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NUMERICAL SIMULATION OF TNT CASTING IN A SHAPED CHARGE SHELL

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Abstract *The present work is devoted to numerical simulation of TNT casting in a shaped charge shell. This kind of device is relevant in military and civilian applications, being used in anti-tank ammunitions and warheads and in petroleum industry for perforating well liners. TNT casting is one of the steps to manufacture the high explosive shaped charge and depending on the cooling conditions, during TNT solidification, defects can be formed. These defects can be cracks, voids and gaps, reducing the device efficiency and increasing the risk of accidental detonation. Then, the heat transfer process during TNT cooling and solidification inside an axis-symmetrical cavity is studied. The apparent heat capacity method is employed on a transient-diffusive heat transfer equation to model the phase change. The shaped charge has a conical void and three different height values of this void cone are analyzed. The boundary conditions are the prescribed temperature on the conical surface and natural convection on others surfaces. The numerical simulations were performed by using COMSOL Multiphysics and Modeling Software, which is based on the finite-element method. The results have shown that the cone geometry have considerable influence in the time of the solidification process and in thermal stress intensity. This influence must be taking into account, during shaped charge and manufacture process designs.*

Keywords: *shaped charge, solidification, apparent heat capacity, explosive, ammunition.*

1. INTRODUCTION

High explosives are substances designed to detonate by the action of a shock wave, furnishing very high amount of power. In order to concentrate the explosion effects in one specific point, the cylindrical shaped charges were developed. Usually, this kind of shaped charge has a conical void in one tip of the explosive and at the opposite tip an initiator is inserted. Then, when the explosive is ignited, the detonation wave propagates from the tip with the initiator to a conical void region. So, the conical void in the explosive directs the reacted gases to a single point. If the explosive surface in contact with the void is coated by a metal liner, where cooper or aluminum are the most used, a hypervelocity jet of liquid metal can be formed after the detonation wave and this jet can reach velocities higher than 8 km/s. In this sense, this device is useful to perforate solid materials. Hereupon, shaped charges have been used to perforate armors and rocks with military and civilian applications, being used in anti-tank ammunitions and warheads and in rock perforation in petroleum industry.

Symmetry is a key aspect of the well-functioning of a cylindrical shaped charge device, affecting the penetration efficiency. Asymmetries reduce the concentration of power, since the asymmetries can break the jet of liquid metal or become the jet thicker. Different kinds of manufacture problems can introduce asymmetries in the shaped charge as inaccuracies of the initiation system, dimensional inaccuracies of the liner, casing and their assembly and also voids, gaps and cracks, which can be formed during explosive cooling and solidification (Ayisit, 2008).

Casting is one of the most used loading techniques to fill shells with high explosives, but during this process defects can be introduced in the product as porosity, voids, gaps and cracks. These defects change the velocity of the detonation wave, decreasing the device efficiency and increasing the risk of accidental ignition (Ayisit, 2008, Annapragada et al., 2008, Caldeira et al., 2016, Ji and Lin 1998, Sun and Garimella, 2005, Sun and Garimella, 2007).

The mathematical modelling for the heat transfer with phase change has been studied for long time. The Stefan problem was depicted in 1891, but it is restricted to a unidimensional transient-diffusive heat transfer equation (Hu and Argyropoulos, 1996), establishing an analytical solution that requires the determination of the phase change frontier position a long of the time. As time goes by and with the intense increment in the computers' capabilities, the development of numerical approaches have been increased using finite differences, finite volumes and finite elements methods allied with following heat transfer with phase change models: the enthalpy method, the apparent heat capacity method and the effective heat capacity method (Caldeira et al., 2016, Catureba et al., 2019, Hu and Argyropoulos, 1996, Susantez and Caldeira, 2019). These three models do not map the phase change frontier a long of the time, but it can be determined by postprocessing of the numerical solution.

Numerical modeling of explosive solidification is an important tool to avoid manufacturing defects related with inefficient cooling and solidification process of explosive loading in ammunitions and in warheads (Caldeira et al., 2016, Catureba et al., 2019, Susantez and Caldeira, 2019, Annapragada et al., 2008, Ji and Lin 1998, Sun and Garimella, 2005, Sun and Garimella, 2007). Nevertheless, most of the solidification studies are devoted to fragmentation ammunitions and not deals with shaped charge ammunitions. The more complex geometries of the shaped charges impose challenges to control and to optimize the cooling and solidification process of explosives, including hot or cold spots near the conical surface, which increase the thermal stress in the explosive, creating conditions to form cracks and voids. Therefore, the purpose of this study is to present the numerical solution of cooling and solidification process of TNT inside a shell with a conical void shape. The effects of the cone height on the solidification process is analyzed.

