

Modeling of Cooling and Solidification of TNT based Cast High Explosive Charges

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ABSTRACT

Cast trinitrotoluene (TNT) based high explosive charges suffer from different defects such as cracks, voids, etc. One of the quality control measures is to cool the castings gradually, so that the entire charge solidifies without a large temperature gradient from core to the periphery of the cast charge. The fact that the solidification of high explosive casting starts from the periphery (cooler side) and travels towards the center enables us to predict the solidification profile of TNT based explosive castings. Growth of solidification thickness and cooling temperature profiles of TNT based cast high explosive charges are predicted as functions of time and space using unsteady state heat transfer principles, associated with heat balance at solid to liquid interface as a moving boundary of solidification. This will enable adoption of proper quality control during solidification of the molten TNT to eliminate inherent drawbacks of cast high explosive charges. The solidification profiles of TNT based cast charges under controlled and natural conditions are predicted and the model is validated against 145 mm diameter TNT cast charge which is found to be in broad agreement with experiments.

Keywords: Solidification, asymptotic growth, unsteady state heat conduction, liquid-solid interface, heat balance, trinitrotoluene, TNT

NOMENCLATURE

C	Specific heat of TNT
h_{sf}	Latent heat of fusion of TNT
k	Thermal conductivity of TNT
ρ	Density
R	Radius of specimen charge
r	Reference radius at any time
T_0	Initial temperature
T_f	Fusion (melting) temperature of TNT
T_w	Wall temperature
δ	Solidification thickness
$\dot{\alpha}$ ($= k/\rho C$)	Thermal diffusivity
l	Liquid
s	Solid
B	Polynomial constant ($B=1$ at $r=0$ & $T_1 = T_0$)
ϕ	Dimensionless temperature parameter
S	Dimensionless sub cooling parameter

Dimensionless Numbers

$$\delta^+ = \frac{\delta}{R}$$
$$t^+ = \dot{\alpha}_s t / R^2$$
$$\alpha^+ = \dot{\alpha}_l / \dot{\alpha}_s$$

1. INTRODUCTION

The two main high explosive loading techniques in military ammunition are pressing and casting. All high caliber bombs, warheads, etc., are filled by casting method in general, with trinitrotoluene (TNT) as casting medium. Some of the serious defects of TNT casting are the shrinkage that

occurs as the filling solidifies, formation of voids and pores due to entrapped air, dissolved gases, and improper feeding of casting material¹. The casting solidifies from outside and the consequent shrinkage is that of an isolated mass at the center of the casting². The shrinkage takes place in the axial direction. Improper control of specific transport mechanisms will lead to cracking of charge due to excessive thermal stresses. It is also seen that in homogeneous crystal growth takes place as the casting solidifies³. These deficiencies in the casting of high explosive will not only alter the detonation profile but may also lead to accidental and premature explosion in dynamic conditions. As such an explosive charge is required to withstand a dynamic load of 200 MPa⁴.

Entrapped air can be removed by mechanical means such as hot probing, vibration, etc. But this may not compensate for the shrinkage. In the casting, shrinkage can be minimized by carefully cooling the charge under controlled conditions⁵. Crystal size can also be controlled by varying the rate of heat transfer⁶, especially towards its softening temperature of around 80 °C. As casting is a heat transfer problem with phase change⁷, prediction of solid-liquid interface position is important for the filling of explosives in shells and moulds as it helps in optimizing the filling conditions.

Plastic bonded explosives (PBXs) are replacing the TNT based explosives to overcome these deficiencies, especially for underwater weapons⁸. However, bulk production facilities are not yet fully established for PBXs. Filling of PBXs in warheads is expensive and time consuming. In view of this fact, TNT based charges are still being manufactured around

the world for military applications. Hence, the present study is of practical importance.

In the present study, growth rate of solidification thickness (or solidification period) and cooling rates are computed. The predicted profiles and the experimental results are compared. A 145 mm caliber TNT based charge, when allowed to solidify under controlled conditions is seen to give better quality explosive charge in terms of explosive loading, increased density and reduced porosity. This results in better explosive parameters.

