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Explosive modelling using LS-DYNA - a user's guide

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Defence R&D Canada – Valcartier

Technical Memorandum
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Abstract

A selective literature review of the Lee-Tarver model of detonation and the JWL equation of state was performed to help users of LS-DYNA model explosives. Some rule of thumb estimates and general guidelines to modeling detonations are also offered.

Résumé

Une revue de la littérature sélective du model de détonation Lee-Tarver et de l'équation d'état JWL a été faite pour aider les usagers de LS-DYNA à modéliser les explosifs. Quelques estimations simples et des avis généraux pour la modélisation des détonations sont également donnés.

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Executive summary

Explosive modelling using LS-DYNA - a user's guide:

Grant W.J. McIntosh; DRDC Valcartier TM 2013-401; Defence R&D Canada – Valcartier; February 2014.

Introduction or background: Numerical simulations of detonations are often required for reasons of time, cost and safety considerations. At DRDC Valcartier, the hydrodynamic finite element program LS-DYNA is used for such simulations. Two commonly used models for explosives and detonations are used in the program, the Lee-Tarver model and the JWL equation of state. The description and parameters for these models are available but are not conveniently located in a single user friendly source. This report attempts to fill this gap.

Results: This report contains descriptions of the models in their various forms and the parameters necessary to model the most commonly encountered explosives.

Significance: A single source will help current and future LS-DYNA users to model more quickly explosives and detonations.

Future plans: Updates if more parameters for other explosives become available could be added to revisions of the document.

Sommaire

Explosive modelling using LS-DYNA - a user's guide:

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Introduction ou contexte : Des simulations numériques des détonations sont souvent requises pour des considérations de temps, coût et sécurité. Au RDDC Valcartier, le programme hydrodynamique d'éléments finis LS-DYNA est utilisé pour telles simulations. Deux modèles souvent utilisés pour les explosifs et les détonations sont disponibles: le modèle Lee-Tarver et l'équation d'état JWL. La description et les paramètres pour ces modèles sont disponibles mais ne sont pas facilement accessibles. Ce rapport essaie de fournir une telle source.

Résultats : Ce document contient des descriptions des modèles et les paramètres nécessaires pour modéliser les explosifs les plus répandus.

Importance : Une source unique aidera les utilisateurs courants et futurs de LS-DYNA à modéliser plus vite les explosifs et les détonations.

Perspectives : Des mises-à-jour si plus de paramètres pour d'autres explosifs deviennent disponibles pourraient être ajoutées aux révisions de ce document.

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1 Introduction

Numerical simulations of detonations are often required for reasons of time, cost and safety considerations. At DRDC Valcartier, the hydrodynamic finite element program LS-DYNA [1] is used for such simulations. The modelling of explosives is quite complicated and as not everyone who uses LS-DYNA is a detonics expert, some guidance on the use of the explosive models contained in the hydrocode is warranted. Two commonly used models for explosives and detonations are found in the program: the Lee-Tarver model and the JWL equation of state. The description and parameters for these models are available but are not conveniently located in a single user friendly source. This report attempts to fill this gap.

2 Simple detonation theory

In this section, a brief outline of the standard theory of detonation will be given as well as suggested references.

A detonation is a rapid expansion of gases which occurs after a self-sustaining shock wave passes through a metastable material (an explosive). Since a shock wave is involved, a characteristic speed is defined, the detonation velocity, V_d . Equally, a shock wave also implies a pressure jump between material before and after the passage of the shock front, the detonation pressure, P_{CJ} . To a first approximation for a given explosive density ρ_o , P_{CJ} is $(\rho_o/4)(V_d)^2$. Typical values for ρ_o are 1 to 2 g/cm³, and for V_d 0.3 to 0.8 cm/ μ s, which gives P_{CJ} on the order of several GPa. The performance of an explosive is directly connected to P_{CJ} , which is function of the explosive chemical used (TNT, RDX, etc.)