2. PHYSICAL PROBLEM AND MATHEMATICAL FORMULATION

The present work simulates the cooling and solidification process of TNT inside an axis-symmetrical shell of a shaped charge ammunition with a conical void. The apparent heat capacity method is employed, considering time dependent heat equation in cylindrical coordinates. The numerical solution was performed by using COMSOL Multiphysics and Modeling Software and three void cones with different heights were analyzed. The explosive domain adopted is represented in Fig. 1, while the mold wall was not considered in the simulations. Heat losses to the surrounding environment by free convection were accounted by Newton's law, with a heat transfer coefficient h_∞ and environment temperature T_∞. The inner cone wall was considered isothermal with temperature T_w. Heat losses through radiation were neglected. Besides that, the explosive density was considered varying due to the phase, while the specific heat and the thermal conductivity were considered constant.
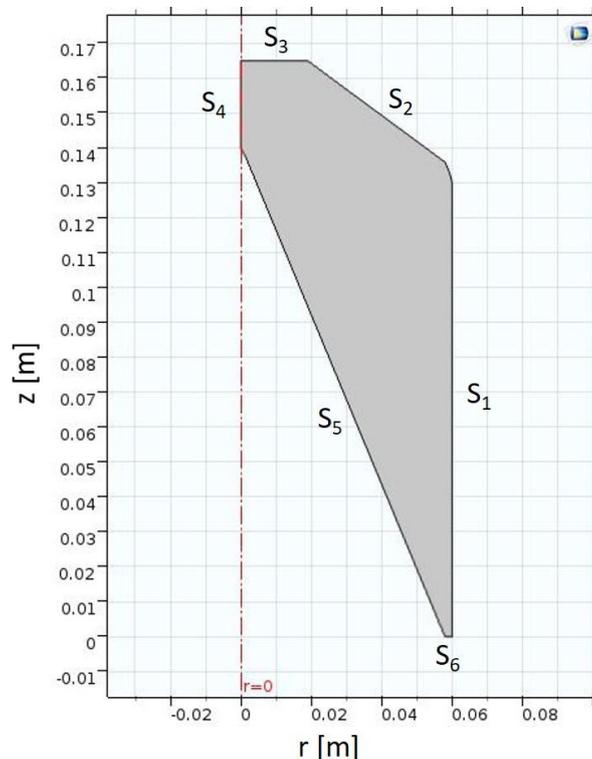

Figure 1. Geometry representing the explosive domain inside the mold.

The explosive was assumed initially with a uniform temperature, T_0. The mathematical formulation for the physical problem is given by:

$$C_{ap} \frac{\partial T}{\partial t} = k\nabla \cdot (\nabla T) \qquad\qquad t \geq 0 \qquad\qquad (1)$$

$$T = T_0 \qquad\qquad t = 0 \qquad\qquad (2)$$

$$-k \frac{\partial T}{\partial n_i} = h_{\infty_i}(T - T_\infty) \qquad S = S_{1,2,3} \qquad t > 0 \qquad\qquad (3)$$

$$\frac{\partial T}{\partial r} = 0 \qquad\qquad S = S_4 \qquad t > 0 \qquad\qquad (4)$$

$$T = T_w \qquad\qquad S = S_{5,6} \qquad t > 0 \qquad\qquad (5)$$

In the apparent heat capacity method, the latent heat of fusion, h_m, is accounted as indicated in Eq. (6):

$$C_{ap} = \begin{cases} \rho_s c_s & T \leq T_m - \Delta T \\ \dfrac{\rho_s h_m}{2\Delta T} + \dfrac{\rho_s c_s + \rho_l c_l}{2} & T_m - \Delta T < T < T_m + \Delta T \\ \rho_l c_l & T \geq T_m + \Delta T \end{cases} \qquad (6)$$

where the thermophysical properties of TNT explosive used are presented in Tab. 1.

Table 1. Thermophysical properties of TNT.

Thermal Properties	Value	Unit	Reference
Thermal Conductivity, k	0.26	W/(m.K)	Caldeira et al. (2015)
Liquid specific heat capacity, c_l	1062.2	J/(kg.K)	Caldeira et al. (2015)
Solid specific heat capacity, c_s	1062.2	J/(kg.K)	Caldeira et al. (2015)
Liquid phase density, ρ_l	1544.6	kg/m³	Caldeira et al. (2015)
Solid phase density, ρ_s	1648	kg/m³	Caldeira et al. (2015)
Melting temperature, T_m	354.05	K	Caldeira et al. (2015)
Latent heat, h_m	98.4	kJ/kg	Caldeira et al. (2015)
Half of phase change temperature range, ΔT	0.872	K	Susantez and Caldeira (2019)

The explosive was considered initially at the liquid phase with a temperature T_0 above the melting temperature T_m. As the time evolves, the TNT solidifies due the contact with the cone wall (S_5 and S_6), considered with a temperature T_w below the melting temperature, and also due the heat transfer to the surrounding ambient air, considered at T_∞. Distinct values for the free convection heat transfer coefficients were used for the heat exchange among the air and outer surfaces (S_1, S_2 and S_3), where the calculations were made regarding their length and slope (Churchill and Chu, 1975, Radziemska and Lewandowski, 2001). The values considered in this work are given in Tab. 2.