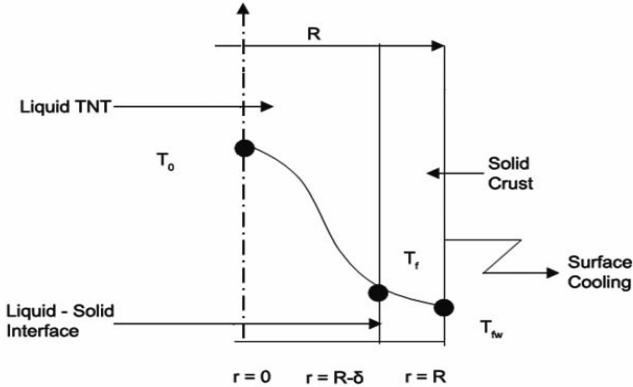


Figure 1. Representative half of explosive charge

2. THEORETICAL ANALYSIS

The physical model of solidification problem is shown in Fig. 1. At time zero, the vertical cylindrical mould of radius R is filled with the molten explosive. Cooling is provided on the outer surface of the mould so that the temperature of the mould wall remains constant at T_w . Solidification, commencing at the inner side of wall of the mould extends towards the central core of the explosive. For $t > 0$, the solidified thickness is δ .

The heat flow in the liquid ($0 \leq r \leq R-\delta$) and solid ($R-\delta \leq r \leq R$) regions of the explosive are governed by the equation of unsteady state heat conduction as⁹.

$$\rho_l C_l \frac{dT_l}{dt} = \frac{k_l}{r} \frac{d}{dr} \left[r \frac{dT_l}{dr} \right] \quad \text{for } 0 \leq r \leq (R-\delta) \quad (1a)$$

$$\rho_s C_s \frac{dT_s}{dt} = \frac{k_s}{r} \frac{d}{dr} \left[r \frac{dT_s}{dr} \right] \quad \text{for } (R-\delta) \leq r \leq R \quad (1b)$$

2.1 Initial Condition

Initially, the explosive contained in the mould is in the molten state at a uniform temperature $T_l = T_o$

$$\text{Thus, at } t = 0, T_l = T_o \text{ for } 0 \leq r \leq R \quad (2)$$

2.2 Boundary Conditions

At any instance of time, the temperature is maximum at the axis of the cylindrical charge, i.e., at $r=0$. This fact, by virtue of symmetry at $r=0$, can be mathematically represented as.

$$\text{At } r = 0, \frac{dT_l}{dr} = 0 \quad (3)$$

Pressure within the mould is constant. Hence, the temperature at the liquid- solid interface remains constant at T_f where T_f is the phase change temperature of TNT.

$$\text{At } r = R-\delta, T_l = T_s = T_f, \text{ where } T_f \text{ is constant } (4)$$

The above condition is presumed, as constant temperature is maintained at the wall.

$$\text{At } r = R, T = T_w, \text{ where } T_w \text{ is constant } (5)$$

2.3 Heat Balance at the Liquid–solid Interface

T_l , the temperature within the liquid phase is higher than the phase change temperature T_f of TNT. Thus, the sensible and latent heats liberated at $r = R-\delta$, the liquid–solid interface are conducted through the solid phase to the coolant at $r=R$. The resulting equation of heat balance is given below¹⁰.

$$k_s \frac{dT_s}{dr} \Big|_{r=R-\delta} = k_l \frac{dT_l}{dr} \Big|_{r=R-\delta} - \rho_s h_{sf} \frac{d\delta}{dt} \quad (6)$$

El-Genk and Cronenberg¹¹ demonstrated that the problem of unsteady state heat conduction with moving boundary can become one of continuous growth, or asymptotic growth, or growth-and-decay depending on the boundary conditions imposed. Because of the adiabatic condition of heat flow at the center, i.e., at $r=0$, continuous growth of the solid crust takes place in the present case. integral method is used to solve Eqn. (1) for liquid phase. In this method, the equation in liquid phase is integrated with respect to r in the appropriate range of r , i.e., $r=0$ to $(R-\delta)$. The resulting equation is given below.

$$\rho_l C_l \frac{d}{dt} \int_0^{(R-\delta)} r(T_l - T_f) dr = k_l (R-\delta) \frac{dT_l}{dr} \Big|_{r=R-\delta} \quad (7)$$

Temperature profiles are assumed for use in and evaluation of Eqns. (6) and (7). These profiles are for $0 \leq r \leq (R-\delta)$

$$\frac{T_l - T_f}{T_o - T_f} = B \left[1 - \left[\frac{r}{R-\delta} \right]^2 \right] \quad (8)$$

and for $(R-\delta) \leq r \leq R$:

$$\frac{T_f - T_s}{T_f - T_w} = \left[\frac{r - R + \delta}{\delta} \right] \quad (9)$$

Temperature profiles given by Eqns. (8) and (9) are obtained subject to the boundary conditions Eqns. (3) - (5).

