Automatic calibration of Ignition and Growth model for a DNAN based melt-cast explosive

Tongtang Cao¹ ², Lin Zhou² and Xiangrong Zhang²*¹
¹Anhui Dongfeng mechanical and electrical technology co, LTD, Hefei 230000, China
²State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081, China
*E-mail: zhangxr@bit.edu.cn

Abstract. To make the calibration of Ignition and Growth model more systematic and efficient for a DNAN based melt-cast explosive, a procedure combining nonlinear software package LS-OPT with hydrocode LS-DYNA was proposed in this paper. Shock initiation experiment was conducted to obtain measured pressure curves. The mismatch between calculated and measured pressure curves was defined as objective function, which was then minimized using optimization algorithm. Calibration results show that the calculated and measured pressure curves agree well both for arrive time to each location and the chemical reaction behind shock front.

1. Introduction
Modeling of reaction and detonation of explosives is important to military and civilian applications. A significant factor affecting the accuracy of the modeling is the material models and the corresponding model parameters. In reaction and detonation modeling, equations of state for unreacted explosive and reaction products together with reactive flow model are used to control the conversion of unreacted explosive to reaction products, and a proper set of model parameters can successfully recur the experiment data. Ignition and Growth model proposed by Lee and Tarver has been widely used to model numerous of shock initiation experiments and has been proved to be a reasonable reactive flow model for shock initiation simulation [1-2]. However, the calibration of Ignition and Growth model is a huge challenge for researchers, because the model owns 15 adjustable parameters and none of them can be determined explicitly from a simple experiment. The calibration is relying on numerical simulations with continual adjustment of model parameters until the mismatch between experimental result and calculated result is acceptable. The process of adjusting the model parameters can be manual or automatic. Compared to the automatic process, manual process is empirical and artificial, and not surprisingly, this process is both inefficient and inaccurate.

In this paper, a procedure combining nonlinear software package LS-OPT with hydrocode LS-DYNA was proposed to automatically calibrate Ignition and Growth model parameters for a DNAN based melt-cast explosive (30% DNAN, 40% RDX and 30% aluminum powder by weight), which is a newly developed insensitive formulation for blast fragmentation warhead. Shock initiation experiment was conducted to measure the pressure curves, which were then used as the basis of calibration of the Ignition and Growth model. Lastly, the measured and calculated pressure curves were compared to illustrate the validity of the procedure.
2. Shock Initiation Experiment

Shock initiation experiment of a DNAN based melt-cast explosives was conducted with a one-dimensional Lagrange analysis measurement system, as shown in Figure 1 (a) and (b). The experimental setup consists primarily of a shock loading system, a signal recording system, and specimens of the DNAN based melt-cast explosive. The shock loading system consists of a detonator, a plane wave generator, a TNT booster, an air gap, and a 13-mm-thick aluminum gap. Output pressure of the shock loading system can be adjusted by changing the height of the air gap. The signal recording system consists of an oscilloscope, a constant-current source, a trigger probe, and four manganin piezoresistive gauges. The trigger probe was placed on the plane wave generator’s surface to trigger the constant-current source and oscilloscope. Each gauge was armored with sheets of Teflon insulation to prevent a short circuit of gauge once the explosive specimen became reactive and conductive. The first gauge was placed between the aluminum gap and the specimen discs, with the other three gauges located between two specimen discs. The specimens consist of three 3-mm-thick discs and a 20-mm-thick disc stacked on top of each other. Each disc is 50mm in diameter. Besides, gauge’s sensitive element should be located at the center of the specimen discs.

Once the plane wave generator was detonated by a detonator, a reactive shock wave was developed in the explosive specimens. The oscilloscope records the voltage-time curves at the four Lagrangian positions of \( h_1 \) (0mm), \( h_2 \) (3mm), \( h_3 \) (6mm), and \( h_4 \) (9mm). According to the calibrated pressure-voltage relationship of manganin piezoresistive gauges, the voltage-time curves can be then converted to pressure-time curves, which is the basis of calibration of Ignition and Growth model in next section.

Figure 1. Experimental setup for shock initiation: (a) picture and (b) schematic view
3. Model Calibration

3.1 Ignition and Growth Model

The Ignition and Growth model requires the following: (1) an unreacted explosive equation of state, (b) a reaction product equation of state, and (3) a reaction rate law governing the chemical conversion of unreacted explosive to reaction products.