Table 2. Model parameters.

Parameters	Value	Unit	Reference
Heat transfer coefficient, $h_{\infty l}$	6.38	W/(m².K)	Churchill and Chu (1975)
Heat transfer coefficient, $h_{\infty 2}$	6.73	W/(m².K)	Churchill and Chu (1975)
Heat transfer coefficient, $h_{\infty 3}$	5.83	W/(m².K)	Radziemska and Lewandowski (2001)
External temperature, T_∞	300	K	Caldeira et al. (2015)
Cone temperature, T_w	300	K	Caldeira et al. (2015)
Initial temperature, T_0	360	K	Caldeira et al. (2015)

3. NUMERICAL SOLUTION

The numerical solution in this work, which makes use of finite element method in COMSOL Multiphysics and Modeling Software was verified by using analytical solution available in the literature and validated by considering experimental results provided by Chen and Shiuan (1992). After the validation, the solution for different shaped charge conical geometries were obtained. The numerical simulations were run in a computer having 64 bits, Windows 10, Processor Intel® Core™i7-7500U CPU@2.70Ghz 2.90 GHz and with 16GB of RAM.

3.1 Verification

First, the analytical solution provided by Rathjen and Jiji (1971) was used for the code verification. In their work, a 2D cartesian geometry, having heat conduction with freezing in a corner was considered. Their solution was applied to a square geometry with 0.1 m side. The boundaries at the abscissa and ordinate axis were considered isothermal with temperature T_w, while the outer surfaces were considered isolated. The TNT thermal properties showed in Tab. 1 were considered for the solution. The analytical formulation was solved considering C = 0.00737, m = 2 and λ = 0.47198. To solve the mathematical formulation presented in Eq. 1 in COMSOL Multiphysics and Modeling Software, the following initial and boundary conditions were applied:

$$T = T_0 \qquad 0 \leq x \leq 0.1 \qquad 0 \leq y \leq 0.1 \qquad t = 0 \tag{7}$$

$$T = T_w \qquad x = 0 \qquad 0 < y < 0.1 \qquad t > 0 \tag{8}$$

$$\frac{\partial T}{\partial x} = 0 \qquad x = 0.1 \qquad 0 < y < 0.1 \qquad t > 0 \tag{9}$$

$$T = T_w \qquad 0 < x < 0.1 \qquad y = 0 \qquad t > 0 \tag{10}$$

$$\frac{\partial T}{\partial y} = 0 \qquad 0 < x < 0.1 \qquad y = 0.1 \qquad t > 0 \tag{11}$$

The comparison between the analytical and numerical evolution of the solidification front are presented in Fig. 2. The discrepancies among the solutions increase as the time evolves having a maximum relative error of 8% for the front analyzed after 3 hours of solidification.
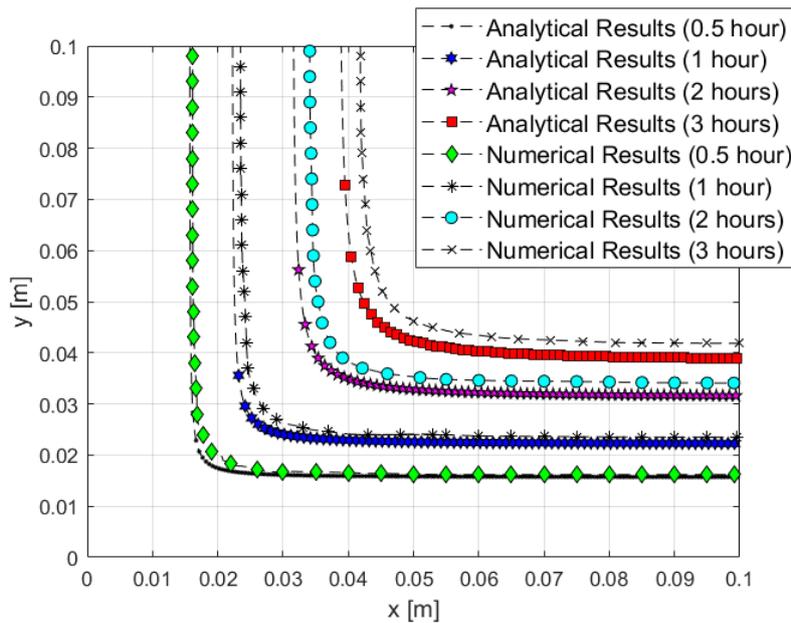

Figure 2. Evolution of solidification front using Rathjen and Jiji (1971) analytical solution and COMSOL *Multiphysics* numerical solution.

