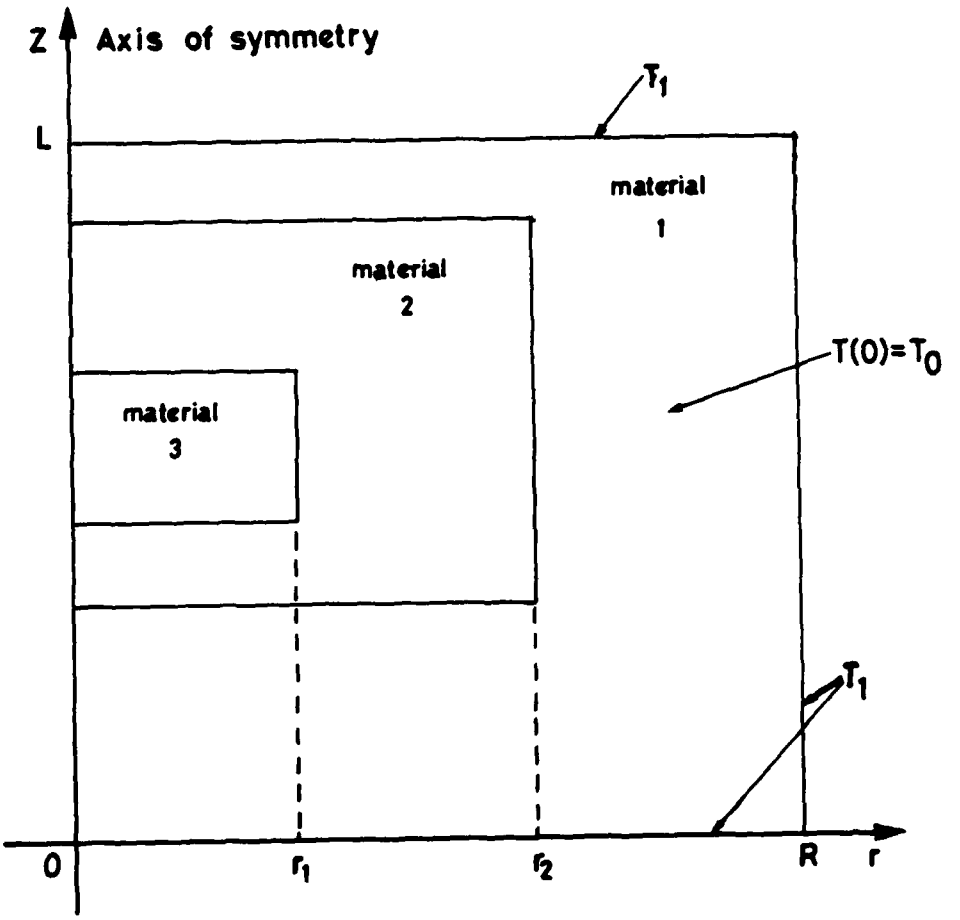

Figure 1. Schematic showing the geometry of the model.

As a first approximation, a zero order burn was chosen. This leads to:

$$S = \rho QZe^{-E/Ru}. \qquad (2)$$

If we neglect the source term for now, Eqn. (1) can be written in cylindrical coordinates as:

$$\rho \frac{C_p}{\lambda} \frac{\partial u}{\partial t} = \frac{\partial u^2}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial u^2}{\partial \theta^2} + \frac{\partial u^2}{\partial z^2}. \tag{3}$$

With cylindrical symmetry of the solution, $\frac{\partial^2 u}{\partial \theta^2} = 0$ and Eqn. (3) simplifies to:

$$\rho \frac{C_p}{\lambda} \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{\partial^2 u}{\partial z^2}, \quad r \geq 0 . \tag{4}$$

Eqn. (4) is valid at all interior modes of the model. At r = o, the physical solution is the one that is non-singular. Using a power series expansion for the radial solution to equation (4) we get,

$$u(r) = u_o + u_1 r + u_2 r^2 + \ldots\ldots$$

For small r, i.e. δr

$$u(\delta r) = u_o + u_1 \delta r + u_2 \delta r^2 + \ldots\ldots \tag{5a}$$

and a Taylor series expansion near zero gives,

$$u(\delta r) = u(o) + \delta r \frac{\partial u}{\partial r}\Big|_o + \frac{\delta r^2}{2} \frac{\partial^2 u}{\partial r^2}\Big|_o + \ldots\ldots \tag{5b}$$

