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Numerical Analysis of Shock Initiation on Highly Energetic Material LX-04

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Abstract. The paper presents investigation of shock initiation effects on highly energetic material LX-04, an HMX based one, by a blunt brass projectile using numerical modelling methods implemented in LS-DYNA software. Multi – Material Arbitrary Lagrangian Eulerian (MM-ALE) formulation has been used to provide the possibility of fulfilment of the elements with multiple materials accordingly to multiple phases of the composition detonated. The work is focused on LS-DYNA's equation of the state keyword *EOS_IGNITON_AND_GROWTH_IN_HE. Proper comparison with experimental data is presented. The introduction into the subject of highly nonlinear transient dynamic finite element analysis, possibilities, and superiority of this kind of modelling are being discussed. Reasons of sustaining the need of data by numerical solutions rather than experimental handling in military applications are given. Some of typical technical issues, occurring during such a fast-performing phenomenon, and the need of experimental validation of the models are typed together with detonation-state determination's observation capabilities.

Keywords: numerical modelling, finite element method, shock initiation

1. INTRODUCTION

Shock initiation is a major property of highly energetic materials, which determines composition's ability to detonate due to pressure growth in its volume caused by an external loading. It is important for safe storage and controlled initiation reasons. This paper discusses numerical analysis of blunt brass projectile impact on initiation of a high explosive. The brass projectile has a diameter equal to 12.7 mm and it is 22.2 mm long. Similar problem was investigated by L.E. Schwer [1] on the Composition-B. The genesis for the creation of appropriate experimental research was caused by the need to create a concept for mines neutralization impact speed determination. Quantity of factors affecting the phenomena that run so violently as an explosion makes the experiment an indispensable part of the results. Many material models and state equations have emerged and they are likely to emerge, which will take into account more and more complex significant phenomena or will seek to minimize the time of numerical calculations while maintaining an acceptable convergence of results with actual experiments.

The Ignition & Growth of Reaction in High Explosives [3] equation, used for this paper's purpose, has been known for many years and the number of collected experimental data is growing. In the LS-DYNA Keyword Manual [4], only LX-17 (TATB 92.5% and Kel-F 800 7.5%) and PBX-9504 (TATB 70%, PETN 25%) and Kel-F 800 5%) and based on HMX as discussed in this work LX-04 (HMX 85% and Viton-A 15%), LX-10 (HMX 95% and Viton-A 5%) and LX-14 (HMX 95.5% and Estane 5702-F1 4.5%) were listed as sufficiently and thoroughly tested and as a result their data can be considered as reliably valid material models. The equation is also used to solve the issues of safety and efficiency of solid rocket fuels. It is used for modelling of shock-to-detonation transition (SDT), which is caused by the pressure growth and energy concentration at the elements what leads to hotspots. Reaction front propagates from such and may strengthen the imposed shock leading to detonation. Impact imposes the energy. LX-04 is a material historically used in the design of shaped charges. Some of the parameters defining the material were listed in Table 1 [9].

Table. 1. LX-04 properties

Property	Value
Detonation velocity	8.46 km/s
Chapman-Jouguet pressure	35.0 GPa
Theoretical maximal density	1.889 g/cm^3

Recent works [10] do compare the Ignition & Growth EOS results with historical and new experimental 1D and 2D data and JWL (Jones-Wilkins-Lee) reaction product EOS predicted by CHEETAH code.

Chemical equilibrium CHEETAH code generated product JWL EOS and the Ignition & Growth product JWL presents good acknowledgement with experiment data, but the Ignition & Growth EOS is normalized to a great deal of experimental data.

2. EQUATIONS OF STATE AND A CONSTITUTIVE MODEL

The Ignition & Growth of Reaction in High Explosives equation of state, represented by the *EOS_IGNITON_AND_GROWTH_IN_HE keywords in the LS-DYNA software, is a key element of the performed analysis. It is based on two JWL, Eq. (1), one for reaction products, the other for unreacted ingredients.

$$p = Ae^{-R_1 V} + Be^{-R_2 V} + \omega C_V T/V \tag{1}$$

where p is the pressure, V is the relative volume, ω is the Gruneisen coefficient, C_V is the average specific heat, and the remaining coefficients are the calibration constants.