Moreover, the differences between the analytical and numerical results shown in Fig. 2 can be devoted to the fact that the apparent heat capacity method considers a mushy region, which means that the phase change proceeds in a temperature range. Otherwise, the analytical solution provided by Rathjen and Jiji (1971), considers that the phase change proceeds at a single temperature.

3.2 Validation

The experimental results provided by Chen and Shiuan (1992) was used to perform the validation procedure. In their work, experimental results for the temperature varying with time at the point P at Fig. 3a is presented for the solidification of TNT performed under controlled cooling. The geometry at Fig. 3a represents the domain, due the axis-symmetry of the projectile shape and of the physical problem. The initial temperature of the TNT projectile was considered uniform at 83 °C. The bottom wall was considered at (T_B) 50 °C while the top wall was considered with a prescribe temperature (T_T) of 105 °C. The lateral surface was considered with a prescribed temperature (T_L) varying linearly between 50 °C and 57 °C from the bottom to the top. A probe heating of 24 cm was used during 4 hours to guide the solidification front at a prescribe temperature (T_h) of 105 °C. After this time, the probe heating was neglected and a symmetry boundary condition was considered for all the extension of z axis. At the COMSOL Multiphysics and Modeling Software, the 2D geometry was considered with the dimension presented in Fig. 3a and the apparent heat capacity method was solved considering the thermal properties presented in Table 1. The temperature contours are presented at Fig. 3b and it can be observed that after 36 hours (40 hours in total considering the duration using the probe heating) the solidification process is not yet finished.
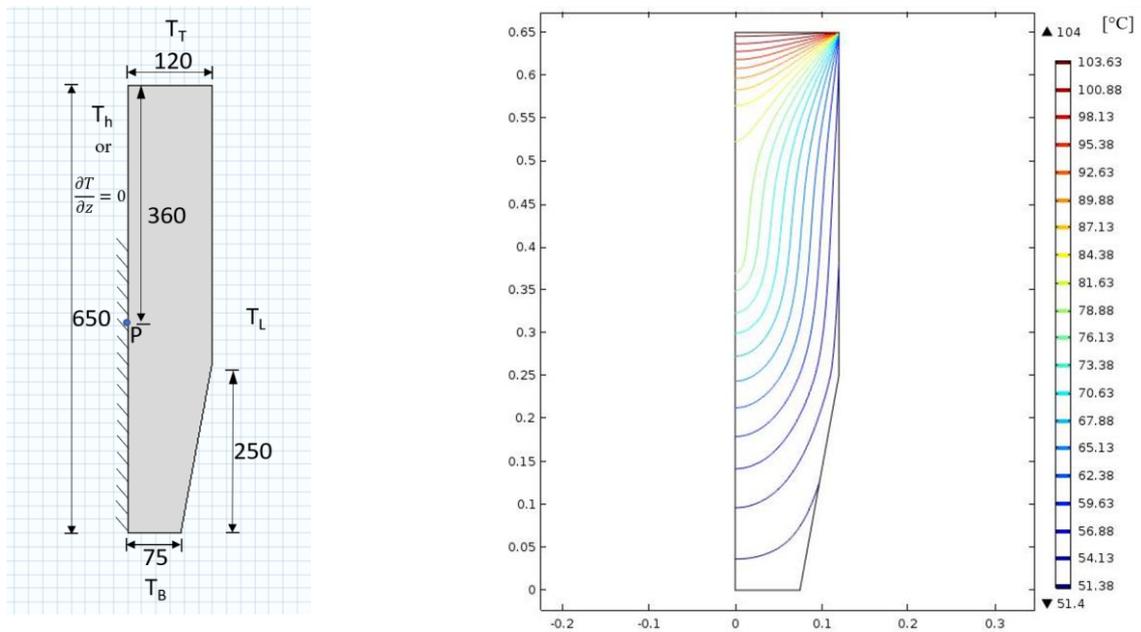

Figure 3. (a) Geometry and boundary conditions for the test problem. (b) Temperature contours at COMSOL *Multiphysics* numerical solution after 36 hours of solidification process.