Equations (6) and (7) are evaluated using Eqns. (8) and (9) to yield differential equations:

$$\frac{d\delta^+}{dt^+} = S \left[\frac{1 - \delta^+ (1 - 2B\phi)}{\delta^+ (1 - \delta^+)} \right] \quad (10)$$

$$\frac{dB}{dt^+} = \frac{2B[S(1 - \delta^+ (1 - 2B\phi)) - 4\alpha^+ \delta^+]}{\delta^+ (1 - \delta^+)^2} \quad (11)$$

$$\text{where } \phi = \frac{k_l(T_o - T_f)}{k_s(T_f - T_w)} \text{ and } S = \frac{C_s(T_f - T_w)}{h_{sf}}$$

$$\delta^+ = \frac{\delta}{R} \text{ and } t^+ = \alpha_s \frac{t}{R^2}; \alpha_s = \frac{k_s}{(\rho_s C_s)}; \alpha_+ = \frac{a_+}{a_s}$$

where ϕ and S are the dimensionless temperature parameter and sub cooling parameter respectively. Equations (10) and (11) are simultaneously solved for δ^+ and B by fourth-order Runge-Kutta method with the initial conditions that at $t^+ = 0, \delta^+ = 0$ and $B=1$

The values of parameters ϕ and s given below are calculated from above relations for $T_0=90^\circ\text{C}$ and $T_w=18^\circ\text{C}$ using approximated thermo-physical properties of TNT¹² which are summarized in Table 1.

$$\phi = \frac{5.5 \times 10^{-4} (90.0 - 80.6)}{6.02 \times 10^{-4} (80.6 - 18)} = 0.1371 \text{ and } S = \frac{0.25475 (80.6 - 18.0)}{23.53} = 0.6777$$

Table 1. Thermo-physical properties of TNT

Melting point (°C)	Specific heat (cal/g°C)	Latent heat (cal/g)	Thermal conductivity [(cal/(s-cm°C))]	Density (g/cm³)
80.6	0.254+7.5x10 ⁻⁴ T (17 < T < 67 °C)	23.53	6.02 x 10 ⁻⁴ (10 < T < 45 °C)	1.56-1.59 (100% liquid)
	0.309+3.5x10 ⁻⁴ T (97 < T < 150°C)		5.5 x 10 ⁻⁴ (45 < T < 75°C)	1.59-1.61 (75% liquid)

3. EXPERIMENTAL

TNT (Special Grade) manufactured in one of the Indian Ordnance Factories was used in the experiments. Melting point, purity and theoretical density of TNT are 80.6 °C, 99.799 % (JSS 1376-02:2004 (Rev. 03)) and 1.654 g/cc respectively, and are assumed to be constant for simplicity. Thermal conductivity of TNT is very poor as compared to stainless steel or even as compared to water.

Before conducting the experiments, solid TNT was melt in a jacketed anchor blade mixer and poured into a preheated jacketed stainless steel mould of 145 mm diameter and 350 mm height. The initial temperature of the mould was kept uniform and only liquid phase was allowed to exist. Explosive charge of diameter 145 mm and height 270 mm is realized from this set up. The upper portion, up to about 60 mm of the solidified charge was of very poor quality with pores, uneven finish and piping. This part of the charge was removed by machining. The final charge was of dimensions ϕ 145 x 190 mm (height).

The experimental arrangement is shown in Fig. 2. The test conditions are reflected.

In Fig. 3. Symmetry enables the solution to be carried out only for a representative half of the charge which is shown in Fig. 3.

The temperature of the charge was monitored and controlled through six PT-100 temperature sensors inserted to a depth of 65 mm at six different equi-spaced radial points along the diameter of the charge and connected to the master controller. Radial points are chosen as the

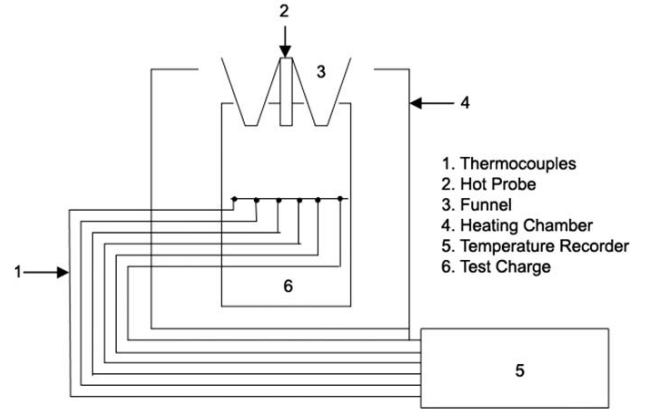


Figure 2. Schematic flow diagram of experiment.

