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Numerical Simulation of the TNT Solidification Process

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ABSTRACT

The solidification phenomenon is present in the casting process of energetic materials. In defence industry, trinitrotoluene (TNT) is used as main charge for high explosive ammunitions. The present study tackles the numerical simulation of the solidification process of TNT by means of a two-dimensional transient model in cylindrical coordinates. The heat conduction problem is solved by using the enthalpy method that rewrites the governing equation in terms of this variable. The transient diffusive equation is then numerically solved by applying finite volumes in an explicit scheme. The analysis the mold thickness and the convective boundary conditions are analysed to assess how they affect heat transfer during solidification. Results obtained allow for a better comprehension of this type of problem.

Keywords: Solidification; TNT; Enthalpy method; Conjugated problem

NOMENCLATURE

C_p	Specific heat
h_c	Convective coefficient
e	Wall thickness
H	Enthalpy per volume unit
k	Thermal conductivity
ρ	Density
r	Radial cylindrical coordinate
R	Radius
z	Axial cylindrical coordinate
L	Length
l	Liquid
s	Solid
T	Temperature
T_i	Initial temperature
T_m	Melting temperature
T_w	Wall temperature
T_∞	Room temperature
T	Time
w	Wall
Δh	Latent heat
τ	Dimensionless time
ξ	Dimensionless position of the solidification front

1. INTRODUCTION

A large part of military explosives are solid compounds that may be cast or pressed to its final shape[1,2]. Generally, whenever an energetic material with relatively low melting temperature is to be delivered in homogeneous, complex shapes, casting is employed, essentially meaning that the explosive is heated until it melts and then it is poured into a mold which is subsequently cooled until the explosive solidify. This is the case of mass production of artillery shells filled with trinitrotoluene (TNT) in the defence industry[3]. Although ammunition loading using solidification phenomenon is a relatively simple procedure, cooling conditions applied to the casting process must ensure that the final product be free of defects such as void formation, residual stress distributions and mold separation which can modify the detonation velocity leading to premature detonation and accidents when handling these explosives[4].

Therefore, it is highly desirable to model phase change processes of energetic materials to predict the total solidification time and the solid-liquid interface position as a function of cooling conditions and mold thickness. Early work related to solid-liquid phase change problems include the one performed by Joseph Stefan in 1891 which leads to the classical mathematical model for the study of melting or solidification known as the Stefan Problem, but due to its mathematical complexity, only few exact solutions are available, such as Neumann´s solution[5]. For this reason, numerical solutions are often employed to solve this type of problem.

The development of numerical models for solidification processes is considered challenging due to the moving solid-liquid interface and the variable fluid properties induced by the thermal evolution[6,7]. With regard to this, fixed mesh techniques are employed as a standard numerical approach to solidification problems, because its main characteristic is to explain the evolution of latent heat by the definition of enthalpy[8].

The enthalpy method is one of the various numerical methods known as weak solutions, which are able to incorporate the effects of phase change into the thermophysical properties, and where the position of the solidification front becomes a consequence of the solution of the temperature field. In this

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method, the heat transfer equation is rewritten in terms of enthalpy, thus eliminating the need for tracking the solid-liquid interface position[2,7].

In addition to the aforementioned difficulties, heat transfer at the mold interface is a priori unknown and since heat flow crossing the boundary between the material being solidified and the mold wall affects directly the evolution of the solidification front, this conjugated problem is also to be addressed. When the phase change material (PCM) and mold surfaces are brought into contact, an imperfect junction is formed. Although uniform temperature gradients may exist in both PCM and mold, the junction between the two surfaces creates a temperature drop, which depends on the thermophysical properties of the materials in contact, on the contact pressure and on initial mold temperature[9].

In this contribution, the solidification process of TNT poured in a mold is analysed by predicting the position of solidification front as a function of time by solving a two-dimensional transient conjugated heat transfer problem in cylindrical coordinates subjected to prescribed temperature or convective boundary conditions. The problem is formulated in terms of enthalpy and solved in a numerical fashion by the method of finite volumes. The conjugated problem is analysed to investigate how the thickness of the mold and the convective boundary condition influence the process and the total solidification time.

