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SPH method in numerical calculus of detonation parameters

V. NASTASESCU^{1*}, GH. BARSAN²

¹Military Technical Academy, Bucharest, Romania ²Land Forces Academy, Sibiu, Romania

Abstract. This paper presents some of our results in using of the Smoothed Particles Hydrodynamics (SPH) method for the numerical modelling of the detonation phenomena. The study of the detonation is very important for evaluation of different explosives and even for their design. The paper also presents, in a synthetically way, some fundamentals of the detonation. The numerical modelling of the detonation can be made by Finite Element Method (FEM), but using of the SPH method brings some important advantages because the large deformations, large distortions occur. If the FEM can be used in Arbitrary Lagrangian-Eulerian (ALE) formulation, the SPH method can easily works and next to it, some specific parameters (density variation, specific energy etc.) can be obtained and analyzed by post-processing. The numerical study allowed us to analyse the influence of some explosive characteristics and of the circumstances (non confined and confined explosive) upon detonation parameters

Keywords: detonation, explosion, FEM, SPH

1. Introduction

There are many reasons for studying the detonation phenomena; also, a study can be made from different point of view. Our paper is focused on the detonation parameters calculus, using in a comparative way, two powerful numerical methods: well known and large used method of finite elements (FEM) and a much newer numerical method, less known and less used in our country, namely smoothed particles hydrodynamics (SPH) method. In this paper, the fundamentals of the FEM and SPH method are considered known by the reader and we'll synthetically present only some fundamentals about explosions and explosives, which represent the application domain of the numerical methods.

^{*} Correspondence address: nastasescuv@gmail.com

1.1. Explosives and Explosions

Any chemical compound, mixture, or device, having the primary purpose to function by an explosion could be named an explosive. Three types of explosions exist: nuclear, mechanical and chemical. A chemical explosion is caused by an extremely fast conversion of a solid or liquid compound into hot gases having a much greater volume than the substances from which they are generated.

Explosives are classified into two categories: low and high. An explosive is said to be a low one, when the rate of advance of the chemical reaction zone into the unreacted explosive zone is less than the sound velocity through this zone. A low explosive burns or deflagrates rather than detonates. In turn, this category is also divided into two categories: gas-producing low explosives and nongas-producing low explosives.

High explosives are those which have the rate of advance of the chemical reaction zone into the unreacted explosive greater than sound velocity through this zone. This rate of advance is termed the detonation rate. There are two types of high explosives: primary and secondary high explosives. A primary high explosive is characterized by an extreme sensitivity to initiation by both heat and shock. A secondary high explosive is initiated only by a relatively high intensity shock. High explosives are most used both in military and civil domains. The most known and used such explosive is TNT.

1.2 Blast Waves

The products of the reacted explosive move into surrounding zone, in the form of propagation waves. There are two types of propagation waves: detonation and de-flagration waves (Fig. 1). The deflagration waves have subsonic velocity and they are expansive waves. Typically, deflagrations propagate at speeds on the order of 1...100 m/s. Across a deflagration, the pressure decreases while the volume increases. The phenomena of detonation is that initial process of an explosion, being a very rapid and stable chemical reaction, which proceeds through the explosive material at a speed, called the detonation velocity.



Explosive.

Detonation waves have supersonic velocity and they are compressive waves. Typically, detonation waves propagate at speeds on the order of 2000 m/s. Across a detonation, the pressure increases while the volume decreases.

Those two zones, representing the reacted and unreacted explosive (Fig. 2), are separated by the shock front or leading surfacee. The thickness of the shock front is about 0.10 mm, for many pure explosive, but it can be larger depending on the high explosive (HE).

This is a boundary between two regions with a discontinuous high pressure. Here, in the shock front (Fig. 2) chemical reactions take place and bulk detonation energy is released. At the rear shock front, a complete thermodynamic equilibrium exists and the detonation products are said to be at Chapman-Jouguet (C-J) state. Normally, the detonation pressure refers to the pressure in the C-J state, which often is lower than the pressure at the shock front.