Jones-Wilkins-Lee (JWL) equation of state was used both for unreacted explosive and the reaction products, in the form [3]:

\[ P = A \left( 1 - \frac{\omega}{R_1 V} \right) e^{-R_1 V} + B \left( 1 - \frac{\omega}{R_2 V} \right) e^{-R_2 V} + \frac{\omega E}{V} \]  \hspace{1cm} (1)

where \( P \) is pressure, \( V \) is relative volume, \( E \) is specific internal energy of explosive, \( A, B, R_1, R_2 \) and \( \omega \) are JWL parameters. The unreacted equation of state is fitted to the available shock Hugoniot data, and the reaction products equation of state is generally fitted to cylinder test or other metal acceleration data. Besides, the parameters of reaction product equation of state can also be determined via thermodynamic equilibrium calculation [4-5]. For DNAN based melt-cast explosive, Table 1 and Table 2 contains the parameters of equation of state for unreacted explosive and reaction products.

| Table 1. Parameters of JWL equation of state for unreacted explosive [6] |
|----------------------------------|
| \( \rho \)(g/cm\(^3\)) | \( A \)(Mbar) | \( B \)(Mbar) | \( R_1 \) | \( R_2 \) | \( \omega \) | \( C_{ve} \) |
|----------------------------------|
| 1.90 | 23827.04 | -0.48782 | 19.886 | 1.9886 | 1.97343 | 1.135E-4 |

| Table 2. Parameters of JWL equation of state for reaction products [6] |
|----------------------------------|
| \( A \)(Mbar) | \( B \)(Mbar) | \( R_1 \) | \( R_2 \) | \( \omega \) | \( E_0 \)(Mbar-cc/cc) |
|----------------------------------|
| 3.925 | 0.171 | 4.508 | 1.6678 | 0.5 | 0.095 |

For chemical rate law, the three-term reaction rate equation is used [7]:

\[ \frac{d\lambda}{dt} = f(1-\lambda)^b \left( \frac{\rho/\rho_0 - 1 - a}{\lambda_{G1\text{max}}} \right)^c + G_1(1-\lambda)^d \left( \frac{\rho \lambda P}{\lambda_{G2\text{max}}} \right)^e + G_2(1-\lambda)^f \left( \frac{\lambda P^z}{\lambda_{G2\text{min}}} \right)^g \]  \hspace{1cm} (2)

where \( \lambda \) is the fraction reacted, \( t \) is time, \( \rho \) is the current density, \( \rho_0 \) is the initial density, \( P \) is pressure, \( I, G_1, G_2, a, b, c, d, f, g, \), \( x, y, z, \lambda_{ig\text{max}}, \lambda_{G1\text{max}} \) and \( \lambda_{G2\text{min}} \) are 15 adjustable parameters. The parameter \( a \) is a critical compression that is used to prohibit ignition until a certain degree of compression (or a certain input pressure) has been reached. In most cases, the parameter \( y \) is set equal to 1 to represent a deflagration, the parameter \( b \) and \( c \) are both set to 2/3 to represent inward spherical grain burning. The three-term reaction rate equation models three stages of reaction generally observed during shock initiation of solid explosives.

3.2 Calibration Procedure

In our procedure, LS-OPT can be seen as a front-end to LS-DYNA to define the objective function necessary to carry out the minimization analysis for calibration. The frame of the procedure can be seen in Figure 2.
LS-DYNA was used to simulate the shock initiation experiment and to obtain calculated pressure curves. To reduce calculation time and save computer memories, we established a two dimensional computational model with 20 meshes/mm, the measured pressure curve of the first gauge was imposed to one of surfaces of DNAN based melt-cast explosive [8-9]. Four observation points at the location of 0mm, 3mm, 6mm and 9mm in computational model were set to output the calculated pressure curves.

System parameter identification is a commonly used feature of LS-OPT, especially for the purpose of calibrating material models. The procedure consists of minimizing the mismatch between target values and corresponding solver output values. In this paper, target values are the measured pressure curves, and output values are calculated pressure curves, which is a variable response, being dependent on the Ignition and Growth model parameters. In LS-OPT, the mismatch between measured and calculated pressure curves was defined as the objective function using curve mapping. Metamodel-based Optimization with Sequential with Domain Reduction was employed to create and optimize an approximate model of the design instead of optimizing the design through direct simulation, which usually requires enormous computation time and memories. Linear polynomial metamodel and D-optimal point selection was chosen in the optimizations. Hybrid genetic algorithm was used to minimize the objective function [10].

The Ignition and Growth model parameters of IMX-101 (also a DNAN based melt-cast explosive) [11] were used as the initial values for calibration in our paper. Except for $b = c = 2/3$ and $y = 1$ were set to constants, the rest 12 parameters were all set to continuous variables and each parameter has a proper upper and lower bounder.

4. Result and Discussion

The calibration required about 13 hour’s computer time on HP Z800 workstation. A total of 15 interactions (20 times calculation for each interaction) were required to obtain the Ignition and Growth model parameters, which were listed in Table 3. Comparison of measured and calculated pressure curves can be seen in Figure 3. It is evident that the arrive time to each position (0mm, 3mm, 6mm and 9mm) of calculated and measured pressure curves agree well, so is for the chemical reaction behind the shock front. Both calculated and measured pressure curves indicated that the detonation has not been completely built until at 9mm depth.

Compared with manual adjustment of model parameters, whose process is always empirical and time-consuming, a notable advantage of our procedure is LS-OPT can automatic adjust model parameters according to computational influence of model parameters on objective function (Figure 4). We can also set these “non-key parameters” (such as freq and es2 in Figure 4, whose influence is 1.6%...
and 1.2%, respectively) as constant to reduce number of model parameters to be calibrated and improve the calibration efficiency.

**Table 3.** Ignition and Growth model parameters for DNAN based melt-cast explosive

| $l$ ($\mu s^{-1}$) | $c$     | $g$     | $G_1(Mbar^{-y} \cdot \mu s^{-1})$ | $G_2(Mbar^{-z} \cdot \mu s^{-1})$ |
|-------------------|---------|---------|-----------------------------------|-----------------------------------|
| $a$               | 0.0     | $d$     | 0.892816                          | 320.957                           |
| $b$               | 0.667   | $y$     | 1.0                               | $\lambda_{G1_{\text{max}}}$= 1.0 |
| $x$               | 5.9345  | $e$     | 0.792461                          | $\lambda_{G2_{\text{min}}}$= 0.0  |

**Figure 3.** Comparison of calculated and measure pressure curves

**Figure 4.** Computational influence of model parameters on the objective function
5. Conclusion
Shock initiation experiment of a DNAN based melt-cast explosive was conducted to obtain the measured pressure curves. In order to get Ignition and Growth model parameters more systematic and efficient, we have proposed a procedure that makes use of the optimization software package LS-OPT driving the hydrocode LS-DYNA. With this procedure, the mismatch between measured and calculated pressure curves was defined as objective function, which was then optimized using hybrid genetic algorithm to minimize the objective function. Comparison of pressures curves from the optimized reactive flow model to calculated pressure curves illustrates the validity of the procedure.

Acknowledgement
This work was supported by the National Natural Science Foundation of China (Grant No. 11772060).

References
[1] Garcia M L, Tarver C M 2006 Three-dimensional ignition and growth reactive flow modeling of prism failure tests on PBX 9502. (Livermore: Lawrence Livermore National Laboratory).
[2] Tarver C M, Green L G 1989 Using small scale tests to estimate the failure diameter of a propellant. (Livermore: Lawrence Livermore National Laboratory).
[3] Kury J W, Hornig H C, Lee E L 1965 Proc., Symp. Detonation, 4nd pp 3-13.
[4] Mader C L 2007 Numerical modeling of explosives and propellants. (Florida: CRC Press).
[5] Lu J P, Kennedy D L 2003 Modeling of PBXN-115 using kinetic CHEETAH and the DYNA codes (Australia: Weapons System Division).
[6] Tong-Tang Cao 2018 Researches on shock initiation characteristics and the reaction rate equation of DNAN based melt-cast explosives (Beijing: Beijing Institute of Technology).
[7] Tarver C M, Hallquist J O, Erickson L M 1985 Modeling short pulse duration shock initiation of solid explosives (Livermore: Lawrence Livermore National Laboratory).
[8] Hussain T, Liu Y, Huang F, et al 2016 J. Energ. Mater. 34(1) pp 38-48.
[9] Tong-Tang Cao, Lin Zhou. Xiang-rong Zhang, et al 2017 J. Energ. Mater. 35(4) pp 430-442.
[10] Stander N, Basudhar A, et al 2015 10ndEuropean LS-Dyna Conf.
[11] Tarver C M 2016 Ignition and growth reactive flow model for IMX-101 (Livermore: Lawrence Livermore National Laboratory).