2. MATERIALS AND METHODS

In this work, the physical-mathematical model studied represents the solidification of TNT inside a steel mold. Initially at liquid phase, it is poured inside a cylindrical shell where due to the conditions imposed on the mold, its solidification process begins. The top surface and center line of the cylindrical domain, which is shown in Fig. 1, are thermally isolated, characterising the condition of null heat flux, whereas the base and cylinder outer surface have a prescribed wall temperature below the solidification temperature of TNT. Figure 1 illustrates the simplified domain adopted in the computational simulation and its boundary conditions.

The physical parameters of the model and the thermophysical properties of TNT are given, respectively, in Tables 1 and 2. The thermal conductivity and specific heat of TNT are constant and phase independent[10].

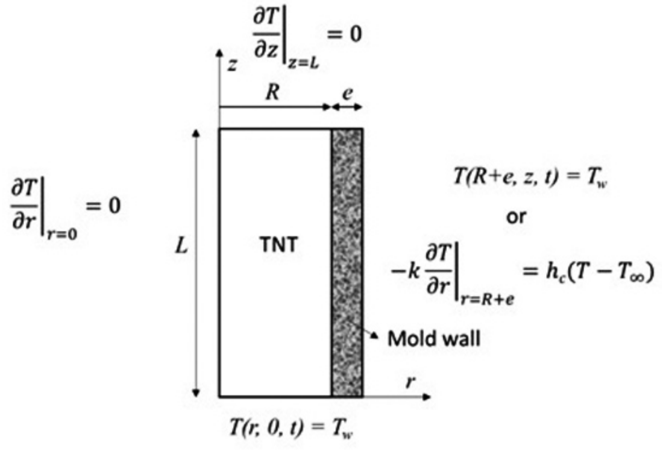

Figure 1. Domain and boundary conditions of the physical-mathematical model.

Table 1. Model parameters[7].

Parameters	Unit	Value
Height, L	m	0.3419
Radius, R	m	0.12
Initial temperature, T_i	K	360
Wall temperature, T_w	K	300

Table 2. Thermophysical properties of TNT[7,10].

Properties	Unit	Value
Thermal conductivity, k	W/(m K)	0.26
Solid phase density, ρ_s	kg/m^3	1648
Liquid phase density, ρ_l	kg/m^3	1544.6
Specific heat, c_p	J/(kg K)	1062.2
Melting temperature, T_m	K	354.05
Latent heat, Δh	kJ/kg	98.4

For the conjugated problem, when the influence of the mold wall thickness on heat transfer is considered in the analysis, a stainless steel mold is considered, whose properties are as shown in Table 3.

Table 3. Mold properties[1].

Parameters	Unit	Value
Thermal conductivity, k_w	W/(m K)	16.27
Density, ρ_w	kg/m^3	8030
Specific heat, $c_{p,w}$	J/(kg K)	502.48

Generally, in the loading of an industrial grenade, the outer surface boundary conditions are characterised by natural convection of the air induced by the hot surface of the grenade or by forced convection, in which direct ventilation is required[11]. Therefore, for the conjugated problem, a convection condition is also analysed on the cylinder outer surface, with external temperature of $T_\infty = 300$K. The air convective heat transfer coefficients considered in this case are presented in Table 4.

Table 4. Convective coefficients[11].

Parameters	Unit	Value
Natural convection	W/(m^2 K)	5.1067
Forced convection	W/(m^2 K)	49.3179

The equation that determines the transient temperature field of the two-dimensional model is the classical heat diffusion equation, described by:

$$\rho c_p \frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(kr\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \tag{1}$$

$$T(r,z,t=0) = T_i \qquad 0<r<R \text{ and } 0<z<L \tag{2}$$

$$\left.\frac{\partial T}{\partial r}\right|_{r=0} = 0 \qquad t>0 \text{ and } 0<z<L \tag{3}$$

$$\left.\frac{\partial T}{\partial z}\right|_{z=L} = 0 \qquad t>0 \text{ and } 0<r<R+e \tag{4}$$

$$T(r,0,t) = T_w \qquad t > 0 \ \text{and} \ 0 < r < R + e \tag{5}$$

In the present work, two different boundary conditions at $r = R + e$ are analysed, the prescribed temperature boundary condition, Eqn. (6), and the convection boundary condition, Eqn. (7).

$$T(R+e,z,t) = T_w \qquad t > 0 \ \text{and} \ 0 < z < L \tag{6}$$

$$-k\left.\frac{\partial T}{\partial r}\right|_{r=R+e} = h_c\left(T - T_\infty\right) \quad t > 0 \ \text{and} \ 0 < z < L \tag{7}$$

In Eqn. (7), h_c is the convective coefficient.

