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Recent Advances on the Solidification Processing of Cast Energetic Materials

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Abstract

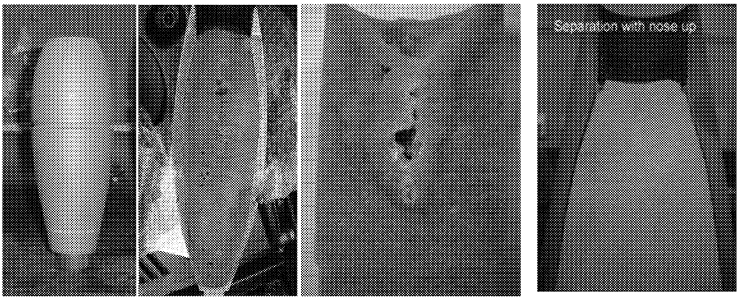
This paper investigates the solidification of highly viscous energetic materials cast into a projectile. Active cooling and heating (ACH) control solidification technology as well as mechanical vibration (MV) are applied to achieve unidirectional solidification and to reduce cracks, gas pores, and shrinkage defects and to decrease the detrimental gap size between the projectile and the solidified energetic material. A comprehensive numerical model was developed to simulate the solidification processes during casting of energetic materials, as well as the resulting induced thermal stresses. The optimized design parameters of the proposed technologies are developed based on numerical modeling and experiment work.

A detailed comparison between the latest experiments performed at the University of Alabama, Solidification Laboratory, obtained with electrical heating and water cooling and with and without mechanical vibration is provided in this paper. In these experiments, a special wax material (*e.g.*, Chlorez 700S) that has similar thermo-physical properties with the IMX-104 explosive material was used. Experiments performed at the USARMY ARDEC using the IMX-104 explosive material with steam heating and water cooling are also presented in this paper. These experiments are being used to further validate the numerical model.

Introduction

Solidification and Casting processes are widely employed in the manufacture of energetic materials. The cooling conditions applied in the casting process can affect the quality of the final cast in terms of void formation, residual stress distributions, and mold separation. Substantial shrinkage is also observed due to the density change upon solidification [1-3]. Residual stresses are known to be closely related to the formation of cold cracks and hot tears during casting. The formation of a gap between the mold and the cast material is of critical importance due to its deleterious effect on heat removal and on crack formation. In the casting of energetic materials all these defects can significantly impair the detonation velocity, Gurney energy, and insensitive munitions characteristics of the formulation, and lead to catastrophic accidents in explosives handling [4-5]. Imposition of carefully controlled cooling condition is thus critical in optimizing the cast quality that could help avoid such destructive effects.

Figure 1 presents the typical mold filling and solidification defects in a 120 mm IMX-104 mortar. The air bubble (entrapped during the mold filling) and the separation and shrinkage formed during solidification are severe. These defects are detrimental to the quality of the 120 mm mortar. Optimization of the process design as well as the design of improved rigging systems is required to minimize/eliminate these defects.



(a) (b) (c) (d)

Figure 1. Casting position (a) and pouring and solidification defects (air bubble and shrinkage cavities ((b) and (c)) and separation (gap) (d)) in the 120 mm mortar.

In the current work, a comprehensive numerical model was developed using ANSYS FLUENT and ANSYS MECHANICAL [6] software to accurately simulate the transport phenomena as well as induced thermal stresses encountered in the casting process of recently developed explosive, consisting of RDX-binder mixtures. An enthalpy method, successfully exploited by many authors [7-8], was used to simulate the solid/liquid phase change process. Instead of working entirely in terms of the temperature of explosive material, an enthalpy function is defined which represents the total heat content per unit mass of the material. The advantage of such a reformation of the problem is that the necessity to track the position of the solid/liquid interface is eliminated. Shrinkage effects and the resulting velocities induced in the melt have been largely neglected in the literature due to the difficulties involved in multiphase pressure-velocity coupling, and the interaction between free surface dynamics and solidification volume change [9]. In order to track the shrinkage shape that is critical in simulation of explosive casting process, NOVAFLOW&SOLID software [10] was used. Effective shrinkage was calculated at each time step and the volume of the solidified material was then subtracted from the liquid phase in the control volumes that contain the interface.