2. Fundamentals of Detonation

Theory of detonation has deep roots in the past. First observations, upon detonation waves, were made by French workers in about 1880. Later, Chapman (1899) and Jouguet (1905), independently gave the first theoretical fundamentals of detonation, considering that detonations travel at a particular velocity which has a minimum value (C-J velocity). The development of detonation theory continued, so Zeldovich (1940), von Neumann (1943) and Döring (1943) independently postulated that the detonation is a combustion wave, sustained by the shock wave.

All the processes which occur regarding formation and propagation of the blast waves and detonation waves as well, present a great complexity and difficulties in theoretical approaching. Thus, although the structure of the detonation wave is highly three-dimensional, many aspects can be studied by carrying out a one-dimensional analysis of a detonation wave.

The main assumptions are: one-dimensional steady flow, constant area tube, the gas is an ideal one, having constant and equal specific heats, adiabatic conditions and body forces are negligible.

The starting point in theoretical approaching is represented by the conservation equations of the mass, momentum and energy. Under above assumptions, these equations are represented by the relations (1)...(3). These equations are written for two states of the explosive, separated by the shock wave (Fig. 3).



Fig. 3. Motion of the shock wave in a medium.

$$\rho_1 u_1 = \rho_2 u_2 = \dot{m} = const. \tag{1}$$

$$P_1 + \rho_1 u_1^2 = P_2 + \rho_2 u_2^2 \tag{2}$$

$$E_1 + \frac{u_1^2}{2} = E_2 + \frac{u_2^2}{2} \tag{3}$$

In the relations (1)...(3), indices 1 and 2 refer to those two states of the explosive (Fig. 3); P,T,ρ and h are the state parameters: pressure, temperature, density and specific energy, respectively.

2.1 Rayleigh Line

By combining the relations (1) and (2), the following relation is obtained:

$$\dot{m}^{2} = (\rho_{1}u_{1})^{2} = (\rho_{2}u_{2})^{2} = \frac{P_{2} - P_{1}}{\frac{1}{\rho_{1}} - \frac{1}{\rho_{2}}} = \frac{P_{2} - P_{1}}{V_{1} - V_{2}}$$
(4)

where V is the specific volume. In the plane P-V, the relation (4) represents a line named Rayleigh line, which goes through two points: point 1 of coordinates P_1, V_1 (known parameters of state 1) and point 2 of coordinates P_2, V_2 (unknown parameters of state 2). For generalization, $P_2 = P$ and $V_2 = V$ and relation (4) becomes relation (5).

$$P = -\dot{m}^2 V + \left(P_1 + \frac{\dot{m}^2}{V_1}\right)$$
(5)

Because left hand side of equation (4) is always positive, two physically inaccessible domains exist as the Figure 4 shows (Strehlow, 1991).



Fig. 4. Rayleigh line in the plane P-V.

Any thermodynamic state is represented by a point (with coordinates P and V) which lies on a single straight line (Rayleigh line). Because the energy has not taken into account and also any equation of state, the Rayleigh line does not represent a complete solution of the considered problem. As the \dot{m}^2 is the slope of the line, the Rayleigh line has two limit positions, for $\dot{m}^2 \rightarrow 0$ and $\dot{m}^2 \rightarrow \infty$, respectively, representing the boundary of the inaccessible domains.

2.2 Hugoniot Curve

Using all those three equations, (1)...(3), and eliminating both velocities u_1 and u_2 , the Hugoniot relation is obtained, in the form of relation (6).

$$E_2 - E_1 = \frac{1}{2} \left(P_2 - P_1 \right) \left(V_1 + V_2 \right)$$
(6)

As the state 2 can be any one, we could write P instead P_2 and V instead V_2 ; so, in the same plane (P-V), represented in the Figure 4, the relation (6) represents a curve named Hugoniot curve or often, just Rankine-Hugoniot curve (Fig. 5 and 6). The relation (6) is written in terms of total enthalpy.

The energy that is released during combustion process is absorbed by the system and rises its temperature. The real enthalpy-temperature relation can be approximated by working fluid-heat addition model (Strehlow, 1991); so, by simple arbitrary heat addition to the working fluid, using the relations:

$$E_1 = c_{p1}T \tag{7}$$

$$E_2 = c_{p2}T - q \tag{8}$$

where c_{p1} and c_{p2} are the specific heat capacity of the explosive in the states 1 and 2, *q* represents a simple heat addition to the flow, so the relation (6) becomes:



Fig. 6 Hugoniot curves (burned and unburne explosive).