Then, for a generic phase-change system containing a solid-liquid interface and the mold wall, the governing equation is now expressed as:

$$\frac{\partial H}{\partial t} = \nabla.\left(k\nabla T\right) \tag{8}$$

where H is the enthalpy per volume unit, defined by Eqn. (9).

$$H = \begin{cases} \rho_s c_{p,s} T & ,T < T_m \ \text{and} \ 0 \le r \le R \\ \rho_l \Delta h + \rho_s c_{p,s} T_m + \rho_l c_{p,l}\left(T - T_m\right) & ,T \ge T_m \ \text{and} \ 0 \le r \le R \\ \rho_w c_{p,w} T & ,R < r \le R + e \end{cases} \tag{9}$$

where the subscripts s, l, and w are, respectively, referred to the TNT solid phase, the TNT liquid phase and the mold wall.

To solve the governing equation, Eqn. (8), the finite volume method is applied. Using the central difference scheme (CDS) interpolation function and explicit formulation, an iterative procedure is obtained. The numerical solution calculates the enthalpy at all volumes of the mesh[12].

It is important to note that both TNT and the mold wall are solved by the finite volume method. Moreover, the solver was programmed in SciLab software.

Then, from the enthalpy field obtained for each step in time, the temperature field is determined by the relation present in Eqn. (10).

$$T = \begin{cases} \dfrac{H}{\rho_s c_{p,s}} & ,H \le H_{sf} \ \text{and} \ 0 \le r \le R \\ T_m & ,H_{sf} < H < H_{lf} \ \text{and} \ 0 \le r \le R \\ \dfrac{H - \rho_l \Delta h - \left(\rho_s c_{p,s} - \rho_l c_{p,l}\right) T_m}{\rho_l c_{p,l}} & ,H \ge H_{lf} \ \text{and} \ 0 \le r \le R \\ \dfrac{H}{\rho_w c_{p,w}} & ,R < r \le R + e \end{cases} \tag{10}$$

where $H_{sf} = \rho_s c_{p,s} T_m$ and $H_{lf} = \rho_s c_{p,s} T_m + \rho_l \Delta h$ are, respectively, the fusion enthalpies per unit volume of the solid and liquid phases.

To present the results obtained and to compare them with the reference data of the literature, the following dimensionless parameters are introduced:

$$\xi = \frac{z}{L} \tag{11}$$

$$\tau = \frac{k\,t}{\rho_s c_{p,s} L^2} \tag{12}$$

3. RESULTS AND DISCUSSION

First, it was considered a 1D model, with heat conduction in the z-direction and boundary conditions as shown in Fig. 1. This enabled the methodology to be validated against the literature[7]. To verify the computational code here developed, it was also considered a 2D problem, in which both extremes in the r-direction have null heat flux. This 2D situation is equivalent to a problem with $R \to \infty$. In this case, heat conduction occurs only in the axial direction. In both scenarios, the dimensionless solidification front position as a function of dimensionless time was calculated and the results were compared with the archival literature[7].

These results are as depicted in Fig. 2, where it can be observed that both 1D and 2D cases lead to the same evolution of the solidification front, as expected due to the symmetry of the 2D problem. Moreover, the results obtained by the enthalpy method are in good agreement with those obtained through the effective capacity method previously employed[7]. The agreement between the 1D and 2D solutions is an important step to verify the quality of the implemented numerical solution.

Next, the problem presented in Fig. 1 with prescribed temperature at the outer surface was solved, considering null wall thickness (e = 0), and the position of the solidification front on axis z was computed, as shown in Fig. 3.