Equating like terms of Eqns (5a) and (5b):

$$u_o = u(o)$$

$$u_1 = \frac{\partial u}{\partial r}\Big|_o$$

$$u_2 = \frac{1}{2} \frac{\partial^2 u}{\partial r^2}\Big|_o$$

Now Eqn. (4) may be rewritten as,

$$\rho \frac{C_p}{\lambda} \frac{\partial u}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2}, \quad r \geq 0 \tag{6}$$

Our power series solution for r must satisfy this equation. Substituting the power series for u and obtaining the derivative with respect to r gives,

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) = 4u_2 + 0(r) \quad \text{as } r \to 0$$

but $$u_2 = \frac{1}{2} \frac{\partial^2 u}{\partial r^2} \Big|_o$$

$$\therefore \quad \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) \Big|_o = 2 \frac{\partial^2 u}{\partial r^2} \Big|_o$$

and Eqn. (6) is recast as:

$$\rho \frac{C_p}{\lambda} \frac{\partial u}{\partial r} = 2 \frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial z^2}, \quad r = 0 \tag{7}$$

for heat flow at the axis of symmetry.

A solution was found to Eqns. (4) and (7) subject to the boundary conditions:

$$\begin{aligned} u(R,z,t) &= T_1 \\ u(r,0,t) &= T_1, \quad t > 0 \\ u(r,L,t) &= T_1 \end{aligned} \tag{8a}$$

together with the initial condition,

$$u(r,z,0) = T_o \qquad 0 \leq r < R, \; 0 < z < L \; . \tag{8b}$$

These conditions are illustrated in Fig. 1.

The numerical solution was obtained by first writing Eqns (4) and (7) in a second order finite difference form [2], based on a Taylor

expansion. The Alternating Direction Implicit (ADI) method [3,4,5,6,7,8,9] was then employed to solve these finite difference equations.

The ADI method was employed due to its unconditional stability [3,5,7,9] and because it is a very time efficient method for the solution of a multidimensional problem. ADI effectively reformulates the finite difference equations into an algebraic problem consisting of a set of linear equations whose coefficients form a tridiagonal matrix. The method involves solving this set of equations in each coordinate direction in turn, such that two net sweeps occur in a two dimensional problem such as this. The first set would be written with one direction expressed implicitly and the other expressed explicitly. In the second set the situation would be reversed. The results after these two sweeps is a single time step advance.

The rz plane of the model was divided up into a rectangular grid of increment δr and δz, in r and z directions respectively*. The material properties were defined at each grid point or node in the plane. Where material interfaces occurred, control volumes [5,6] were placed around the boundary node of interest (see Fig. 2). For the control volume, the sum of the heat flow into the node was equated to the mass of the control volume times the specific heat capacity times the rate of temperature change simulating a non-explosive material. This is first order accurate differencing. Second order differencing at the interface may be employed in a later version of HEAT. For the node shown in Fig. 2 this would lead to the following set of first order difference equations for r expressed implicity and z expressed explicitly and without the source term.

$$u^{n+1/2}_{i-1j}\left(\frac{\lambda_2}{\delta r}A_1\right) + u^{n+1/2}_{ij}\left(-\frac{\lambda_2}{\delta r}A_1 - \frac{\lambda_1}{\delta r}A_2 - \frac{2V}{\delta t}\right) + u^{n+1/2}_{i+1j}\left(\frac{\lambda_2}{\delta r}A_2\right) =$$

$$u^{n}_{ij-1}\left(-\frac{\lambda_2}{\delta z}A_1\right) + u^{n}_{ij}\left(\frac{\lambda_2}{\delta z}A_1 + \frac{\lambda_1}{\delta z}A_2 - \frac{2V}{\delta t}\right) + u^{n}_{ij+1}\left(-\frac{\lambda_2}{\delta z}A_2\right)$$

where $A_1 = 2\pi (i - 3/2)\,\delta r\delta z$

$A_2 = 2\pi (i - 1/2)\,\delta r\delta z$

$V = \pi\delta r^2\delta z(i - 5/4) + \pi\delta r^2\delta z\,(i - 3/4)$

λ_i = thermal coefficient in material i

u^n_{ij} = temperature at node i,j at time n.