The comparison among numerical simulations and results of the Chen and Shiuan (1992) for the temperature of the point P evolving with time is presented at Fig.4. The solidification process at point P is only showed for the time after turn off the heating probe. The numerical results present the same behavior of experimental results with possible errors in numerical solution due to the uncertainties in thermophysical properties and boundary conditions. The agreement between the results are considered good and the numerical solution provided by COMSOL Multiphysics and Modeling Software is validated.
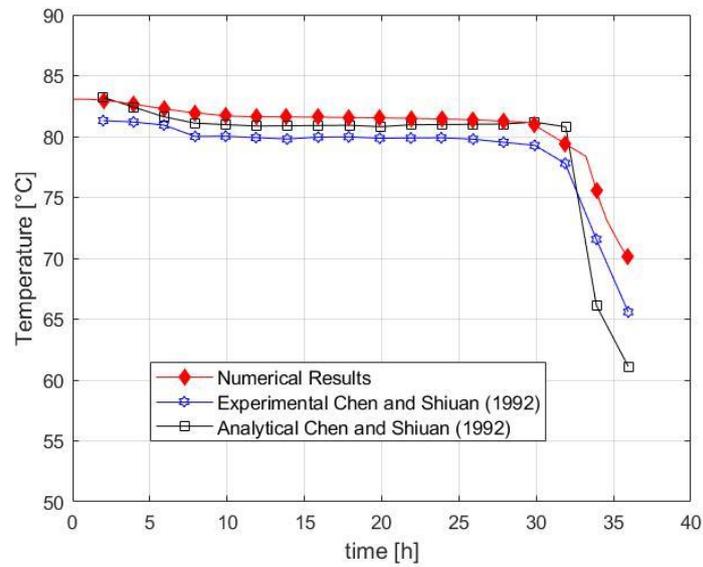
Figure 4. Temperature measurements and analytical results provided by Chen and Shiuan (1992) compared with COMSOL *Multiphysics* numerical solution for point *P* at Fig. 3a.

3.3 Shaped Charge Explosive

In order to solve the mathematical formulation described in Eq. (1) together with restrictions (2) to (5), the simulations were performed in COMSOL Multiphysics and Modeling Software using finite element method. Three distinct values of cone height were investigated as shown in Table 3. The geometry used in simulations are illustrated in Fig. 5 with the respective dimensions.

Table 3. Conical shapes investigation.

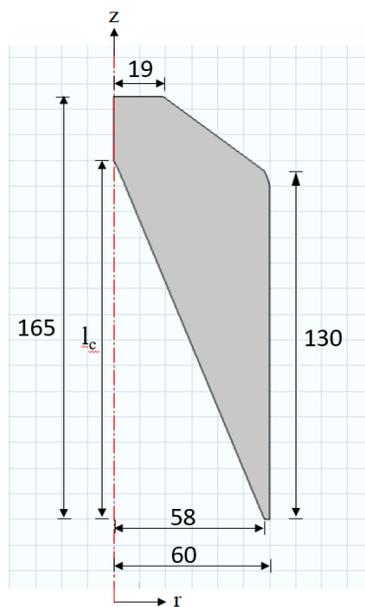| Case	Geometry parameters	Height %	Value	Unit
1	Cone height, l_{c1}	96	158	mm
2	Cone height, l_{c2}	85	140	mm
3	Cone height, l_{c3}	73	120	mm

Figure 5. Drawing with dimensions in millimeters used at the simulations.

The temperature distribution and the evolution of the solidification phase (black contour in the figures) for the three conical shapes investigated in Tab. 3 are illustrated in Figs. 6 to 8. The simulations were performed considering extremely fine triangular meshes with 11916, 13277 and 14973 number of elements for cases 1, 2 and 3, respectively, all having a maximum element size of 0.001 m and a time step size of 1 second. Figs. 6 to 8 show the temperature distribution and solidification front in the cross section of the shaped charge shell for three different investigated cases. Right and left parts in these figures are the places full of TNT. Because of the model is axial symmetric, plots on the right and left sides of the centerline of the shaped charge shell are same. Fig. 6 shows that the solidification front moves from the boundary to inward of the domain, forming a toroidal liquid region that is vanishing in less than 2 hours of phase change. This temperature evolution influences the thermal stress inside the solid explosive. In Fig. 7, the cone wall has a smaller height compared to case 1. Comparing Fig. 6 and 7, it is possible to observe that after half hour of phase change, case 2 has liquid above the vertex of the cone, indicating that the solidification process is faster in case 1 than in case 2. It is expected, since the amount of explosive in case 1 is less than that of case 2. Figure 8 presents the numerical results for the case of the void cone that has the smallest height compared to the other cases. In this case, the solidification process has as a uniform region with an ascendant movement. The phase change process ends up before 3 hours of solidification. This cone geometry induces the slow solidification process since it is the case with more explosive mass. It also leads the symmetrical ascendant movement of phase change fronts. Therefore, this geometry is more suitable to avoid thermal stress sites. The compromise between avoiding thermal stress sites and obtaining the correct pressure and velocity should be taken into account in the shape charged designs.