In the relation (9), γ is the ratio of specific heat capacity (c_p , c_v) for an ideal gas and q is a known parameter. Adopting this hypothesis, for calculus referring to TNT, the γ value is 2.727.

We have to notice that always $V_1 \neq 0$ and $P_1 \neq 0$, so the point 1 can be considered the origin of all explosive transformations. P_1 can be the athmospheric pressure, underwater pressure and at its limit can be even zero, but never $V_1 \leq 0$. As the Figure 6 shows, the Hugoniot curve does not pass through the so-called origin (q > 0). A complete representation, in the P-V plane, of the solution for a process represented by the equations (1)...(3) is presented in the Figure 7. The Hugoniot curve is the locus of all possible solutions for the equations (1)...(3), or for the equation (9). The points where the Rayleigh line is tangent with Hugoniot curve defines the C-J points (Fig. 7): one above P_1 is C-J detonation point and other, below P_1 , being the C-J deflagration point (points B and C respectively, Fig. 7). Intersections of the Rayleigh line with Hugoniot curve (points D, F, G, E, Fig. 7) define some points experimentally grounded. Large discussions can exist around Rankine-Hugoniot diagram, but these are beyond of this paper.

2.3 Detonation Theories

The detonation process can be imagined as a shock wave moving through an explosive. The Chapman-Jouguet (C-J) theory is the main and the oldest detonation theory. This successfully is used nowadays, but next to it other theories appeared, like Zeldovich-von Neumann-Doering (ZND) theory and overdriven detonation (ODD) theory. All these theory are synthetically presented in the Figures 8...13.



Fig. 7. Rankine-Hugoniot diagram.



Fig. 8. Pressure-specific volume in C-J theory.



Fig. 10. Pressure-specific volume in ZND theory



Fig. 9. Pressure-distance in C-J theory.



Fig. 11. Pressure-distance in ZND theory.



Fig. 12. Pressure-specific volume in ODD theory. Fig. 13. Pressure-distance in ODD theory.

In accordance with Chapman-Jouguet (C-J) theory, detonation process is characterized by a shock moving through explosive, so this is compressed and heated, initiating the chemical reaction. This process is considered to be instantly and all the time in an equilibrium and in a steady propagation in the explosive. In C-J conditions, a complete release of the stored chemical energy occurs. C-J theory is based on some assumptions; among these, the shock wave is supposed to move at a speed of local sonic velocity. In equilibrium conditions, the moving velocity of the shock front has a minimum value.

This velocity value is called detonation velocity or C-J velocity. So, the state behind the shock front is characterized by the C-J state.

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The Zeldovich-von Neumann-Doering (ZND) theory is a result of C-J theory developing. ZND theory accepts that the shock wave moves through explosive, but the shock wave compresses the explosive to a high pressure (much greater than C-J pressure), at which the explosive remains still unreacted. This high pressure is called von Numman spike (vNS) and it is a characteristic parameter of von Numman spike point. According to ZND theory, the reaction begins at the spike point and finishes at C-J point, reaching the equilibrium. The detonation products expand backward.

In some conditions, the front of detonation wave can be highly compressed without any reaction. The maximum pressure in an explosive, without any reaction is considered to be the pressure value corresponding to von Numman spike (vNS). When an explosive is subjected to a higher pressure than that of vNS point, another detonation pattern is considered to be induced.

This detonation pattern is called strong detonation or overdriven detonation (ODD). In the case of overdriven model, the reaction starts at HPS pressure. In the C-J and ZND models, the propagation of detonation is viewed as a steady process, while in overdriven model, the propagation of detonation is an unsteady process. This reaction finishes in ODD point, on Hugoniot curve of detonation products.