By comparing Figs. 2 and 3, it is possible to observe the influence of the boundary condition of prescribed temperature at the outer surface of the domain. The vertical asymptote in Fig. 3 indicates that a solidification front moves in the radial direction from the mold wall to the center of the domain and when the solidification front approaches the z-axis, then $\xi \to \infty$.

Following, it was analysed the effect on the solidification process caused by different diameters of the grenade, considering null wall thickness (e = 0). It is well known that when the diameter tends to infinity, the one-dimensional solution is recovered. Simulations were performed for radius values of R = 0.36 m, R = 0.72 m and R = 1.08 m and the results shown in Fig. 4 in the dimensionless form.

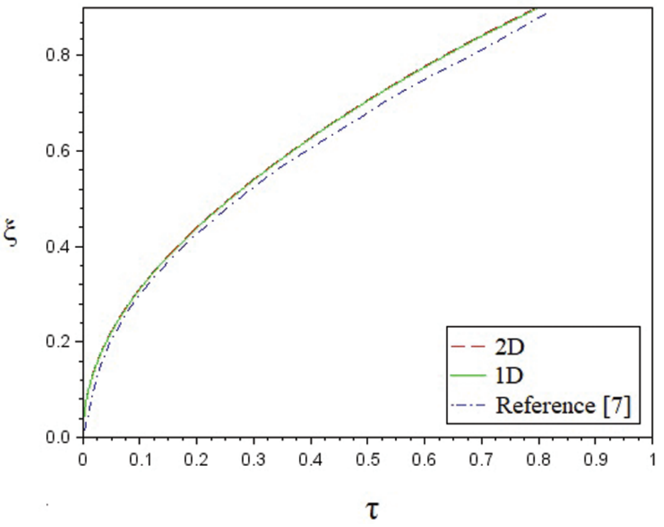

Figure 2. Evolution of the solidification front for 1D and 2D verification problems.

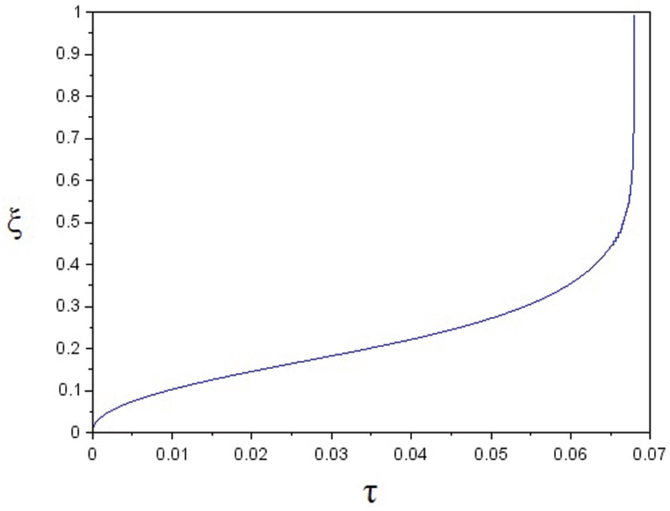

Figure 3. Evolution of the solidification front on *z* axis (*e* = 0).

Figure 4 shows that by increasing the grenade diameter, the influence of the prescribed temperature boundary condition at the outer surface of the domain decreases. Thus, the evolution of the solidification front tends to the one obtained for the 1D situation. For the case $R = 0.72$ m, very close curves are already obtained and for $R = 1.08$ m, the curves practically overlap. Therefore, the influence of the r-direction on the evolution of the solidification front along z axis can be considered irrelevant when $R/L > 3.2$ on the evolution of the solidification front on z axis. However, in most used mortar grenade calibers 60 and 120 mm with lengths, respectively, equal to 130 and 341 mm, R/L are minor than 3.2. Consequently, the radial movement of the solidification front is very important during the high explosive filling process of these ammunitions.

For the conjugated problem, in which the presence of the mold is considered, three different thicknesses were evaluated: $e = 0.005$ m, $e = 0.01$ m and $e = 0.02$ m. It was considered that the heat transfer between the mold and the TNT occurred only by conduction. The same boundary conditions shown in Fig. 1 were used, being the prescribed temperature the one employed at $r = R+e$. It was then obtained the evolution of the solidification front in the axial direction at $r = 0$, as shown in Fig. 5.