The effect of the explosive reaction is determined by Eq. (2) controlling the course and quantity of reacted gases, where the individual of the three parts are active only for specific fractions of reacting material.

$$\frac{dF}{dt} = I\,(1-F)^b \left(\frac{\rho}{\rho_0} - 1 - a\right)^x + G_1(1-F)^c F^d p^y + G_2(1-F)^e F^g p^z \tag{2}$$

where F is the ratio of unreacted substance to the products of detonation, t is the time, ρ is the density, ρ_0 is the initial density, and I, G_1, G_2, a, b, c, d, e, g, x, y are the constant calibration factors.

Material information must be included in a keyword together with the equation's keyword. In the case of relatively low pressures, up to 2-3 GPa it is recommended to use the *MAT_ELASTIC_PLASTIC_HYDRO (MAT010) keyword. Experimental data and determined coefficients constituting the input for both cards were based on Ref. [5].

The equation of state, used to determine the characteristics of brass, is the Gruneisen equation of state defined for the materials subjected to compression as Eq. (3).

$$p = \frac{\rho_0 C^2 \mu \left[1 + \left(1 - \frac{\gamma_0}{2}\right)\mu - \frac{a}{2}\mu^2\right]}{\left[1 - (S_1 - 1)\mu - \frac{S_2 \mu^2}{\mu + 1} - \frac{S_3 \mu^3}{(\mu + 1)^2}\right]^2} + (\gamma_0 + a\mu)E \tag{3}$$

and for tension as Eq. (4).

$$p = \rho_0 C^2 \mu + (\gamma_0 + a\mu)E \tag{4}$$

where $\mu = (\frac{\rho}{\rho_0} - 1)$, *E* is the thermal energy, and the remaining parameters *C*, γ_0, S_1, S_2, S_3 and *a* are the constant parameters.

Johnson-Cook constitutive model considers several effects, characteristic for fast-performing processes, such as the impact of strain velocity or softening of material under the influence of adiabatic heating. The stress in the brass projectile is described as in Eq. (5).

$$\mathrm{\sigma = (A + B\varepsilon^n)(1 + c ln\dot{\varepsilon}^*)(1 - T^{*m})} \tag{5}$$

where *A*, *B*, *C*, *m*, *n* are the material constants, ε is the equivalent plastic strain, $\dot{\varepsilon}^*$ is the dimensionless plastic deformation speed, and T^* is the temperature is defined in Eq.(6).

$$\mathrm{T^* = \frac{T - T_{room}}{T_{melt} - T_{room}}} \tag{6}$$

where *T* is the temperature resulting from the work of plastic deformation under adiabatic conditions, T_{room} represents the ambient temperature, and T_{melt} is the melting temperature of the material.

This model also includes five material failure constants. Fragmentation is assumed as a criterion for destruction when the total relative strain reaches the value calculated in Eq. (7).

$$\mathrm{D = \sum \frac{\Delta\varepsilon}{\varepsilon^f}} \tag{7}$$

where $\Delta\varepsilon$ is the increase in plastic strain equivalent which occurs during the integration of the cycle, ε^f - is the equivalent of deformation at the fracture moment, under the conditions of strain rate, temperature, pressure and stress equivalent.

The deformation at the moment of failure defines Eq. (8).

$$\mathrm{\varepsilon^f = [D_1 + D_2 exp D_3 \sigma^*][1 + D_4 ln \varepsilon^*][1 + D_5 T^*]} \tag{8}$$

where $D_1 - D_5$ are damage model material failure constants and $\sigma^* = \frac{P}{\sigma_{\mathrm{eq}}}$ is the triaxial ratio between the hydrostatic pressure defined as $P = \frac{1}{3}\,\mathrm{tr}(\sigma)$ and the equivalent stress (Von Mises).

The corresponding constants for the Johnson-Cook constitutive model were determined in Ref. [6].

3. MODEL AND RESULTS

The 2D model used in the analysis, presented in Fig. 1, has designated grid areas filled with individual materials. It was realized with the use of shell elements. An axisymmetric axis is Y-axis of the model.