Time = 0.5 hour

Time = 1 hour
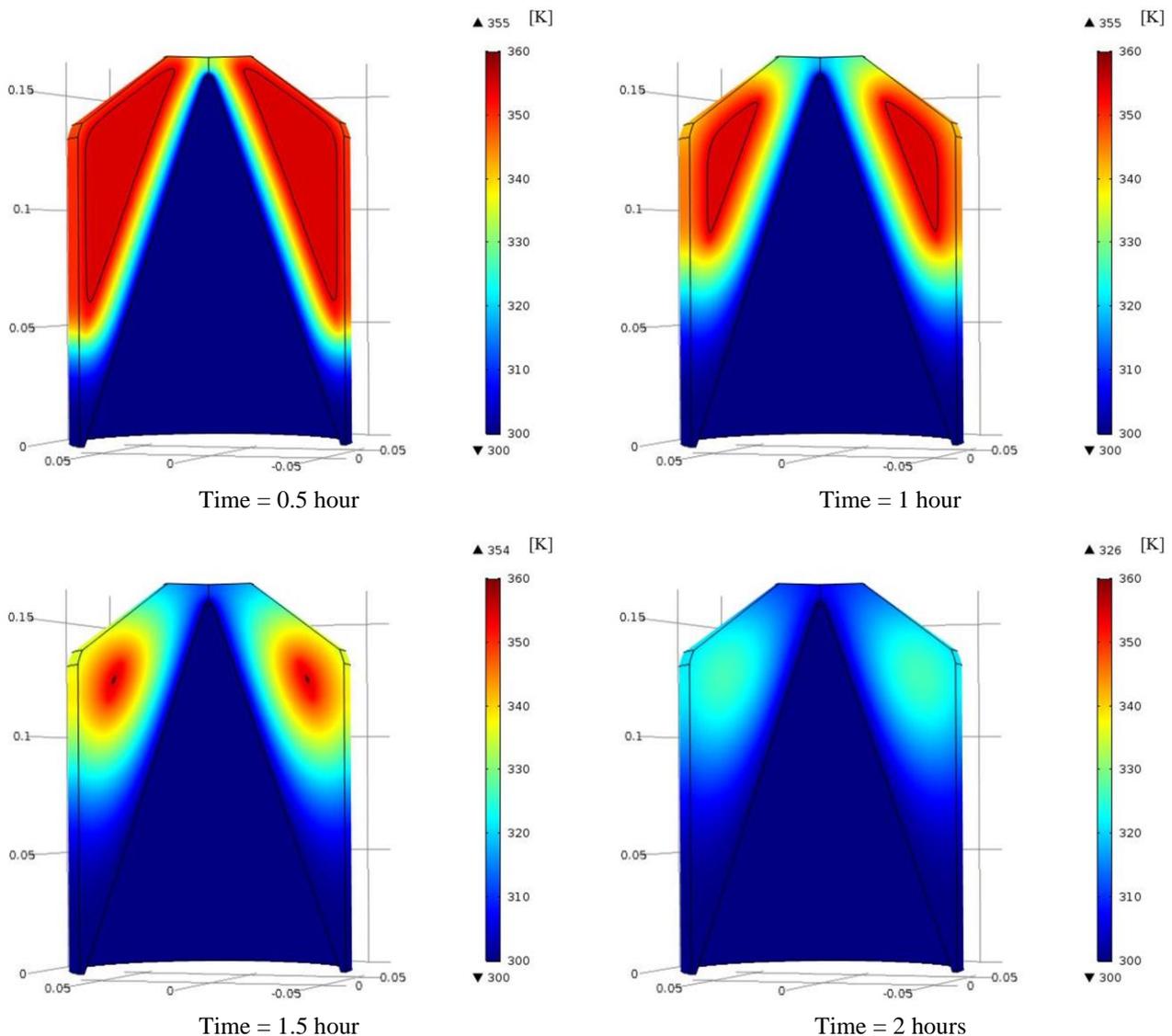