Experimental measurements of physical properties such as thermal conductivity, specific heat, thermal expansion coefficient, and liquid viscosity were conducted using Diamond TMA (www.tmadiamond.com), Hot Disk Instrument, and Brookfield viscometer. The stress-strain relationship was measured using simple compression technique developed in-house [11].

A new technology named “Active cooling and heating” (ACH) that can be used for melt cast process of energetic materials in order to improve product quality is described in this paper. The purpose of the ACH is to use controlled (active) heating and cooling of the mold to try to achieve unidirectional solidification with minimum solidification related defects including gap separation and solidification shrinkage. Figure 3 illustrates the experimental mold setup and cast wax material that shows no shrinkage and gap separation. Optimal cooling parameters predicted by numerical simulations can be easier controlled using the ACH technology. Maintaining higher temperature along a riser and gradually decreasing temperature at the bottom part will keep solid front flat propagating upward. This helps to reduce the excessive thermal stress formed due to large temperature gradient and provides control of shrinkage shape. New design of the riser geometry with electrical or steam heating was proposed after calculation of the thermal modulus distribution inside the projectile.

Numerical Model

The studied energetic material IMX-104 is assumed to be isotropic, incompressible and Newtonian fluid with a very high viscosity due to the high volume fraction of solid particles. The constituents of IMX-104 are DNAN (2, 4-dinitroanisole), NTO (3-Nitro-1, 2, 4-triazol-5-one) and RDX. Of these three constituents only DNAN undergoes solid/liquid phase change while NTO and RDX remain in solid, crystalline form during the entire process. The solidifying melt was modeled as a single material with temperature-dependent density, thermal expansion coefficient and Young's modulus, with all other properties remaining the same in both solid and liquid phases. The variation of density with temperature was described by Boussinesq approximation. The numerical model was based on solving the system of governing equations for conservation of mass, momentum, and energy:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \tag{1}$$

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \vec{u}) = -\nabla p + \nabla \cdot \left[\mu \left(\nabla \vec{u} + \nabla \vec{u}^T\right)\right] + \rho_\infty \vec{g} \beta_l (T - T_\infty) + \frac{(1 - f_l)}{\left(f_l^3 + \varepsilon\right)} A_{mush} \vec{u} \tag{2}$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \vec{u} h) = \nabla \cdot (k \nabla T) \tag{3}$$

where A_{mush} is the mushy zone constant, f_l the liquid fraction, ε =0.001 is used to prevent division by zero, and $h = c_p T + f_l \Delta H$, the specific enthalpy of the melt.

In the absence of detailed visco-elastic-plastic material properties, the material was treated as an isotropic thermo-elastic material:

$$\frac{\partial}{\partial t}\left(\rho \frac{\partial \vec{w}}{\partial t}\right) = \nabla \cdot \left[\mu \left(\nabla \vec{w} + \nabla \vec{w}^T\right)\right] + \nabla\left(\lambda \nabla \cdot \vec{w} + (3\lambda + 2\mu)\beta_s T\right) - \left\{\nabla \cdot \left[\frac{\sigma_{ij}^d \sigma_{kl}^d}{\vec{\sigma}^2}\left(\frac{9G^2}{H' + 3G}\right)\nabla \vec{w}\right]\right\} + \vec{b} \tag{4}$$

where $\lambda = \frac{\upsilon E}{(1+\upsilon)(1-2\upsilon)}$, μ are Lame's coefficients, H' is the plastic modulus, G is the shear modulus and b is the body force.

In order to analyze the shrinkage and void formation caused by the density change during solidification, the algorithm employed must be capable of tracking a moving free surface. The volume of fluid (VOF) method is employed in this work since it can handle free surface movement and has been previously applied to study solidification shrinkage. For the casting problem considered, only two phases, i.e., IMX-104 and air is present in the system. When the density change upon solidification is taken into consideration, the governing equations for conservation of mass, momentum, and energy will have the additional source terms due to the density difference between the solid and liquid phases of IMX-104. The resulting system of equations is solved by NOVAFLOW&SOLID software.