The above very simplified theory is for a plane, infinite, one dimensional detonation. In two and three dimensions, complications arise, in particular, there is a size effect, in which a detonation ceases if the explosive size becomes too small (critical diameter). One can think of this as energy loss out the sides due to expansion being greater than the energy release by the explosive's decomposition and thus the reaction is no longer self-sustaining. A related effect is due to confinement – a confined explosive reacts more violently than an unconfined one.

There are many explosive substances but there are only a few which meet the strict criteria for safe handling in practical quantities. Today's explosives are safe to manipulate (pick up, carry, etc.) but this also results in them being difficult to detonate. All practical explosives require some intense shock to set them off and this shock is supplied by a detonator.

A large part of the science of detonics is devoted to the study of just how explosives react when subjected to a shock. At an engineering level, it was observed that for a given explosive, a detonation occurs if a high enough pressure (P) is applied for a long enough time (t). There seems to be a critical value of P^2t . (a sensitivity) for each explosive. The sensitivity of an explosive, its propensity to detonate under a shock load, is a factor of many parameters - the explosive compound itself (type, crystal size); the size, shape, location and number of defects and voids; the degree of confinement; the ambient temperature.

The available literature on explosives is enormous. There has been a great deal of both theoretical and experimental work performed over the last century but a coherent picture of the detonation process has slowly emerged. One of the best introductions to practical detonics science is by Cooper [2]. Another good reference is by Meyer [3]. An older standard reference is by Cook [4]. Another older reference is Federoff [5]. There are a couple of books available in French, by Calzia [6] and Cheret [7]. More detailed explanations of detonation theory can be found in Fickett and Davis [8]. Mader [9] has written a treatise on numerical modeling of detonations but it emphasises his work and it is difficult to separate general principles from his particular implementation of them (in particular the Forest Fire model and the HOM equation of state).

A great deal of experimental parameters for explosives have been summarised in works produced by three large American laboratories – LASL [10], LLNL [11] and NSWC [12]. These were all compiled in the 1980's.

Just about everything on explosives has been mentioned in the proceedings of the International Symposia on Detonation [13]. Finally, there are literally thousands of internal laboratory reports from around the world. These are more difficult to find but are often cited in the above mentioned references.

3 Initiation of detonation modelling

A basic question is often asked: does an explosive detonate subjected to a given stimulus? To answer it, the evolution of a detonation from an unreacted state to a fully reacted state must be followed.

Most models describe the reaction as follows. The unreacted explosive is subject to a compression. The compression can be calculated a number of ways but information about the mechanical properties and the shock Hugoniot of the unreacted explosive are generally needed. The compression, i.e. an increased pressure and possibly a temperature increase, leads to the start of an exothermic reaction. The explosive changes from an unreacted solid (burn fraction $F=0$) to gaseous reaction products (burn fraction increasing to $F=1$) according to some rate law (dF/dt). This rate law is the heart of a model. The most common ones are the Lee-Tarver model (described below) and the Forest Fire model (described by Mader). The mixture of unreacted and reacted explosive is described usually by assuming a local pressure and temperature equilibrium and a volume which is a simple addition of the volume of the two states weighted by the burn fraction. The reaction continues until $F=1$ and then the reaction products expand as described by a products equation of state, of which there are many – BKW, JWL, JWLb, LJD, Sack-Tuesday and others

Within LS-DYNA, only the Lee Tarver ignition and growth model (EOS 7) [14] is available to model the initiation of an explosive. A similar model is available for propellants (EOS 12) but has very limited material data available. The Lee-Tarver model covers the principles described above. It begins with a description of the unreacted explosive which is described by a JWL equation of state of the form:

$$P = Ae^{-R_1 V} + Be^{-R_2 V} + (\omega c_v T) / V$$

where A , R_1 , B , R_2 , ω and c_v are constants for a given explosive (subscripted e) and V is ρ_o/ρ . One should remember at this point that the use of an equation of state in LS-DYNA also requires a constitutive material model. Since the above equation already describes the material response, only null material (Mat 9) is needed to use the Lee-Tarver model. The explosive then burns according to:

$$\partial F / \partial t = I(1-F)^b (\rho / \rho_o - 1 - a)^x + G_1(1-F)^c F^d p^y + G_2(1-F)^e F^g p^z$$

where the three terms are applied for specific F ranges: the first when $0 < F < F_{igmax}$, the second term when $0 < F < F_{g1max}$ and the third when $F_{g2min} < F < 1.0$. In the literature, there is also a two term rate law which can be trivially modeled with the three term law by setting G_2 to zero and F_{g1max} to one. Finally, the detonation products are also described by the above JWL equation of state with different constants (subscripted p). The constants for the four most commonly used military explosives are given in Table 1 (cm-g- μ s-MBar units).

(cm-g- μ s-Mbar)	Composition B	C-4	TNT (Cast)	PETN
ρ_o	1.630	1.601	1.61	1.75
A_e	1479.0	778.1	17.98	37.46
B_e	-0.05261	-0.05031	-0.931	-1.313
r_{1e}	12.0	11.3	6.2	7.2
r_{2e}	1.20	1.13	3.1	3.1
ω_e	0.9120	0.8938	0.8926	1.173
c_{ve}	$2.487 \cdot 10^{-5}$	$2.487 \cdot 10^{-5}$	$2.050 \cdot 10^{-5}$	$2.263 \cdot 10^{-5}$
T_o	298	298	298	298
A_p	5.5748	6.0977	3.712	6.17
B_p	0.0783	0.1295	0.032306	0.16926
r_{1p}	4.5	4.5	4.15	4.4
r_{2p}	1.2	1.4	0.95	1.2
ω_p	0.34	0.25	0.30	0.25
c_{vp}	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-5}$
E_o	0.081	0.09	0.070	0.101
I	44.0	$4 \cdot 10^6$	50	20

a	0.01	0.0367	0	0
b	0.222	0.667	0.222	0.222
x	4.0	7.0	4.0	4.0
F_{igmax}	0.3	0.022	1.0	1.0
G_1	514.0	140	40	400
c	0.222	0.667	0.222	0.222
d	0.667	0.333	0.667	0.667
y	2.0	2.0	1.2	1.4
F_{glmax}	1.0	1.0	1.0	1.0
G_2	0.0	0	0	0
e	0.	0.667	0	0
g	0.0	0.667	0	0
z	3.0	3.0	0	0
F_{g2min}	1.0	0.0	1.0	1.0
Ref.	Murphy et al. (10 th det) [15]	Urtiew [16]	Lee-Tarver [14]	Lee-Tarver [14]

Table 1 Lee-Tarver model parameters for four explosives

Parameters for other explosives can be found in the literature as follows:

PBX9404 (HMX based) – Lee-Tarver [14]

Propellant B (AP, HMX, Al, binder) – Tarver & Green [17]

RX-26_AF (HMX, TATB) – Green et al. [18]

RX-03BB (TATB based) – Lee-Tarver [14]

LX-17 (TATB based) – Murphy [15]

PETN/Al – Tao et al. [19]

TNT/Al – Tao et al. [19]

PBX-9502 (TATB based) – Tarver & McGuire [20]

EDC35 (TATB based) – Tarver & McGuire [20]

If explosive is NOT characterised for the Lee-Tarver model, one could try a composition with a similar explosive component but adjust ‘a’ to match an experiment. If no experiment is available, estimate ‘a’ as $1 - \rho/\rho_{\text{tmd}}$ where tmd refers to the theoretical maximum solid density.

If one must model a completely new composition, then experimental data is required. Most new explosives are subjected to a series of tests including measurements of their mechanical properties and shock tests. The best one can then do is to model the pressure response of the unreacted explosive using its mechanical properties and try to estimate P^2t for comparison to critical values or to compare to the pressures generated by the shock tests. If exceeded, one must assume detonation and use the techniques in next section

4 Explosive expansion modelling

Once it is determined that the explosive detonates (by assumption, calculation or observation), we must now model its effects. When an explosive detonates, it is suddenly converted into a hot, dense gas which, because of its high pressure, wants to expand and do work on its surroundings. This expansion is assumed to be isentropic –i.e. no external energy is added to the system nor is any internal energy subtracted. Many equations of state (eg BKW, HOM, LJD, JCZ, JWL) are available to describe the expansion. They all have some theoretical justification for their forms but at the end of the day, they are all fitted to experimental data. Each equation of state must, at a minimum, describe the detonation point (P_{CJ}) and eventually behave as an ideal gas for very large expansions.

To describe a detonation in LS-DYNA, two things must be specified: when to start the expansion and how the expansion proceeds. These are handled with material model 8 (HE burn) and JWL equation of state [21] respectively. Two other equations of state are available: the Sack-Tuesday equation of state (rarely used) and JWLb (a variation of the JWL EOS for very high pressure compressions).

To specify when the expansion starts, the HE burn model can use one of two methods (or both). The first method is called a programmed burn. The location(s) and time(s) of ignition are user specified (*INITIAL_DETONATION control card). These could be individual points, along a line or the entire explosive. The detonation wave propagates according to the Huygens principle, reaching an element at time D/V_d where D is closest distance between an ignition point and the element and V_d is the detonation velocity, and then as the wave crosses the element, burn fraction F increases from 0 to 1 in time approximately L/V_d where L is the length of the element. An example of this option would be modeling of the explosive in a shaped charge

The second method is called a beta (or CJ) burn in which any compression of the explosive causes an ignition of the compressed element(s) and burning will occur as described in the LS-DYNA manual (or Mader, p. 316). This option could be used to describe a detonation caused by a fragment impact on an HE round.

For both burn models, a diffraction problem can occur. This happens if parts of the explosive do not have a direct view of the nearest ignition point. These parts are prematurely lit by straight line ignition algorithm. To prevent this, it is best to always run a detonation simulation with shadow burn option on (using *CONTROL_EXPLOSIVE_SHADOW control card...)

The pressure in the expanding product gases is best modeled by the JWL equation of state. The JWL model describes the expansion along the isentrope which passes through the Chapman-Jouget (detonation) point by

$$P_{CJ} = A_p e^{-r_1 V} + B_p e^{-r_2 V} + C V^{-(\omega+1)}$$

The energy along this isentrope can be found by integration ($dE = -p dV$), namely,

$$E_{CJ} = (A_p / r_1) e^{-r_1 V} + (B_p / r_2) e^{-r_2 V} + (C / \omega) V^{-\omega}$$

and the JWL equation of state is generated by assuming a simple linear dependence of energy on pressure for values off the isentrope

$$E = E_{cJl} + (V / \omega)(P - P_{cJl})$$

which, upon expansion and rearrangement, becomes

$$P = A_p \left(1 - \frac{\omega}{r_1 V}\right) e^{-r_1 V} + B_p \left(1 - \frac{\omega}{r_2 V}\right) e^{-r_2 V} + \frac{\omega E}{V}$$

Parameters exist for many explosives, many more than have been characterised for initiation parameters. See Table 2 for many common explosives (cm-g-μs-MBar units). The mechanical properties (bulk modulus K, shear modulus G, yield, stress σ_y) are only approximate values.

(cm-g-μs-Mbar)	Comp B	C-4	PETN	TNT	NM	Octol 78/22	Tetryl	HMX
ρ_o	1.717	1.901	1.500	1.630	1.128	1.821	1.730	1.891
P_{cJl}	0.295	0.280	0.220	0.210	0.125	0.342	0.285	0.420
V_d	0.798	0.8193	0.745	0.693	0.628	0.848	0.791	0.911
K_{bulk}	0.10			0.077	liquid	0.113	0.052	
G_{shear}	0.05			0.03	liquid	0.05	0.026	
σ_{yield}	0.01			0.00711	liquid	0.01	0.0216	
A_p	5.242	6.0977	6.253	3.712	2.092	7.486	5.868	7.783
B_p	0.07678	0.1295	0.23290	0.03231	0.05689	0.13380	0.10671	0.07071

C	0.01082	0.01043	0.01152	0.01045	0.00770	0.01167	0.00774	0.00643
r_1	4.2	4.5	5.25	4.15	4.40	4.50	4.40	4.20
r_2	1.1	1.4	1.60	0.95	1.20	1.20	1.20	1.00
ω	0.34	0.25	0.28	0.30	0.30	0.38	0.28	0.30
E_o	0.0850	0.090	0.0856	0.07	0.0510	0.0960	0.0820	0.1050
Ref.	[11], [12]	[11]	[11]	[11], [12]	[11]	[11], [12]	[11], [12]	[11]

Table 2 JWL Parameters for common explosives

Other JWL coefficients can be found in the LLNL [11] and NSWC [12] handbooks and in the following references:

HMX/Polyurethane – Bailey [22]

EDC37 (HMX based) – Merchant [23]

SEP (PETN/paraffin) – Itoh & Liu [24], [25]

TNAZ – Baker [26]

If one has to model an explosive that is NOT characterised, an initial try can be made with an explosive with a similar explosive composition and detonation properties. If no similar explosive is available but the formulation of the new explosive is known, calculations of the equation of state can be made using the thermochemical program TIGER [27] or its descendants (CHEETAH, JAGUAR). TIGER can generate the parameters for the BKW or JCZ equations of state and then a fit can be made to the JWL model. If one is lucky enough to have unanalysed cylinder test data, programs exist to calculate JWL coefficients (eg. Jacques [28]).

5 Conclusions

Explosive modelling using LS-DYNA is widely performed. A judicious choice of parameters will enable a dedicated modeller to answer the two fundamental questions: does an explosive detonate? And if so, what does the explosive do to its surroundings? This report tried to explain the nature of the models and constants in order to prepare LS-DYNA input that makes sense.

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List of symbols/abbreviations/acronyms/initialisms

ρ	Density
σ_{yield}	Yield Stress
ω	JWL equation of state parameter
A	JWL equation of state parameter
B	JWL equation of state parameter
C	JWL equation of state parameter
E	Energy
F	Burn fraction
G_{shear}	Shear modulus
$G_1 \text{ or } 2$	Lee-Tarver model parameter (reaction rate)
I	Lee-Tarver model parameter (reaction rate)
K_{bulk}	Bulk modulus
P	Pressure
V	Relative volume with respect to initial state OR velocity
a	Lee-Tarver model parameter (ignition compression)
b	Lee-Tarver model parameter (exponent)
c	Lee-Tarver model parameter (exponent)
c_v	JWL equation of state parameter (heat capacity constant volume)
d	Lee-Tarver model parameter (exponent)
e	Lee-Tarver model parameter (exponent)
g	Lee-Tarver model parameter (exponent)
$r_1 \text{ or } 2$	JWL equation of state parameter
x	Lee-Tarver model parameter (exponent)
y	Lee-Tarver model parameter (exponent)
z	Lee-Tarver model parameter (exponent)
CJ (subscript)	Refers to Chapman-Jouget state
d (subscript)	Refers to detonation
e (subscript)	Refers to unreacted explosive state
o (subscript)	Refers to original state
p (subscript)	Refers to reacted explosive products state

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A selective literature review of the Lee-Tarver model of detonation and the JWL equation of state was performed to help users of LS-DYNA model explosives. Some rule of thumb estimates and general guidelines to modeling detonations are also offered.

Une revue de la littérature sélective du model de détonation Lee-Tarver et de l'équation d'état JWL a été faite pour aider les usagers de LS-DYNA à modéliser les explosifs. Quelques estimations simples et des avis généraux pour la modélisation des détonations sont également donnés.

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LS-DYNA, Lee-Tarver model, JWL equation of state, explosives

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