2.4 Equations of State for Explosives

For the calculus and analysis of the detonation waves and their effects as well, it is necessary to know the equations of state (EOS) of the explosive. There are some such of equations of state: polytropic ($\gamma - law$) equation of state, Jones-Wilkins-Lee (JWL) equation of state, Becker-Kistiakowsky-Wilson (BKW) equation of state, Jones-Wilkins-Lee-Baker (JWLB) equation of state and others. A part of them are already implemented in the professional numerical programs (Ls-Dyna, Autodyn etc.), like as JWL and JWLB EOS.

The most used equation of state is JWL EOS, which will be synthetically presented bellow. This EOS is obtained by combining of the isentropic equation of state with Mie-Gruneisen EOS for solids. The final form of JWL EOS is:

$$P = A \left(1 - \frac{\omega}{R_1 V} \right) \cdot e^{-R_1 V} + B \left(1 - \frac{\omega}{R_2 V} \right) \cdot e^{-R_2 V} + \frac{\omega h}{V}$$
(10)

where A, B, R_1, R_2 and ω are named JWL parameters, being constants which are experimentally determined for each explosive. The parameters ρ (density), h

(specific energy), u_D (detonation velocity) and P_{CJ} (Chapman-Jouguet pressure) are the input parameters, these depending on the taken into account explosive. For TNT these constants have the values presented in the Table 1.

Table						JWL paran	neters of	the INI (explosive
	ρ	Ε	u_D	P_{CJ}	A	В	R_1	R_2	ω
	kg/m ³	GJ/m ³	m/s	GPa	GPa	GPa	-	-	-
TNT	1630	7,00	6930	21,00	337,1	32,31	4,15	0,95	0,300

Table 1. JWL parameters of the TNT explosive

As the JWLB EOS is concerned, it was developed in 1991 by Baker for describing of the high pressure regime produced by overdriven detonations. For many explosives, all the input data are presented in the technical literature. Being about the overdriven detonation, the output parameters obtained by using the JWLB equation of state are greater than those obtained using the JWL equation of state.

Regardless the used EOS, any numerical model would have to be calibrated in relation to the experimental results or some benchmarks.

3. Analytical Calculus

Starting from that one-dimensional model, an analytical calculus calculus can be carried out, based on the Chapman-Jouguet (C-J) theory. Here are some calculus relations, from literature [2], [5], [12], for detonation parameter calculus:

a) the density ρ_2 of the explosive, in the Chapman-Jouguet point (ρ_{CJ}):

$$\rho_{CJ} = \frac{\gamma + 1}{\gamma} \rho_1 \tag{11}$$

b) the pressure P_2 in the C-J point (P_{CJ}):

$$P_{CJ} = 2(\gamma - 1)\rho_1 E_1 \tag{12}$$

c) the specific energy E_2 in the C-J point (E_{CJ}):

$$E_{CJ} = \frac{2\gamma}{\gamma + 1} E_1 \tag{13}$$

d) the sound velocity ($c = c_2$) in the C-J point (c_{CI}):

$$c_{CJ} = \sqrt{\gamma(\gamma - 1) \cdot E_{CJ}} \tag{14}$$

e) the detonation velocity (u_D) :

$$u_D = \sqrt{2(\gamma^2 - 1) \cdot E_1} \tag{15}$$

Such calculus relations are useful in the analysis process of the detonation, providing the quantitative results for comparing with the experimental results or with results obtained by other ways.

In the Table 2, some results comparatively are presented, using different ways. The comparison is referring to the measured values and presented in many papers. The most known and referred paper is [2] and [3], where also some empirically or semi-empirically formulas are given. The results of the analytical calculus are based on the theory synthetically presented above, using the relations (10)...(13).

	Measured	Empirically	Analitycal Calculus		
	Values	Calculated Values	C-J Theory	JWL EOS	
P _{CJ} [Pa]	2.10*10 ¹⁰	$2.23*10^{10}$	2.42*10 ¹⁰	$2.01*10^{10}$	
E _r [%]	0.00	6.19	15.14	-4.14	
<i>u</i> _D [m/s]	6930	-	7435	-	
<i>E_r</i> [%]	0.00	-	7.29	-	

Table 2. Comparative results

By far, the numerical methods, like FEM and the newer SPH method are the most powerful, efficient and versatile methods, with great possibilities for post-processing of the results.