Experimental Results

The experimental setup with ACH at the University of Alabama (UA) is shown in Figure 2. Figure 3 illustrates the experimental mold setup and the cast wax material that shows no shrinkage and gap separation. A special wax material (*e.g.*, Chlorez 700S) was used in these cast experiments. The wax material has similar thermo-physical properties with the IMX-104 explosive material and it can be safely used in the UA lab for process optimization. Electrical heating (60 W and 150 W heaters) and water cooling systems were applied in the experiments to control the solidification process in such a way to minimize both the gap separation and the shrinkage defects in the top portion of the mortar.

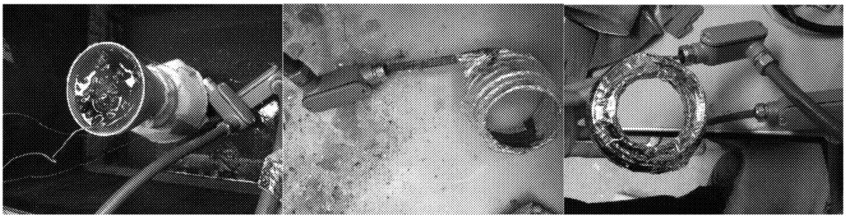

(a) (b) (c)

Figure 2. Experimental setup for the active cooling and heating (ACH) of the 120 mm mortar: (a) top view of the solidified mortar in the water tank and (b) 60W electrical heating system and (c) 150W electrical heating system.

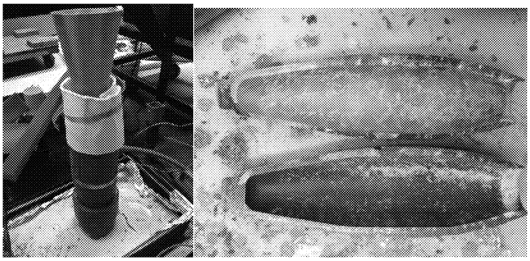
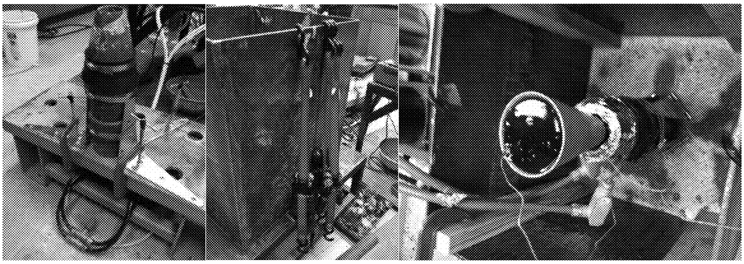

(a) (b)

Figure 3. Experimental mold setup (a) and (b) Cast wax (Chlorez 700S) material without shrinkage and gap separation (preheated mold, 60W electrical heating, without water cooling).

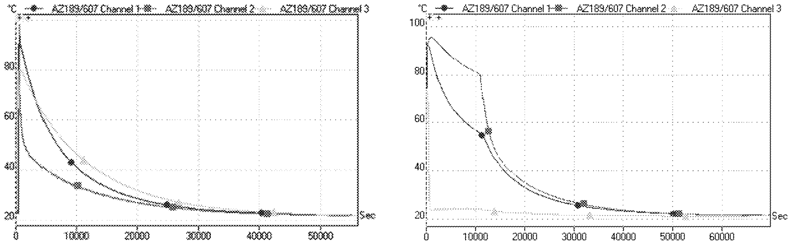
Figure 4 show the experimental setup of the mortars with MV and with and without water cooling. The process conditions are explained in the following paragraph. The wax material was melt in a furnace at 423K for 9 hours. The mold (mortar case) was preheated to 423K. The heating cable was set at 373K for 2 hours after pouring the wax material. Water cooling was done in three steps (similar heights) (i) water flow rate at 1.26 l/min for 20 min (ii) 0.95 l/min for 30 min; (iii) 0.63 l/min for 40 min.