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* The values for r and z were determined after a series of test jobs. It was then decided that a minimum of 10 cells per material layer was required.

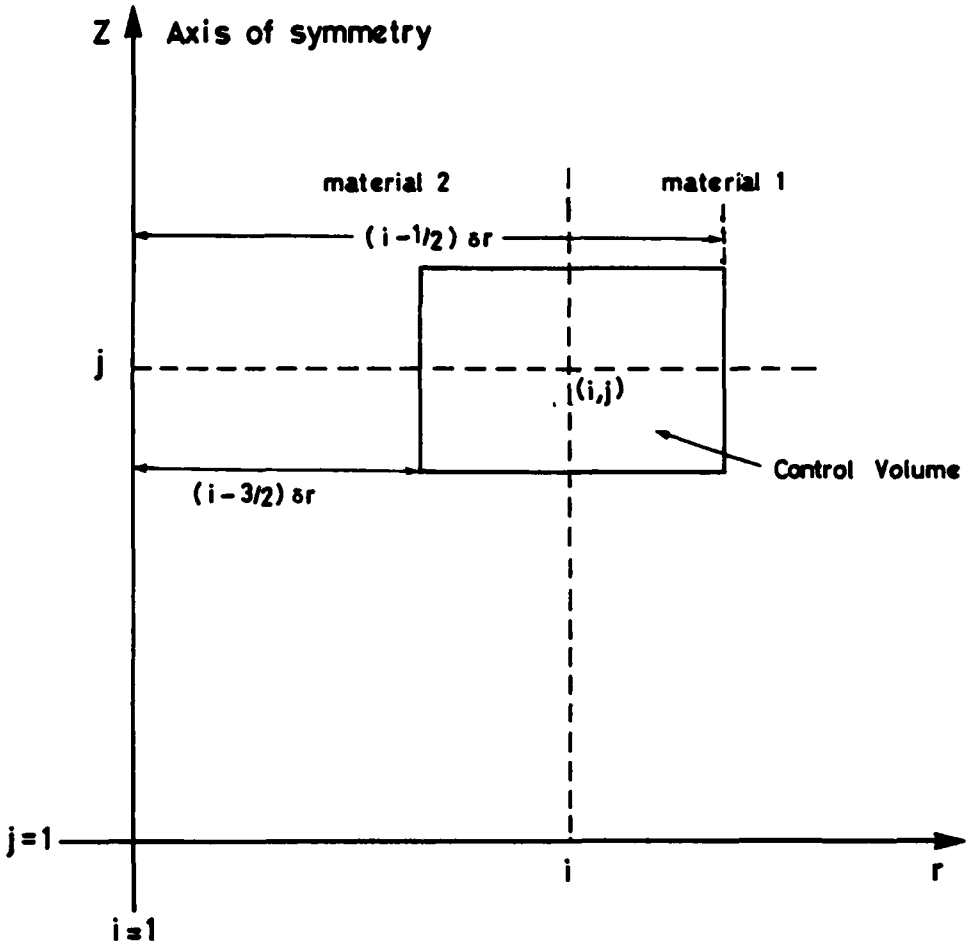

Figure 2. Description of the control volume at (i,j).

With the boundary conditions and initial conditions set, Eqns. (8a) and (8b), the tridiagonal coefficient matrix was solved employing the Thomas Algorithm [10,11]. This is a fast solution technique, in which the structure of a tridiagonal matrix is used to advantage.

At the end of each incremental time step, the temperature increase due to the source term was determined at all the nodes within the explosive. Given this new temperature distribution, melting was determined and, if necessary, accounted for, by using the latent heat of fusion in conjunction with the melting point for each material. If, on the other hand, the temperature within the explosive had risen to a very high value (arbitrarily set at $773^{o}K$), total decomposition was assumed and the simulation stopped. The final time step information was then saved.