4. Using of the SPH Method

The theoretical fundamentals of SPH method are considered to be known [10], [11], [13]. The using of the SPH method will be presented for a given problem consisting in determination of the detonation parameters for 1 kg of TNT, pressed by not confined, having a spherical shape. For a mass of 1 kg and a density of 1630 kg/m3, the calculated radius is 0.0527 m.

In this paper, we present the results for a spherical shape of TNT because the theoretical studies and many experimental results were made, first of all, for this TNT shape. Next to this aspect, the results presented in this work are obtained in ideal conditions, like an explosive placed unconfined, in vacuum.

We have to emphasize that the explosive shape together with boundary conditions has a great influence upon the detonation parameters and generally upon the explosion parameters. What is presented here is useful for approaching of others explosive shapes, in different surrounding conditions.

4.1 Numerical Models

There are some numerical models for SPH method and for FEM, as well. For models having as small as possible number of nodes and elements, the present of symmetry has to be taken into account. From this point of view, the spherical shape has a lot of

symmetry planes. For a right and simplified model, the symmetry planes would have to be the same with coordinate planes.

Considering the spherical explosive shape, for both two numerical methods (FEM and SPH), the simplest model is a 2D axisymmetric model. Such models are presented below (Fig. 14). Even this model type can be simplified, because it also has a symmetry axis (x-axis), like in the Figure 14, c) and e).

For FEM analysis, a plane finite element with four nodes was used, with three finite element side dimensions: 1 mm, 0.50 mm and 0.25 mm. It is very interesting to notice how the finite element size influences the detonation parameters.

The same three dimensions were adopted for the distance between particles in the case of SPH method. Next to it, different smoothing lengths were used, so their influence was put in evidence.



In the case of using of the FEM (models presented in the Fig. 14-b and c), the boundary conditions are presented in the Figure 14-a. In the case of using of the SPH method (Fig. 14-d) no boundary conditions are necessary; for the model presented in the Fig. 14-e, for the particles lying on the x-axis, the Y-displacements have to be restricted. The lack of the boundary conditions for the SPH model (Fig. 14-d) comes from the theoretical formulation of the SPH method in the version of 2D axi-symmetric. Also, this aspect depend on how the particles were generated. Generally, the such pre-processors don't put the particles just on the boundary, but at half the internodal distance.

4.2 Numerical Results

Our results comparatively are presented, using SPH method and FEM. Each of these methods were used in three versions of the discretisation. This is referring to the inter nodal (particle) distance and respectively, to the finite element size. These characteristics are presented in the Table 3.

The numerical analysis was performed using Ansys/Ls-Dyna program; a dedicated material model (MAT_HIGH_EXPLOSIVE_BURN) was used, together

with JWL EOS. The used material constants are those presented in the Table 1. As the smoothing length is concerned (a very important parameter in SPH method), different values were used, inclusive the value automatically calculated by the program. The analysis time was choosen of $1.00*10^{-5}$ seconds, as all the TNT mass to be totally burned.

Table 5. The characteristics of the numerical models								
	Vers	ion_1	Versi	ion_2	Version_3			
	SPH_1	FEM_1	SPH_2	FEM_2	SPH_3	FEM_3		
Distance/Size [m]	0.00100	0.00100	0.00050	0.00050	0.00025	0.00025		
Mass [kg]	0.9985	0.9992	0.9997	0.9993	0.9997	0.9993		
Nodes number	4410	4569	19012	18009	69268	71309		
Elements number	4410	4440	19012	17750	69268	70800		

Table 3 The characteristics of the numerical models

The numerical results are referring to some very important parameters, which can be known for each particle or node, but these parameters can be represented like a parameter field, for all domain.



Fig. 16. The pressure field by FEM.

Figures 15 and 16 show a very good concordance between results obtained by SPH method and by FEM. Practically, at the same moment $(4.3*10^{-6} \text{ s})$, the SPH maximum pressure (Fig. 15) differs by an error of 6.19% in relation to FEM maximum pressure (Fig. 16). As the resultant velocity is concerned, the same very good concordance between values obtained by SPH method (Fig. 17) and by FEM (Fig. 18) exists; the error is only 1.12%.