The cylindrer of LX-04 material measuring 40 mm in diameter and 30 mm in length has been developed as having appropriate dimensions, so that the observation of the results in the time steps, in which the phenomena accompanying the explosions are measured, is possible. The observations were carried out on finite element mesh having the sizes of 0.25 mm, 0.125 mm, and 0.0625 mm.

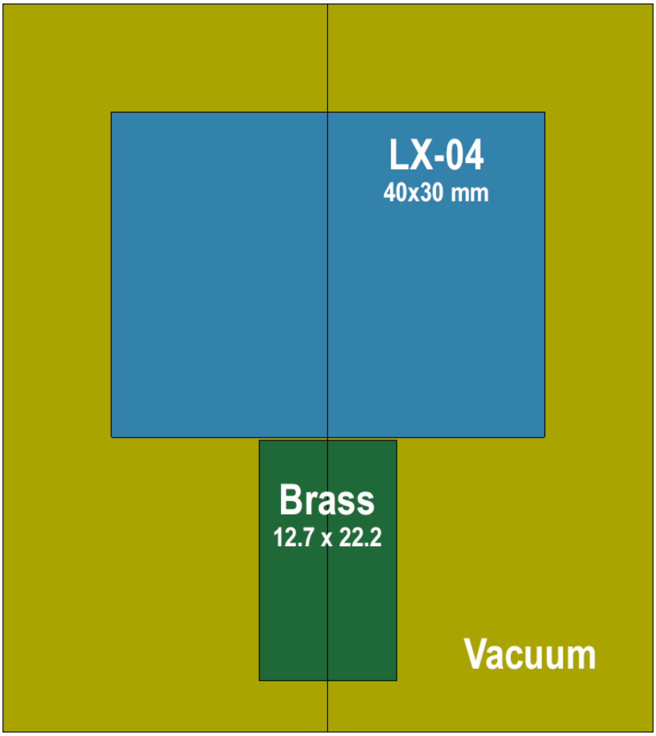

Fig. 1. An axisymmetric model with the axis marked and reflection

As a result, the obtained geometry was not different from the one presented in [1], which as a purpose-based operation was used to calibrate control parameters of simulations using the data for state equations for Composition-B and Multi-Material Arbitrary Lagrangian Eulerian formulation settings to approximate the results obtained by L.E. Schwer.

The model has open boundaries, which means that the given boundary conditions allow the detonation products to leave the space, reducing the area of the environment, which is not interesting from the point of view of this study. However, the problem is still the decreasing time step, which decreases with in the increase of the impact speed and the change of material to the material with a higher detonation speed, as in the case of Composition-B and LX-04. The simulation time has significantly increased for these reasons.

L.E. Schwer in [7] noted that incorrectly interpreted in the description in the *MAT_JOHNSON_COOK (MAT015) keyword, the EPSO parameter should not be selected in a time-dependent manner. In [1], the author implicitly accepts the suggestion of Almond and Murray [8] as the assumption of 250% of the time-dependent value, which was also used for LX-04. The advection method (METH parameter in *CONTROL_ALE) was assumed to be equal to 3, due to being the first-order method. METH = 2 Van Leer + half index shift (second order) and METH = -2 Modified Van Leer, which are recommended for explosives, generate the same Go and No-Go speeds. The Johnson-Cook failure model was also included. The model prepared in this way served as an input model for simulation using the parameters for LX-04.

Table 2. Go and No-Go speeds and converging study of a finite element mesh

El. size [mm]	No-Go [m/s]	Go [m/s]	El. quantity
0.25	825	830	32280
0.125	840	845	129120
0.0625	850	855	516480

Determining whether a reaction occurred is quite an interesting issue. In experimental conditions, we deal with sound or light phenomena. This clearly states that the process is proceeding. However, it does not give the opportunity to explore every area of the object freely. To record phenomena occurring inside the detonating material, copper-manganese and nickel-type extensometers and high-class oscilloscopes are used. Numerical simulations generate the ability to create cross-sections, record waveforms of specific points and pressure waves. In addition, LS-DYNA enables the use of the *DATABASE_EXTENT_BINARY card to store eight historical variables in the case of the Ignition & Growth in High Explosive state equation, which allows for even deeper observation of the event.