It should be noted that although this code was written as second order accurate within a single material, the interface calculations are only first order accurate. The final model is therefore only accurate to first order.

3. VALIDATION

HEAT was validated by using three separate techniques. Each one of these techniques verified a particular aspect of the code. The combined results of these tests provided a high level of confidence in the model predictions.

Fig. 3 shows the geometric details of a simplified shell. In all cases studied the time step was initially set to 0.1 seconds. If after 50 cycles, the temperature rise was less than 10% at every node, the time was increased by 10%. The initial time step was chosen as a compromise between keeping the truncation errors low and still maintaining computational speed. This procedure allows the time step to increase as long as the solution is slowly varying. The shell was discretised into a square grid of 0.002 m (2 mm) for δr and δz giving each material a minimum of 10 cells. All cells must be the same size in this model.

The first method of validation involved employing the model to solve the heat conduction equation where the solution was either known or easily recognizable. This is a standard technique. For instance, this model predicted a constant temperature when the initial and boundary conditions were set equal at time $t = 0$ and the heat source was inactive. Conversely, if the heat source was active, the temperature within the explosive region of the model gradually increased.

Problems which had a particular symmetry in a plane perpendicular to the rz plane, displayed symmetry in that plane on output, as expected. Incorporating lower thermal conductivity constants slowed the rate of temperature rise within the model. All these qualitative observations provide confidence in the model.