Figures 5 and 6 present the temperature experiments for the setup with MV system as illustrated in Fig. 4, without and with water cooling, respectively. In Figures 5 and 6, T1 (or channel 1) is the thermocouple located inside of the cast material (neck area), T2 (or channel 2) is the thermocouple inside the thermal isolation (neck area), and T3 (or channel 3) is the thermocouple located in the middle height of the mortar case beneath the thermal isolation area. It can be seen from Figs. 5 and 6 that the addition of both heating and vibration had positive effects on the temperature evolution profiles of the 120 mm mortar. Fluidity of the wax material (that helps feeding the solidification shrinkage) was significantly increased due to the use of mechanical vibration.

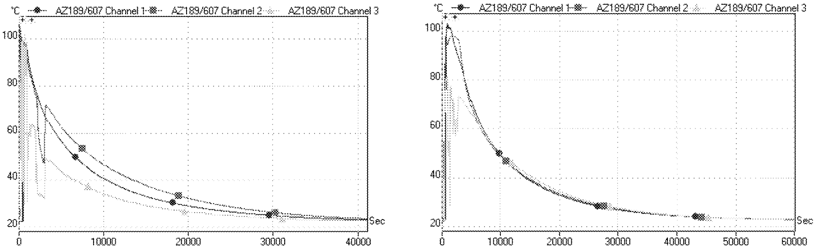


(a) (b) (c)

Figure 4. Experimental setup with MV: (a) mortar assembled on the MV system (without water cooling) (b) water cooling tank connected to the MV system and (c) mortar assembled (with 150W electrical heating) inside the water cooling tank.

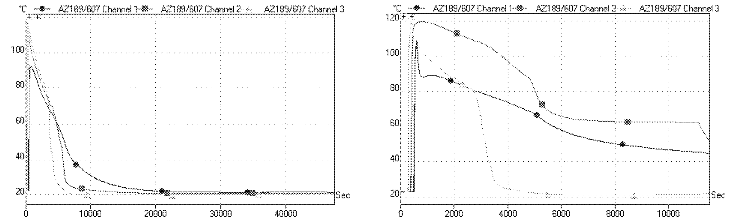


(a) without MV without heating (b) without MV with heating

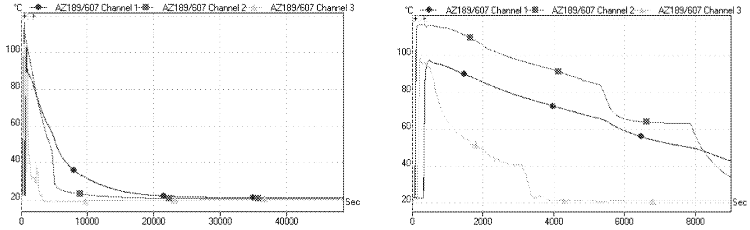


(c) with MV without heating (d) with MV with heating

Figure 5. Temperature measurements in the wax experiments (without water cooling).



(a) without MV without heating (b) without MV with heating

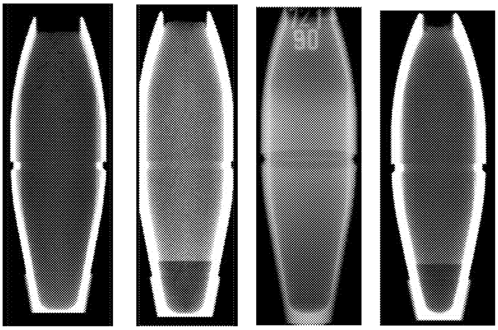


(c) with MV without heating (d) with MV with heating

Figure 6. Temperature measurements in the wax experiments (with water cooling).

Controlled directional solidification was achieved in the 120 mm mortar (Figs. 5 and 6) by using the electrical heating and water cooling technology (ACH). The solidification shrinkage in the top portion of the mortar was completely eliminated. Also, no gap separation was observed in these mortars.