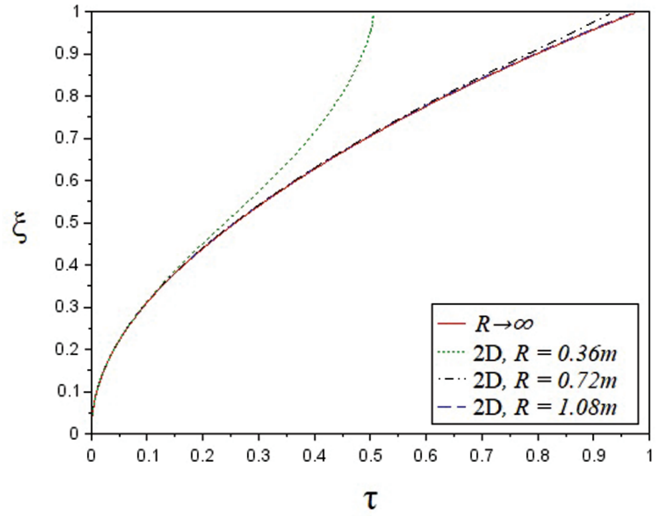

Figure 4. Effect of the domain radius on the evolution of the solidification front along *z* axis (*e* = 0).

The inclusion of the mold wall thickness in the computational simulation does not seem to affect significantly the results obtained without the wall presence. This is somewhat expected due to the very high thermal conductivity of steel when compared with the very low thermal conductivity of TNT.

Since the curves in Fig. 5 overlap, to obtain a better comparison of results, total solidification times as a function of the thickness of the mold are shown in Table 5. It is noticed that even for the relatively large thickness of $e = 0.02$ m, the time added to complete the solidification process was only 0.73 per cent.

Table 5. Total solidification time.

Mold thickness (m)	Time (s)
-	53510.0
0.005	53635.2
0.01	53736.0
0.02	53900.4

Figure 6 shows the solidification of TNT as simulated with a fixed wall thickness of 0.01 m, for three values of inner radius.

Figure 6 indicates that a small change in the inner diameter of the grenade causes a significant change in the total solidification time, since increasing the inner diameter consequently increases the mass of material to be solidified under the same boundary conditions.

Finally, the influence of natural and forced convection on the solidification process was analysed, for the situation of a mold thickness equal to 0.01m, by imposing a convective boundary condition described by Eqn. (7). A heat transfer coefficient of 49.3179 W/(m^{2}K) was considered for the case of forced convection while a value of 5.1067 W(m^2 K) was considered for the case of natural convection. The results obtained are as shown in Fig. 7.

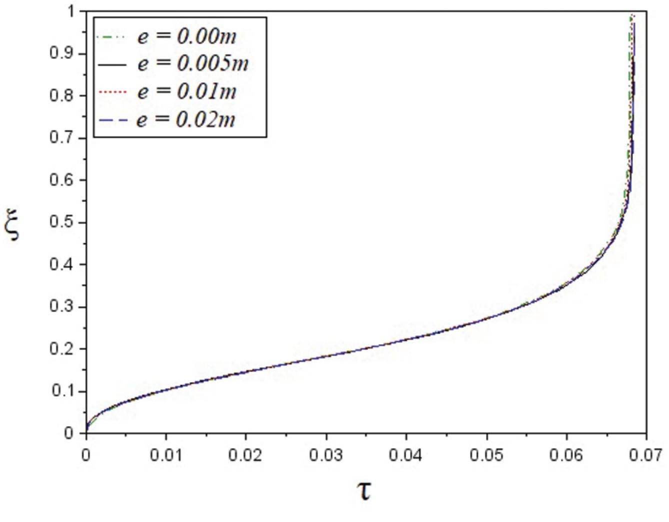

Figure 5. Effect of the wall thickness on the evolution of the solidification front along *z* axis.