As the theory says and as the Figures 15...18 also show, the pressure and velocity evolve over time, especially in that zone of shock propagation.

The Figure 19 presents the pressure time evolution in five selected points (Fig. 20), which are placed along radius, having the coordinate y=0 (see Fig. 14). These points have the coordinates x in rising sense, towards the sphere center (x=0; y=0).



Fig. 17. The resultant velocity field, by SPH method Fig. 18 The resultant velocity field, by FEM.







In the Figure 21, the element (particle) mass/radian distribution is presented. Looking at this figure, taken at the starting time when density is the same for all particles, we see a x-or radius-distribution, which is a right one for a 2D axisymmetric model [18] (in reality, the particles have a variable volume, resulting a variable mass, owing to the 2D axisymmetric concept). The using of the SPH method allows us to analyse some very important parameters of the detonation process. So, only a SPH model automatically can take into account the variation of the mass, the density and others. In the Figure 22, the density field at the analysis start time is presented.

Fig. 21. Element mass/radian distribution.



As it was expected, the density is the same in all particles. After beginning of the burning (like in the Fig. 23), the density is modified; where the burning is over, the

density is lower than its initial values, in the shock wave the density is greater than its initial value and where the explosive is unburned the density has its initial value. Along the path presented in the Figure 23, the density has the variation versus distance, which is presented in the Figure 24.

For the same path presented in the Figure 23, the pressure variation versus distance, at the analysis time of $4.3*10^{-6}$ s, is presented in the Figure 25.

We can notice that behind the shock wave (where the maximum pressure occurs), the pressure goes down and in front of the shock wave the pressure has its initial values (in our case, zero).



Among the parameters of the SPH method, the smoothing length (h) is one of the most important one. This parameter has a great influence upon the results and even computer time as well. Until now, the smoothing length has no dedicated value for an analysis type etc. There are some general recommendations [11], [13] which could have to be taken into account. The user is helped by an available option of the program as this automatically to choose the smoothing length and this to be a variable one [11], [13]. The influence of the smoothing length upon numerical results is presented in quantity in the Figures 26 and 27.

		Measured	Empirical Calculated	Analitical Results		Numerical Results by SPH Method		
		values	Values	Theoretical	JWL	SPH_1	SPH_2	SPH_3
P_{CJ}	[MPa]	21000	22300	24200	20100	21460	24600	27900
	E _r [%]	0.00	6.19	15.14	-4.14	2.19	17.14	32.85
<i>u</i> _D	[m/s]	6930	-	7435	-	7094	6161	6503
	E _r [%]	0.00	-	7.29	-	2.37	-11.10	-6.16
$ ho_{CJ}$	[kg/m ³]	-	-	2228	-	2250	2372	2433
	E _r [%]	_	-	0.00	-	0.99	6.46	9.20
V =	$ ho_0$ / $ ho$	-	-	0.732	-	0.724	0.687	0.670

Table 4. Comparison of the numerical results with experimental and analitycal results.

So, it is necessary that the SPH method to be calibrated by analysing the numerical results with experimental results, or with the benchmark results, or/and with the analytical (theoretical) results.

The numerical results, obtained by using of the SPH method and presented in this paper, are based on the calibration of the SPH method by comparison the numerical results with the experimental and theoretical results. As the smoothing length (h) is concerned, for SPH_1 version we used automatical determination by the program, for SPH_2 and SPH_3 versions, the smoothing length was constant, having the value 1.50 and 2.50 respectively.

5. Conclusions

The phenomenon of the detonation is a very complex one, which can be analysed for improving of its parameters, for the sake of improving of its effects upon structures. Nowadays, the explosives are used in many civil activities like controlled building demolition, in mechanical technology like explosion plating, welding, hardening, controlled plasticization of tubes and others.

The appearing and using of the SPH method offer us a new, efficient and versatile tool for numerical analysis of the fluids and structures. For numerical analysis of the detonation process, the SPH method is a very good one not only for results in a good concordance with the experimental results, but for its new parameters which can be analysed, like density variation, volume and mass variations etc. A great advantage of the method consists in avoiding of the difficulties coming from large deformations and great nonlinearities.

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