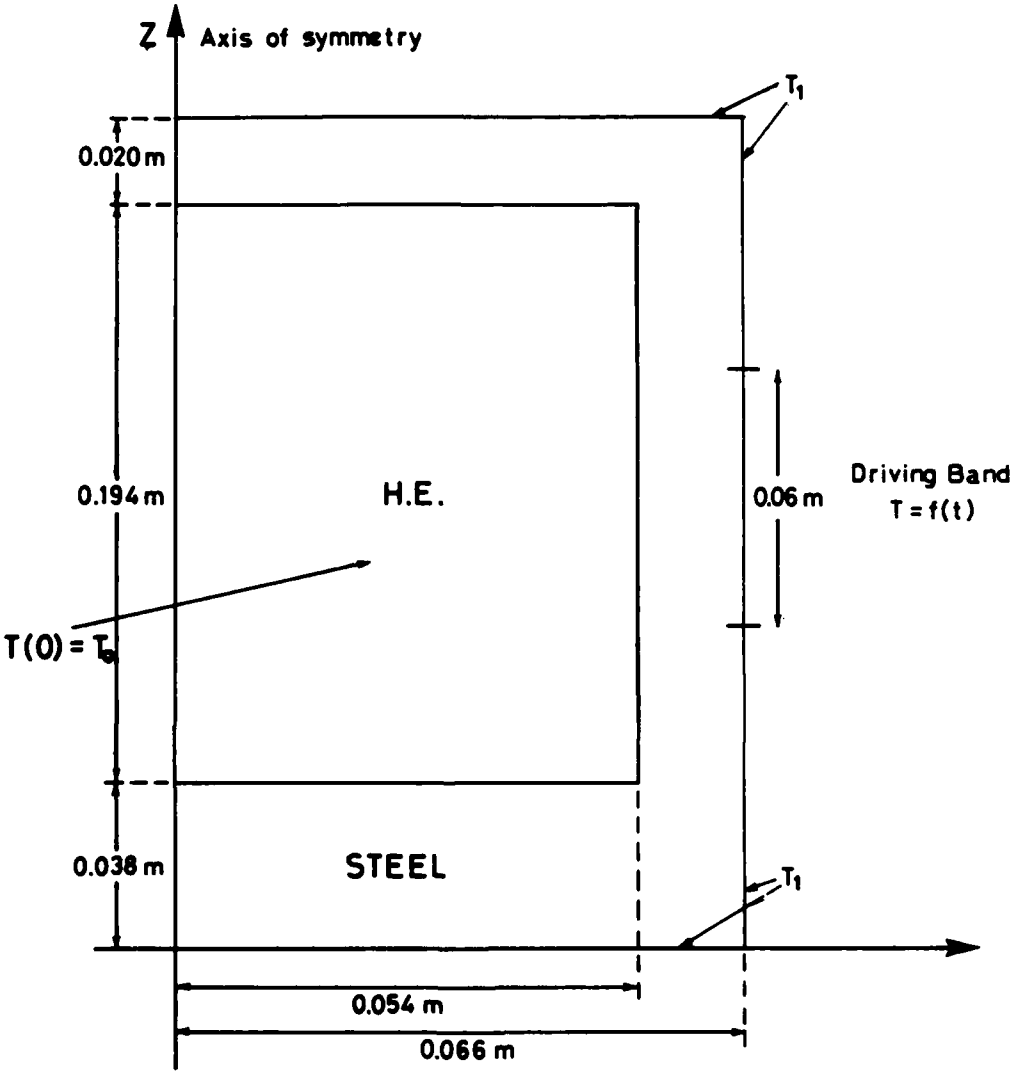

Figure 3. Simplified version of a filled shell with a driving band.

TABLE 1

Temperatures at the given radii and times within a steel cylinder as calculated by an analytic one dimensional solution and from a HEAT simulation in brackets. HEAT valves are taken from a cross-sectional slice at the centre line i.e. z = 0.127 m. Both results are for a boundary temperature of 798K and an internal temperature of 298K. The steel cylinder had a radius of 0.066 m and a height of 0.254 m.

	RADIUS(m)			
Time (s)	0	0.02	0.038	0.056
23.2	302.3 (299)	321.3 (309.2)	410.6 (383.4)	630.5 (601.3)
57.2	366.8 (313.5)	409.2 (339.8)	520.1 (448.2)	689.7 (647.7)
106.9	481.1 (344.5)	516.0 (372.5)	601.5 (480.4)	722.9 (664.2)
179.7	600.5 (386.6)	622.5 (412.2)	675.9 (510.5)	751.4 (677.1)
286.4	699.4 (435.6)	710.4 (458.2)	737.1 (544.8)	774.8 (691.5)

TABLE 2

Table showing the time to detonation as determined by an effectively 1-dimensional calculation [14] and HEAT using stated constant boundary conditions. The 1-dimensional code used 5 cells (0.012 m each) in the radial direction and 50 cells (variable dimensions between 0.037 m and 0.002 m) in longitudinal direction, and with a time step of 0.1 s. Our model used a constant cell dimension of 0.002 m, 33 cells along the radial direction and 127 cells in the longitudinal direction. The time step was monotonically increased from 0.1 s.

Boundary Temperature (K)	Time to Detonation (s)	
	1-dimensional calculation	2-dimensional calculation (HEAT)
573		42.1
598	33.3	35.4
608	31.3	
623	28.9	32.1
648	25.8	29.1
698		24.7
798	16.9	19.2
2000	7.0	8.3

In the second method, the temperature calculated from an analytical solution for a one dimensional inert single material was compared with this model in an inert single material phase only. The results are given in Table 1.

A definite difference between the analytic and numeric solutions can be seen in Table 1. This discrepancy is due mainly to the heat sinking effect of the neighbouring material cells in the two dimensional case. Initially the difference is not great (about 5%), as the heat conduction is predominantly in the radial direction. Later on, longitudinal heat flow becomes important, and the discrepancy between the one dimensional and the two dimensional models grows to around 60%. At this stage the effect of a two dimensional calculation is apparent. The result is a lower calculated temperature at the nodes for the two dimensional model. This demonstrates the need for a two dimensional analysis when considering the temperature rise within a cylinder.

In the third method, HEAT is compared with the solution from another numerical model [14]. Although the latter model is two dimensional, it contains the wrong geometry for our problem and hence can only be used to provide a one dimensional solution. Nevertheless, the comparison is still instructive. Table 2 shows the times to detonation for HEAT and for this one-dimensional model.

TABLE 3

Table showing the time to detonation as determined by HEAT. Either a constant boundary condition or a slowly decreasing temperature profile for the boundary condition were used. Appendix A provides the form of this temperature profile.