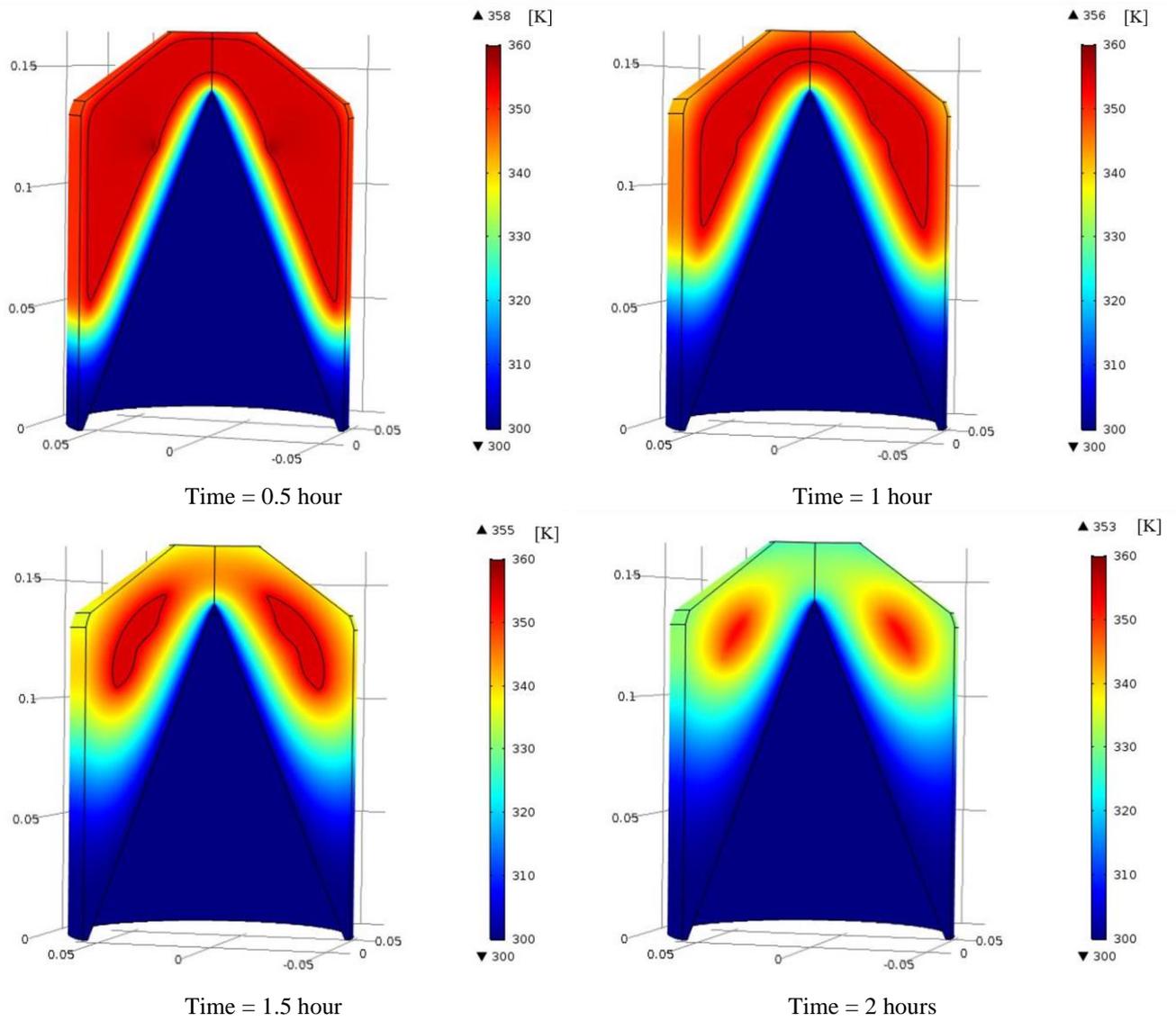
Time = 1.5 hour