So, there are several possibilities of detonation determination - observation of pressure compression wave, velocity observation, using historical variables or finding elements where pressure exceeds Chapman-Jouguet pressure.

Correspondingly, lower values of the velocity of impact excitation agree with the results of the Susan test [9] (similar initiation test with slightly different character), where Composition B achieves a score of 55 m/s before any reaction occurs, and LX-04 only requires 43-46 m/s.

Figure 2 presents the bullet with increased velocity in material emerging in the central point of contact of the projectile with the composition caused by the pressure growth associated with the impact, from where the pulse propagation followed, leading to the detonation of the entire volume of the material.

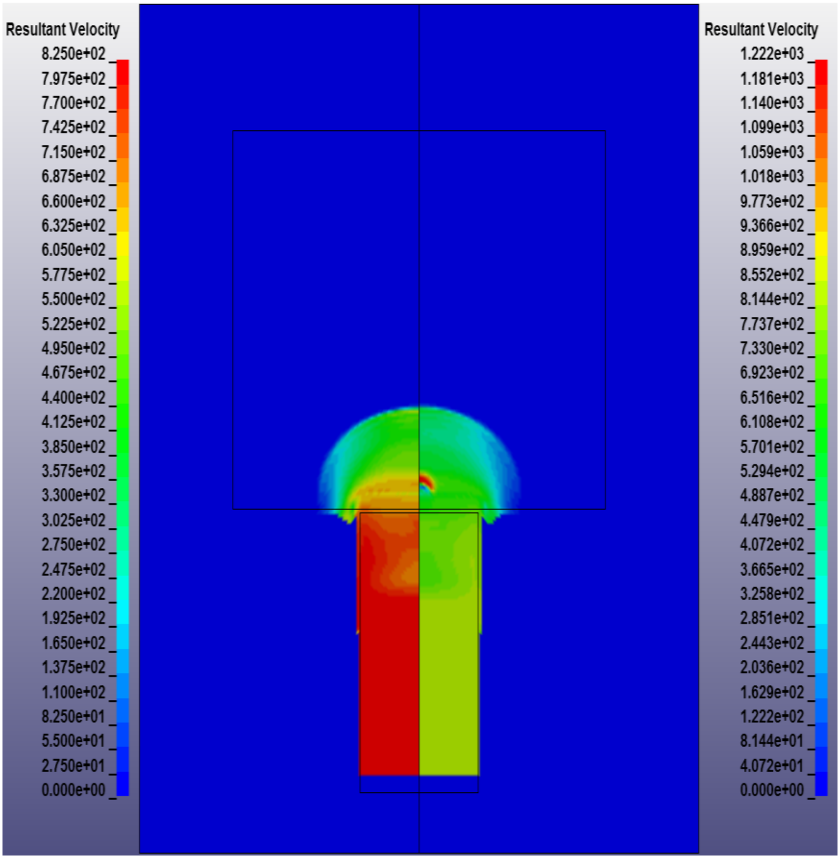

Fig. 2. Velocity contours in 0.25 mm mesh elements at a time stamp of 2 microseconds for the projectile speed of 825 m/s (No-Go) on the left and 830 m/s (Go) on the right.

Figure 3 presents one of the possible methods to determine the shock to detonation time by comparing the reacted to unreacted material fraction in elements. Fully developed detonation is shown.

The tracers of pressure have been placed, equally spaced in the material at the symmetry axis. By the means of the created pressure plots (Fig. 4), recorded with sufficient frequency to properly catch the initiation moment and peak pressure it is possible to find the run-to-detonation distance. Maximal pressure, exceeding Chapman-Jouguet pressure for the material, determines that detonation surely occurred.

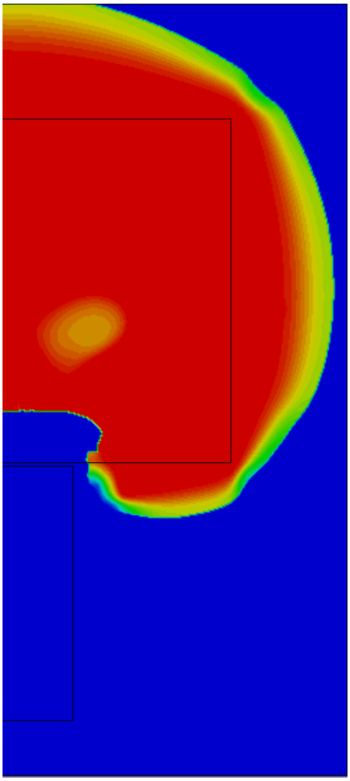

Fig. 3. Historical variable representing fraction of reacted material using a 0.125 mm mesh

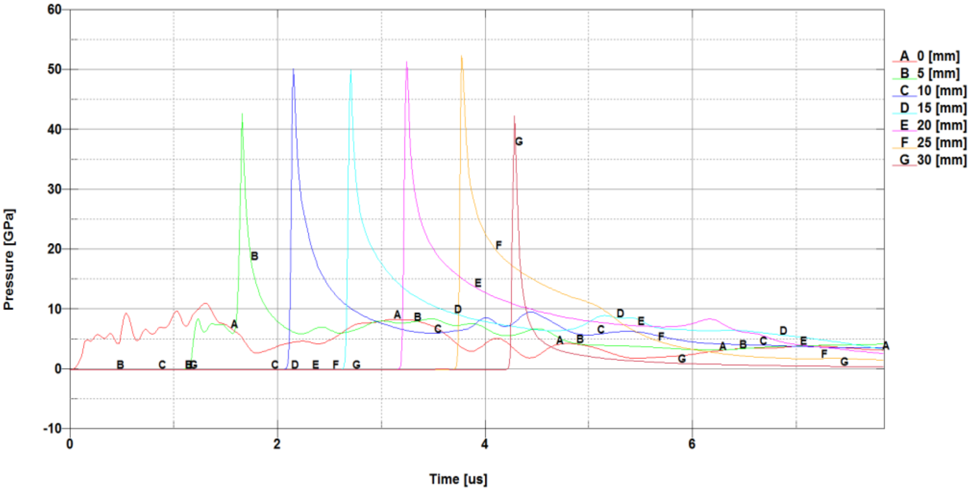

Fig. 4. Pressure value plots in discrete places in the material on the symmetry axis for 830 m/s impact velocity

According to the plot from Fig. 5 from [5] the shock pressure of approximately of 6 GPa as in the case of 830 m/s impact velocity in this work is corresponding to 6.5 mm run-to-detonation distance, which agrees with the simulation results. The peak is reached on the element closest to the axis as it is expected resulting in ignition and growth. Such a peak characteristic for detonation does not appear in case of lower impact speeds.

4. CONCLUSIONS

The explosion is a highly non-linear problem and requires large amounts of computing power and optimization of numerical techniques. Hence, highly developed, modern technologies enable such calculations. LS-DYNA, which is used in one-, two- and three-dimensional non-linear structural collisions at high speed, explosions and other dynamic problems is an important tool in the simulation process.

HMX-based explosives were created to generate high detonation velocities, for a strong impulse, and the polymers doped are mixed for increased stability. LX-04 is characterized by a significant amount of plasticizer in the Viton-A form, which makes the material less susceptible to impulses than materials lacking it. Simulation still cannot be a full replacement for prototyping, but well-performed allows for a quite precise determination of the performance and capabilities of the examined objects.

The blunt geometry of the projectile significantly simplifies the mesh formation process and can serve as a good introduction to the exploration of the possibilities of the Ignition & Growth in High Explosives model.

It allows for the use of larger grid sizes and for shortening the calculation time of individual configurations. The minimum element size of 0.25 mm used in this work, ensures a good balance between the calculation time and the convergence of results. The mesh convergence test performed showed the differences between the velocity for which (Go) detonation occurs between 0.25 and 0.125 mm mesh smaller than 2% (Table 2).

It seems risky to conduct this type of consideration without testing mesh convergence and the impact of the method on the MM-ALE solver. The obtained results of the detonation speed limit show a good comparison with the results of other commonly performed tests.

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