Initial Boundary Temperature (K)	Time to Detonation (S)	
	Constant conditions	Decreasing Conditions
573	42.1	
598	35.4	-
608		57.2
623	32.1	45.7
648	29.1	35.4
698	24.7	27.6
798	19.2	20.5
2000	8.3	16.6

The time to detonation is larger when calculated by HEAT. This is not surprising considering the interpretations made from Table 1. The effect of including the second dimension is to slow the heating rate and hence increase the time to detonation. As the detonation time is the critical parameter required from these calculations, the superiority of the two dimensional model becomes apparent. Even though this time difference, as shown here, is small, the effect is real and should be included in the calculation.

4. EMBELLISHMENTS, RESULTS AND DISCUSSION

A constant boundary temperature is unrealistic. Heat transfer from the barrel to the shell, for instance, is most likely to occur through the intimate contact of the driving band. Hence the boundary condition should specifically include this region, and for completeness, should also contain a cooling function for the temperature profile since the barrel will cool as the shell heats (see Appendix A).

The cooling function was determined from experimental data and gives temperature as a function of time. The length of the driving band was determined from drawings. The effect of these changes can be seen in Table 3. Here, a comparison between constant temperature and reducing temperature boundary conditions is made. It should be noted that with the constant boundary temperature condition a detonation will always occur provided that this initial boundary temperature is greater than the self-ignition temperature. In the reducing temperature condition, detonation only occurs above a critical initial temperature, below this temperature self-sustained decomposition cannot begin. The critical ignition temperature in this case is a function of the geometry of the shell and the charge and their thermal properties, as well as of the decomposition properties of the explosive, Eqn. (2).

In addition, the form of the cooling function, the length of the driving band, and the geometry of the problem, are all critical parameters in determining whether a mass detonation will occur. For this reason, the results of Table 3 can only be taken as a guide. Nevertheless, the indication is that a significant change in the predicted stability of the shell is found if the boundary conditions are more realistic.

The length of the driving band in the previous calculations was 0.06 m. As the actual heat input may well occur beyond the boundaries of the driving band, it was decided to investigate time to detonation for a longer driving band. We chose an extended length of 0.08 m. Some simulations from Table 3 were then repeated using the increased length. The results are compared in Table 4.

TABLE 4

Time to detonation as determined by HEAT for a driving band of length 0.06 m or 0.08 m. The initial boundary temperatures are given. The rate of boundary temperature decrease is the same for both calculations.

Initial Boundary Temperature (K)	Time to Detonation (s)	
	Driving Band 0.06 m	Driving Band 0.08 m
558	-	-
598	-	47.4
608	57.2	
623	45.7	37.0
698	27.6	26.1
798	20.5	19.2

With the larger driving band, more energy can be put into the system. As the thermal characteristics of the shell remain constant, the time to detonation must decrease. It is also interesting to note that the difference in the predicted times is not large when the initial temperature is far above the cook-off temperature. This happens because at those temperatures cook-off occurs so rapidly that not all the available energy is used or needed. At lower temperatures, energy balance becomes critical more quickly for the narrower band and hence the time differences increase. The extent of influence of the driving band is significant in the determination of the time to detonation and should therefore be carefully considered.

To improve efficiency, the input and output of HEAT was modified. A useful feature that was included allows the user to restart the calculation from the last time step saved. This means that the model can be run for a small number of cycles and the output viewed. The simulation can then be continued again if necessary, therefore eliminating the need to attempt one large simulation run only, which is not always desirable.

5. CONCLUSION

A model to solve the two-dimensional transient heat equation in cylindrical coordinates has been developed and programmed in FORTRAN 77 to run on a VAX 11/780 computer. This model (HEAT) has been tested and compared with

results for single material or multimaterial media with distinct boundaries. The model has been demonstrated to solve problems with either constant boundary conditions, or with time dependent temperature profiles along a region of the boundary.

The model uses second order finite differences within a single material but only first order finite differences at material boundaries. These approximations will influence mesh size determination. They do not affect accuracy of the results directly.

The model should prove to be valuable in the determination of heat conduction into filled shells, particularly where heat sinks are of concern and where simpler one dimensional codes will not suffice. In these cases, the calculated temperature rises will be more realistic. The model can also be used as a basis for other more general problems of cylindrical symmetry. For example, voids and tapered profiles may be incorporated.

6. ACKNOWLEDGEMENTS

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Conduction (heat transfer)	Gun barrels
Mathematical models	Premature functioning

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