Time = 2 hours

Figure 6. Temperature distribution (in Kelvin) and evolution of solidification phase (black contour) considering case 1.

Figure 7. Temperature distribution (in Kelvin) and evolution of solidification phase (black contour) considering case 2.
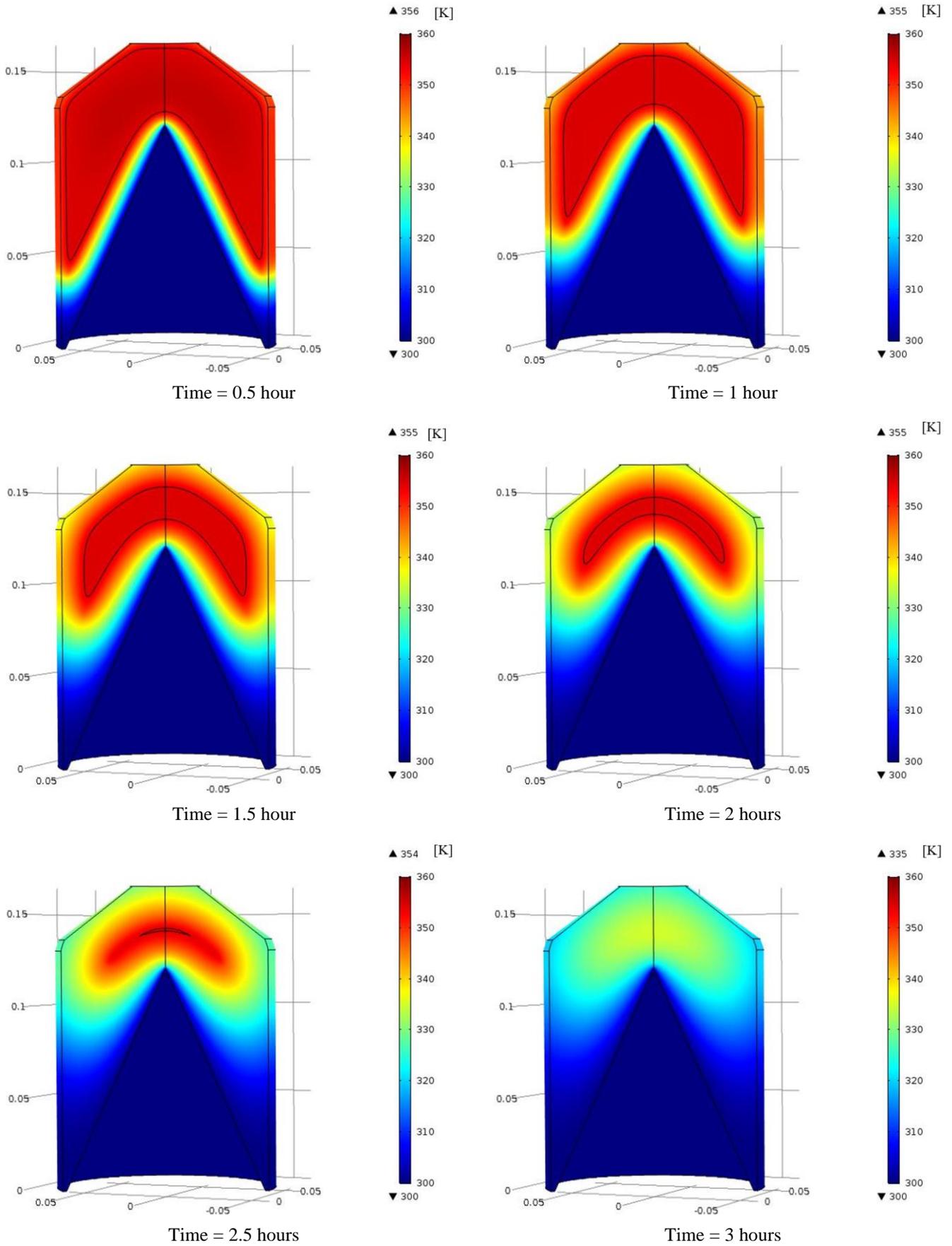
Time = 0.5 hour

Time = 1 hour

Time = 1.5 hour

Time = 2 hours

Time = 2.5 hours

Time = 3 hours

Figure 8. Temperature distribution (in Kelvin) and evolution of solidification phase (black contour) considering case 3.

4. CONCLUSIONS

Shaped charge is a device developed to concentrate the power provided by an explosive detonation in a single point or region. Once the conical region of the explosive is coated by a metal, it can be transformed into a liquid jet of metal by the explosive detonation, which is usually employed to perforate solid surfaces. Depending on the cooling conditions during the explosive solidification, thermal stress spots can be formed, leading to manufacture defects that increase the risk of accidental ignition. It is recommendable to have a slow solidification process with an ascendant front to avoid air entrapment closes to the base that can leads to the detachment of the explosive. Regarding that, the purpose of this work was to obtain a numerical solution for the solidification of shaped charge TNT explosive considering conical shapes with three different heights. The apparent heat capacity method was the mathematical model used to represent the phase change process in COMSOL Multiphysics and Modeling Software and the evolution of the solidification front was observed for different times. The 2D numerical solution was verified using the analytical solution for the heat conduction with freezing in a corner and validated using experimental results for TNT solidification in a shell. Three distinct height of the cone were investigated for the TNT solidification showing that the cone geometry has a considerable effect on the time dependent solidification process and also on the formation of possible thermal stress sites. In the design of shaped charge, this effect must be taking into account. Further work needed to be performed in order to evaluate the amount of thermal stress induced by the shape of the void cone.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE