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Genetic Algorithm Optimisation of a TNT Solidification Model

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ABSTRACT

The control of the solidification process of energetic materials is important to prevent manufacturing defects in high explosive ammunitions. The present work aims to propose an optimisation procedure to determine the value of the model parameter, avoiding the traditional trial and error approach. In this work, the solidification of TNT has been numerically modelled employing apparent heat capacity method and the model parameter was optimised using genetic algorithm. One dimensional numerical model has been solved in Comsol Multiphysics Modeling Software and the genetic algorithm code was written in Matlab. The Neumann's analytical solution of the solidification front was used as a reference to build the fitness function, following the inverse problems concepts. The optimum model parameter has been predicted after 20 generations and among 30 candidate solutions for each generation. The numerical solution performed with the optimised model parameter has agreed with the analytical solution, indicating the feasibility of the proposed procedure. The discrepancy was 3.8 per cent when maximum difference between analytical and numerical solutions was observed.

Keywords: TNT; Grenade; Solidification; Genetic algorithm; Solidification process; Neumann's analytical solution

NOMENCLATURE

C_{ap}	Apparent heat capacity [J/m^{3}K]
c	Specific heat [J/kgK]
f	Fitness function [m^{-1}]
Δh	Latent heat [J/kg]
k	Thermal conductivity [W/mK]
L	Length [m]
L_1	Length of the investigated region [m]
S	Solidification front [m]
T	Temperature [K]
ΔT	Model parameter [K]
t	Time [s]
z	z-coordinate [m]
α	Thermal diffusivity [m^2/s]
λ	Parameter in the Neumann's analytical solution
ρ	Density [kg/m^3]
τ	Dimensionless time
0	Initial
anal	Analytical
num	Numerical
m	Melting
s	Solid phase
l	Liquid phase
w	Wall

1. INTRODUCTION

High caliber bombs and warheads are manufactured by casting method and, during this casting process, trinitrotoluene (TNT) is generally used. During solidification of TNT pores may occur, the volume of the TNT shrinks and crystal growth takes place. These defects can alter detonation profile and cause premature explosion under dynamic conditions. Porosity can be eliminated employing hot probing and vibration. Moreover, to minimise the shrinkage and control the crystal size, the filling conditions must be optimised. For those reasons, modeling the phase change process is very important during TNT solidification[1].

To model the melting and solidification process, analytical and numerical approaches have been proposed. The Neumann's analytical solution is useful for one dimensional problems. Otherwise, numerical solutions are preferred for multidimensional problems in complex geometries. Among the numerical approaches, the most used are the apparent heat capacity method, the effective heat capacity method and the enthalpy method[2].

Kumar & Rao[1] developed a model to predict the solidification time and temperature profile of cast explosives. This model was verified with experiments on 145 mm diameter TNT cast charge, which determines that 50 °C was the optimum cooling temperature to have higher charge density. Rathjen & Jiji[3] suggested an analytical solution for the solidification of a liquid with constant wall temperature. Caldeira[4], *et al.* made a numerical study estimating the porosity formation during TNT solidification using the effective heat capacity method. In this work, the Particle Swarm optimisation was employed to solve the inverse problem. Zhang[5], *et al.* presented an analytical model predicting the location of solidification front and solidification time for heterogeneous materials. It was

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observed that as porosity increases, the total solidification time also increases. Furthermore, if the shapes of the pores are polygonal, then the solidification takes much longer time. Ji & Lin[6] have numerically modelled the solidification process of TNT, considering the natural convection inside the liquid TNT. The enthalpy method and Darcy law were used and the results reveals that when natural convection was taken into account the solidification time was increased. Chen & Shiuan[7] made a numerical and experimental study about solidification of TNT. It has shown that the process of controlled cooling was better than the process of natural cooling. Sun[8], *et al.* made a numerical and experimental study on the solidification of TNT and cyclo-trimethylene-trinitramine (RDX)-blinder explosive. This research has considered the heat transfer, the fluid flow and the stress field in the shell. The results have showed that within 10 per cent of the casting time, more than 80 per cent of the explosive solidified due to the high solidification rate at the beginning of the process. Nevertheless, for (RDX)-blinder explosive, the effect of the convective heat transfer on the temperature field is negligible due to the high viscosity. Sun[9], *et al.* have presented an experimental and numerical study considering convection effect and thermal stresses for the energetic materials during solidification. The analysis has concluded that was possible to suppress the separation of the cast material from the mold controlling the cooling conditions. Annapragada[10], *et al.* investigated the effect of cooling conditions on the void formation, base separation and thermal stresses for the solidification of high Prandtl number melt in their numerical and experimental study. The buoyancy effect inside the investigated energetic material was taken into account. The suggested new cooling conditions gives 25 per cent reduction in the base separation.

Optimisation methods, having benefits of avoiding the traditional trial and error approach, have been used in many fields including solidification. As an effective optimisation method genetic algorithm is also used in researches. Shahane[11], *et al.* used genetic algorithm method in their numerical study about die casting to find the initial and cavity wall temperatures for the optimum product quality. Santos[12], *et al.* applied genetic algorithm method to continuous casting process in their numerical and experimental study. The optimum settings of water flow rates in different sprays zones for the quality of the solidified strand have been determined.

In the present work, the solidification process of TNT has been numerically modelled using apparent heat capacity method in Comsol Multiphysics Modelling Software which uses finite elements. The optimum value of the model parameter, ΔT, which defines the half of phase change temperature range for TNT, has been determined using genetic algorithm, implemented in Matlab. This work aims to propose an optimisation procedure to determine the value of the model parameter, avoiding the traditional trial and error approach.

2. MATERIAL AND METHOD

2.1 Problem Definition

The region of a mortar grenade, which is initially filled with hot liquid TNT, during the casting process is shown in Fig. 1. Then, after a cooling process the TNT is solidified.

Motivated by the engineering problem as shown in Fig. 1 and aiming to determine the model parameter, a simplified theoretical problem is proposed. One dimensional TNT solidification process has been modelled using apparent heat capacity method. The bottom part of the grenade has the boundary condition of constant temperature lower than the solidification temperature. Solidification starts from the bottom and proceeds towards the top.

The governing equations and boundary conditions are as follows

$$C_{ap}\frac{\partial T}{\partial t}=\frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) \tag{1}$$

$$T=T_0 \quad 0\le z\le L \quad t=0 \tag{2}$$

$$T=T_w \quad z=0 \tag{3}$$

$$\frac{\partial T}{\partial z}=0 \quad z=L \tag{4}$$

where C_{ap} is the apparent heat capacity, k is the thermal conductivity and L is the length of the numerical domain.

In the grenade shown in Fig. 1 the length filled with liquid TNT, L_1, is equal to 0.13m. However, to mimic the semi-infinite domain considered in the Neumann's analytical solution, the adopted numerical domain length must be much larger than L_1. Then, L = 1.3 m is used. Nevertheless, the relevant length is L_1.

The apparent heat capacity C_{ap} is as given in the Eq. (5).

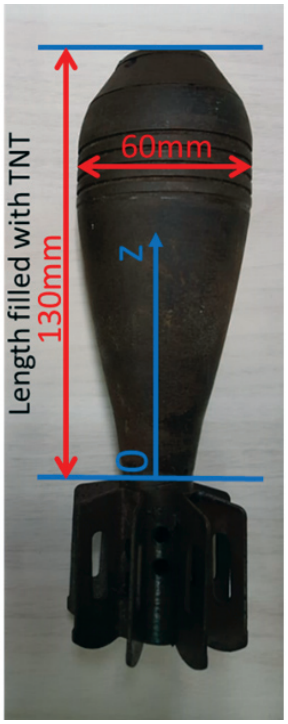

Figure 1. 60 mm mortar grenade.

$$C_{ap} = \begin{cases} \rho_s c_s & T \le T_m - \Delta T \\ \dfrac{\rho_s \Delta h}{2\Delta T} + 0.5\rho_s c_s + 0.5\rho_l c_l & T_m - \Delta T < T < T_m + \Delta T \\ \rho_l c_l & T \ge T_m + \Delta T \end{cases} \quad (5)$$

The parameters of the model and the thermophysical properties of TNT are as given in Table 1[4]. The optimum value of ΔT has been determined using genetic algorithm.