length to diameter ratio is more than 1.5. This is also because of the reason that the interior quality of the charge is established by testing the mould product by dissection for density equality, blowholes, cracks and shrink holes radially¹³. The rate of cooling was controlled by an indigenously developed 8085 microprocessor based control system which regulated the flow of hot water/steam or compressed air through a set of solenoid valves either to heat or cool respectively. The maximum scatter of temperature observed during the cooling process was about 4°C (±2%). The central core temperature was considered for generation of experimental temperature profile. The predicted and experimental solidification profiles are compared in Fig. 4. Cooling trends of charge at the top of the charge (30 mm) are monitored, both under natural and controlled conditions were monitored and plotted in Fig. 5.

Different solidification periods were computed by varying T_w in the model in order to study the effect of wall temperature. The same is shown in Fig. 6.

The cast charges cooled under different conditions were cut into smaller discs and the densities were determined

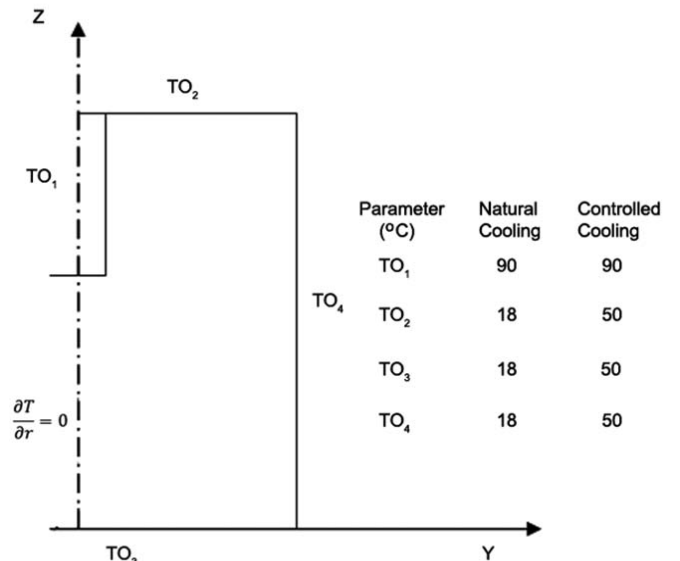


Figure 3. Geometry and boundary conditions of test problem.

by using Archimedes's principle. The density values along with the porosity values (with < 1% variation) are furnished in Table 2.

Porosities in the specimen samples were calculated using the formula.

4. RESULTS AND DISCUSSION

In the solid, the temperature decreases due to the growth of frozen layer, while in the liquid, the distributions change

Table 2. Charge analysis

Position	Natural cooling		Controlled cooling	
	Density (g/cc)	Porosity (%)	Density (g/cc)	Porosity (%)
25 mm from top	1.50	9.31	1.57	5.07
100 mm from top	1.55	6.28	1.60	3.26
175 mm from top	1.55	6.28	1.60	3.26

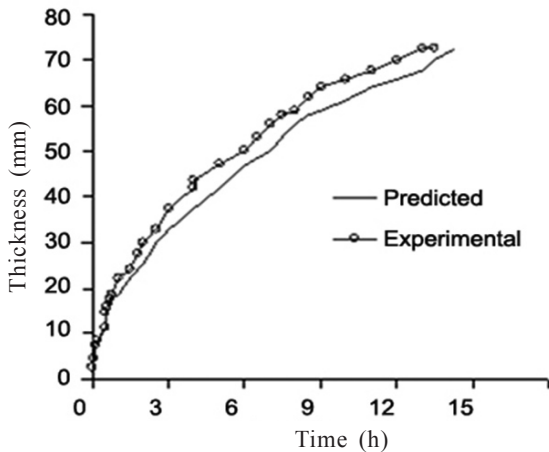


Figure 4. Solidification profile.