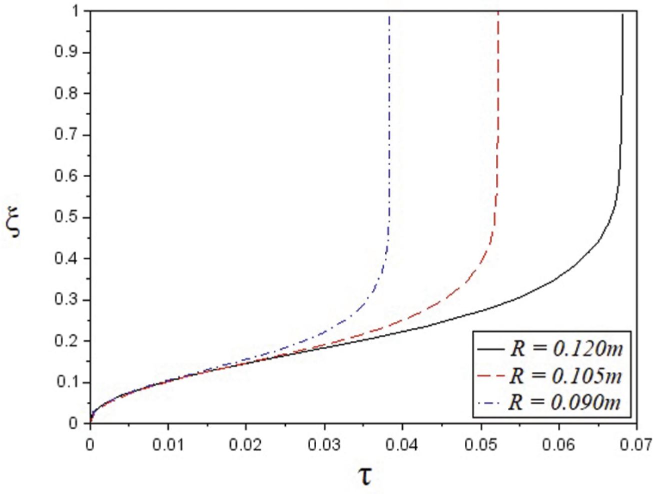

Figure 6. Effect of the grenade diameter on the evolution of the solidification front along *z* axis (*e* = 0.01 m).

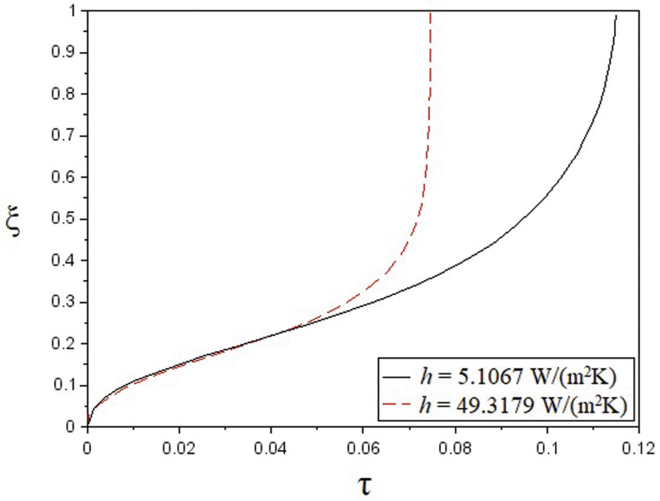

Figure 7. Evolution of the solidification front on *z* axis for natural and forced convection (*e* = 0.01m).

It is noticed in Fig. 7 that by increasing the convective coefficient, the total solidification time decreases. Therefore, the value for the convective coefficient is an important parameter to control the solidification process.

Since the diameter of the ammunition cannot be changed due to commercial specifications, the control of the solidification process by altering the convective coefficient can be achieved in practice by imposing suitable values for the room temperature and air velocity in the air blowers. Thus, the final product can meet the quality standards demanded by the defence industry.

4. CONCLUSIONS

This work has shown that the enthalpy method is a very simple and effective technique for handling phase-change problems with conjugated heat transfer. This method avoids the tracking requirements of the moving solidification front present in other methods, since the thermophysical properties of the phase change material and of the mold material are incorporated in the enthalpy variable.

The proposed numerical solution implemented in SciLab software has shown good agreement with the literature, indicating the good quality of the program. By systematically increasing the diameter of the explosive charge while maintaining its height fixed, it was established that a limiting radius to height ratio for modelling the solidification process as a 2D problem as far as the evolution of the solidification front along *z* axis is concerned. It was determined that for values greater than or equal to $R = 3.2\,L$ the 2D solution along z-axis matches the results obtained by the 1D model. In other words, when $R \geq 3.2\,L$, the total solidification time can be computed by either 1D or 2D models since both computed times are equal.

Although the thickness of the mold can influence the heat transfer process, this was not the case for this problem, since the thermal conductivity of stainless steel is much higher than its counterpart for TNT. Therefore, no significant effects were observed as far as total solidification time is concerned. On the other hand, the inner diameter variation greatly affects the total solidification time.

The effects of the convective boundary condition on the solidification process are relevant on the studied problems. The quality of the final product can be guaranteed by controlling the speed of the solidification front, which can be achieved by imposing suitable values for the room temperature and air blower velocity.

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In current study, he had conducted the modelling and data analysis.