Figure 7 showed some of the experiments performed at USARMY ARDEC facility using IMX-104 material cast into 120 mm mortars. The experiments were performed under different solidification conditions. Improved process conditions (Figs. 7 c and 7d) eliminated the major solidification related defects shown in Figs. 7a and 7d.



(a) (b) (c) (d)

Figure 7. USARMY ARDEC Experiments: (a) macro-shrinkage (top portion) (b) longitudinal macro-cracks (c) and (d) no macro-defects.

Numerical Simulation Results: Design Improvements

NOVAFLOW&SOLID [10] and ANSYS'S FLUENT [6] were used in this study to perform all casting simulations needed to improve the mold design. The results of the original design are shown in Refs. [12-14]. The new design consists of several improvements including the geometry modification of the top riser, mold preheating and application of mechanical vibration as well as application of electrical or steam heating techniques in the neck area between the top riser and the mortar. The results of the ACH with electrical heating are shown in Figures 6-8 in Ref. [14]. It was demonstrated in Ref. [14] that the active heating can be applied to improve feeding and therefore can eliminate the macro-shrinkage in the neck area.

Figures 8 and 9 present the results with the without steam heating. The steam heating technology needs to be used for safety reasons. Based on the results in Figure 9, it can be concluded that steam heating can successfully replace the electrical heating.

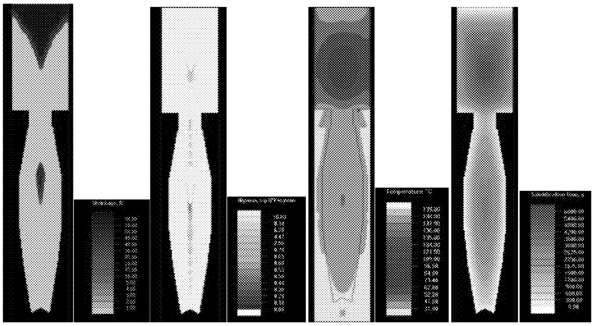

(a) (b) (c) (d)

Figure 8. Predicted micro-shrinkage (a), macroshrinkage (b), temperature (c) and solidification time (d) in the 120 mm mortar cooled in water (no steam heating, Al riser preheated at 110 C).

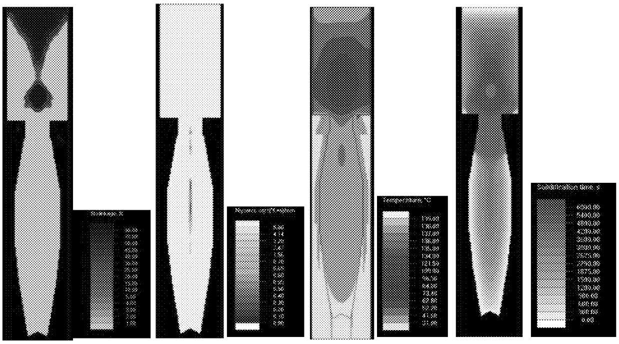

(a) (b) (c) (d)

Figure 9. Predicted micro-shrinkage (a), macroshrinkage (b), temperature (c) and solidification time (d) in the 120 mm mortar cooled in water (steam heating, Al riser preheated at 110 C).

Concluding Remarks and Future Work

Experimental and modeling studies have been performed to improve the design and process conditions of energetic materials cast into a projectile. The proposed improvements led to significant decrease in casting and solidification shrinkage defects in the cast projectiles. The improved process design consists of using ACH technologies with proper modifications in the top riser geometry, pouring rates, mold preheat temperature, and water cooling conditions. MV was also studied. It was shown that: (i) ACH with MV can improve the directional solidification conditions of the mortar that can further decrease the solidification shrinkage, cracking tendency and gap separation and (ii) steam heating can replace successfully the electrical heating.

Future work will include a detailed study regarding the mechanical vibration (MV) and steam heating effects on the solidification of energetic materials cast into projectiles.

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