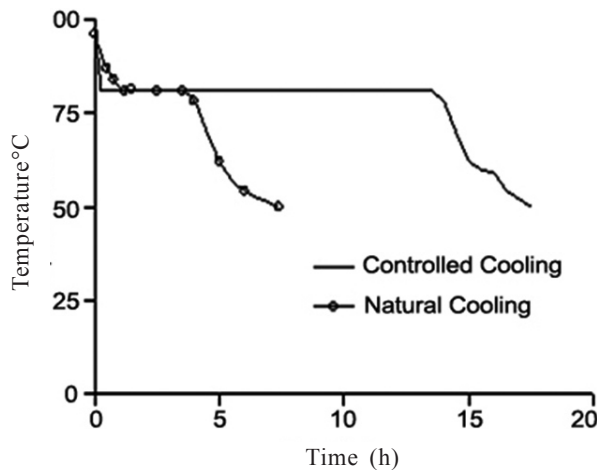


Figure 5. Core temperature profile.

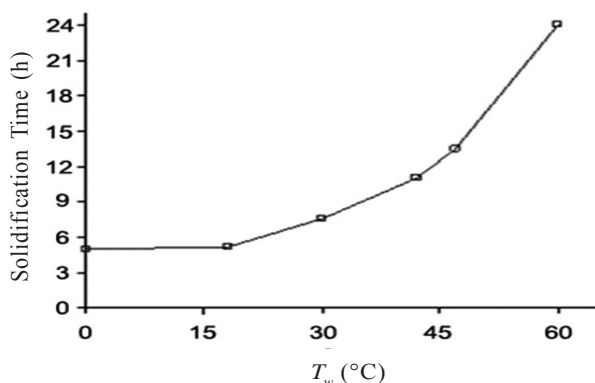


Figure 6. Effect of T_w on solidification time.

relatively little during the course of the solidification. The temperature gradient in the solid near the interface initially is much greater and then decreases at later times and finally approaches the temperature gradient in the liquid phase. As the casting solidifies from periphery to the core, the thickness of solid TNT grows towards the center. Initially, solidification of TNT is expected to be faster than at later stages in view of its poor conductivity. Therefore, solidification (the motion of the solid-liquid interface) slows down and finally sieges, when equilibrium temperature is attained¹. This can be very clearly seen from Fig.4, where initially solidification rate is relatively fast and slowed down as time lapsed. The deviation that is seen between the predicted and experimental profiles may be due to the uncertainties in the approximated thermo-physical properties and experimental conditions.

From the temperature profiles under plant (natural cooling) and laboratory (controlled cooling) conditions as can be seen from Fig. 5, it indicates that in the former case solidification is complete in about 4 h and 30 min and the temperature falls to 50 °C in about 7 h indicating that the process of solidification takes place between 50 °C and 60 °C¹⁴. This only resulted in poor quality charge. Whereas, in controlled cooling where the outside temperature was maintained, the charge took about 13 h to completely come to uniform phase change temperature along the diameter. This period is arrived at from Fig. 4, where the charge took this time to solidify. Then the liquid phase quickly solidified simultaneously throughout the diameter without leaving any voids. This yielded good quality charge without cracks and voids. Cooling the charge at lower T_w reduces the solidification time due to higher temperature gradient. However, this results in large amount of porosity in the charge, since only little time is available for the molten TNT to fill the pores caused by occluded air. As a result a very inferior quality charge is obtained^{15,16}. At the same time if the T_w is high, solidification time is appreciably high as can be seen from Fig.6, while not bringing about any significant change in the charge quality. Under natural cooling conditions, density of solid TNT achieved is 1.55 g/cc while under controlled (T_w around 50°C) conditions, density increases to 1.60 g/cc. It is known that every 0.01 g/cc density variation brings in about 2 % variation in explosive energy¹⁷. Thus, 0.05 g/cc increase in density by adopting controlled cooling will better the explosive energy by 10 %. Reduction of porosity from 2% to 0.5%, would result in an improvement of VOD, detonation pressure and Shaped charge jet velocity by 1.2%, 4.5%, and 1.7% respectively¹⁸.

5. CONCLUSIONS

The model predicts the solidification time and temperature profile of cast explosives more or less accurately. The predicted profile of cooling is in good agreement with experimental profile. By predicting the solidification time, the density of the charge and the porosity can be estimated and thus corrective measures can be exercised by optimizing the plant conditions.

It can be concluded that for an explosive of 145 mm caliber, the optimum cooling temperature is about 50 °C and the solidification time is around 14 h at 50 °C for obtaining higher charge density, which in turn boosts the explosive parameters like velocity of detonation, detonation pressure, etc.

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