Table 1. Parameters and thermophysical properties of TNT[4]

Property	Symbol	Value
Initial temperature	T_0	360 K
Wall temperature	T_w	300 K
Melting temperature	T_m	354.05 K
Density of solid	ρ_s	1648 kg/m^3
Density of liquid	ρ_l	1544.6 kg/m^3
Specific heat	$c_s = c_l$	1062.2 J/kg K
Thermal conductivity	$k_s = k_l$	0.26 W/m K
Latent heat	Δh	98400 J/kg

The solidification front is obtained using the Neumann's analytical solution depicted by Özışık[13]. Figure 2 is the schematic view of the problem.

This analytical solution provides the temperature distribution in solid and liquid phases, respectively, T_s and T_l, and the position of the solidification front $S(t)$ as a function of time, $S_{anal}(t)$.

$$T_s(z,t) = T_w + (T_m - T_w)\left(\frac{erfc(\frac{z}{2\sqrt{\alpha_s t}})}{erfc(\lambda)}\right) \quad (6)$$

$$T_l(z,t) = T_0 + (T_m - T_0)\left(\frac{erfc(\frac{z}{2\sqrt{\alpha_l t}})}{erfc(\lambda\sqrt{\frac{\alpha_s}{\alpha_l}})}\right) \quad (7)$$

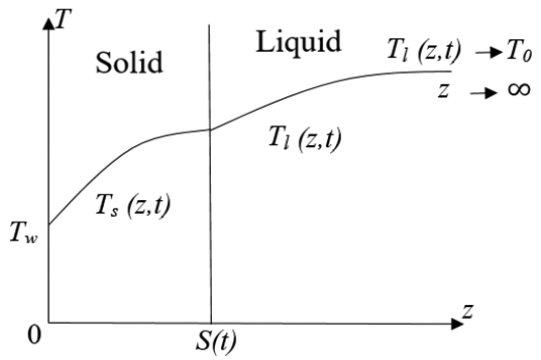

Figure 2. Solidification in a half space[13].

$$S_{anal}(t) = 2\lambda\sqrt{\alpha_s t} \quad (8)$$

The value of λ is calculated from the Eqn. (9).

$$\frac{e^{-\lambda^2}}{erf(\lambda)} + \frac{k_l}{k_s}\sqrt{\frac{\alpha_s}{\alpha_l}}\frac{T_m - T_0}{T_m - T_w}\frac{e^{-\lambda^2(\alpha_s/\alpha_l)}}{erfc(\lambda\sqrt{\alpha_s/\alpha_l})} = \frac{\lambda\Delta h\sqrt{\pi}}{c_s(T_m - T_w)} \quad (9)$$

The consistent λ value for the present problem is 0.47385401. $S_{anal}(t)$ data obtained from analytical solution has been used in the fitness function in the genetic algorithm method.

The total solidification time, under the studied conditions, was equal to 35 h and the time step in the numerical simulation was equal to 0.5 h. The position of the solidification front along of the time was computed interpolating the numerical temperature profile in each time, considering that the position of the solidification front is the position of T_m.

In order to predict the position of the solidification front correctly, 21 points after bottom end of TNT with equal distance has been defined on the domain as seen in Fig. 3.

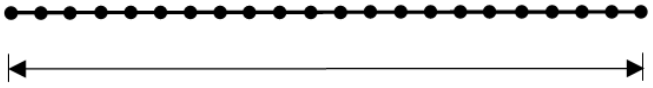

Figure 3. Prediction of the position of solidification front.

2.2. Genetic Algorithm Method

Genetic algorithm is an optimisation method, which can be used in an inverse problem approach to predict unknown parameters of a model. In this sense, reference analytical or experimental data can be employed to build the fitness function. In this work, the optimum ΔT value has been obtained applying the genetic algorithm method, adopting the Neumann's analytical solution as a reference data in the fitness function. This optimisation method is as depicted in Fig. 4.

The genetic algorithm mimics the natural selection of individuals inside a population to build an optimisation problem that maximises a fitness function[14-15].

The fitness function for this study is given in Eq. (10) and genetic algorithm settings are as presented in Table 2.

$$f = 1/\sqrt{\sum_{t=0}^{t=35h}[S_{num}(t) - S_{anal}(t)]^2} \quad (10)$$

Table 2. Genetic algorithm settings

Generations	20
Population size	30
Number of genes of each chromosome	60
Crossover probability	0.8
Crossover type	1 point
Mutation probability	0.025
Tournament selection parameter	1

The initial population is usually randomly generated and each candidate solution for ΔT is represented by a single individual (or chromosome)[14-15]. The chromosome is an array of binary numbers (or genes) and is as represented in Fig. 5.

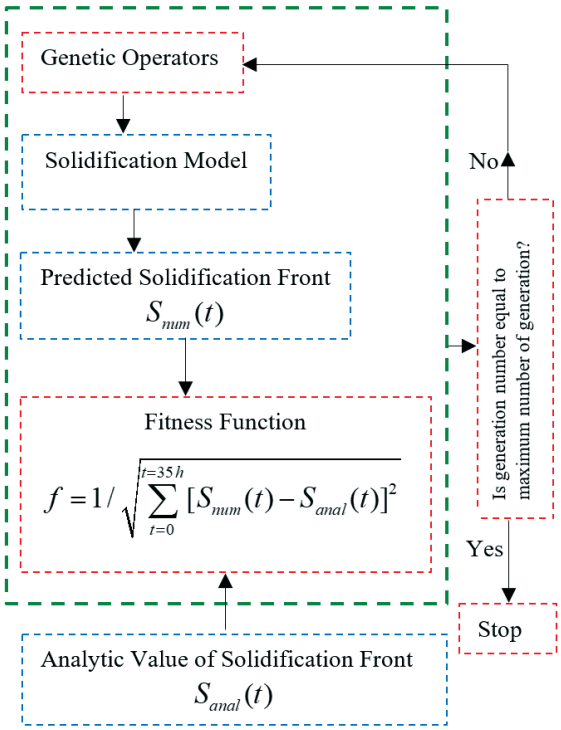

Figure 4. Optimisation flow chart.

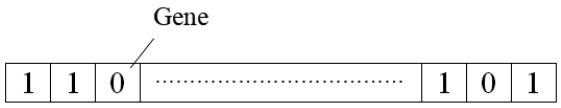

Figure 5. Chromosome.

The optimum value of ΔT has been investigated in a feasible search space from 0 to 5K.

The best individuals are selected for the next generation, according to fitness function[14-15]. Tournament selection method has been performed for two randomly selected individuals and the tournament selection parameter is set as 1 to guarantee that the best individual will be in the next generation. This parameter can be set from 0 to 1 and increasing this value, the probability of the fittest individual survive to the next generation also increases.

The crossover probability establishes the probability of a selected couple change genes between chromosomes. It can occur in one, two or more chromosome points, but in this work a single point was chosen.

In order to recall lost information and ensuring the search space large enough, mutation is applied sweeping population and changing value on the gene from 0 to 1 or vice versa due to mutation probability for a binary representation[14-15].

The best individual for each generation was cloned to the next generation to protect the best one. It is an elitism procedure.

3. RESULTS AND DISCUSSION

Before starting to analysis, mesh dependency analysis has been performed for ΔT = 2K as seen in Table 3.

The sensibility of the results and the computational time are proportional to the number of elements. However, after performing a mesh dependency analysis, a mesh with 25602 elements has been chosen to conduct the numerical simulations regarding sensibility and computational time.

Table 3. Solidification front for various number of elements

Solidification front S (m) at t = 35 h	Number of elements
0.1393	202
0.1381	804
0.1377	3216
0.1374	12801
0.1372 (Chosen)	25602
0.1371	51204
0.1373	102408
0.1373	204816

The proposed procedure has identified the optimum value of ΔT and the corresponding fitness value, respectively, equal to 0.872055630912406 K and 123.6549 m^{-1}.

The dimensionless form of the analytical solution and the numerical solution with the optimised ΔT for the evolution of the solidification front along of the time is as shown in Fig. 6.

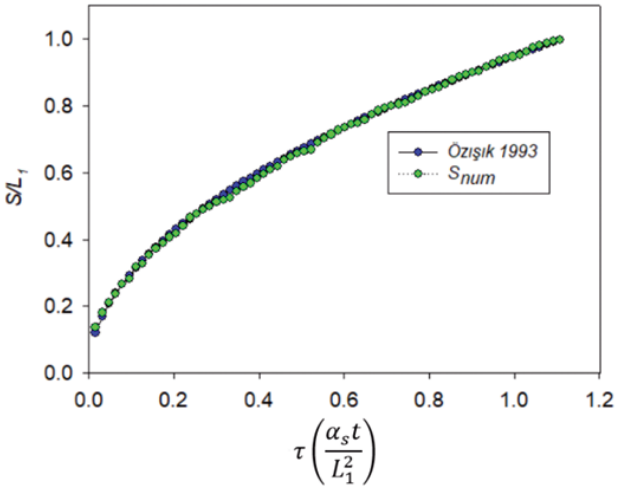

Figure 6. Evolution of the solidification front, S_{num} and S_{anal}.

The numerical and Neumann's analytical solutions have predicted almost the same curve for the evolution of the solidification front along of the time as shown in Fig. 6 and the maximum difference between these curves is 0.0208. However, this value is 0.0591 in the case of ΔT = 2 K.

The maximum and average fitness values, considering Eqn. (10), for each generation is illustrated in Fig. 7. Average value of the fitness function shows an increasing trend with the number of generations. This means that the optimisation method is effective. On the other hand, the optimum value of the ΔT has been reached at the fifth generation.

4. CONCLUSIONS

In this study solidification process of TNT has been modelled in Comsol Multiphysics Modeling Software. Apparent heat capacity method has been used in the model. The model parameter ΔT was an unknown parameter of the model.

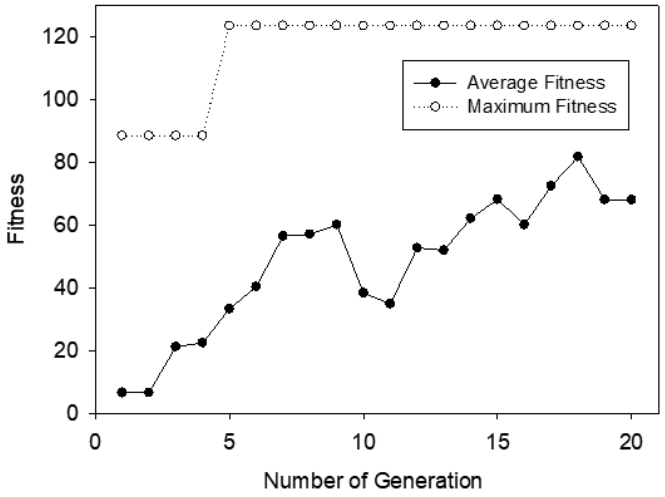

Figure 7. Fitness values.

A genetic algorithm optimisation procedure was proposed to determine the unknown parameter, considering the inverse problem concepts and minimising the differences between the numerical and the analytical solutions for the evolution of the solidification front along of the time. The genetic algorithm has adopted 30 individual in the population and 20 generation. The efficiency of the genetic algorithm was proven since the optimum model parameter value was determined in five generation. The Neumann's analytical solution has been used as a reference solution in the fitness function. It has been shown that for the optimised ΔT, numerical results for the solidification front are almost the same of the analytical ones. Then, the proposed optimisation procedure is one useful way to determine the unknown parameter, avoiding the traditional trial and error procedure.

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She had performed the numerical analysis of this study and adapted genetic algorithm method to this research.

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