UPON ANALITICAL AND NUMERICAL CALCULUS OF THE MAIN PARAMETERS OF THE DETONATION PROCESS

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Abstract. This paper presents some results of scientific research undertaken by the authors, regarding the numerical modeling of the detonation process, both the Finite Element Method (FEM) and the method of free particles, in version of Smoothed Particle Hydrodynamics (SPH) method. After a synthetic presentation of detonation, as part of explosive process, whose parameters and effects must be known, the authors describe the fundamentals of the analytical calculus and approaching ways of the numerical analysis. So, Rankine-Hugoniot relations, Chapman-Jouguet and Zeldovich-von Neumann-Doering theories and equations of state of explosives during the energy conversion process, are successively presented. The paper continues with numerical modeling using MEF in several variants of the mesh, using several equations of state and varying a number of parameters in the initial data characteristics of explosives. Concrete examples are considering two explosives: TNT and PETN. The main parameters analyzed are the pressure and the detonation speed together with their variation in time and in space. The analysis of the above parameters is made in the context of the key input process, a particular concern of the influence of the pressure and velocity at the Chapman-Jouguet point of balance and the internal specific energy of explosive upon the pressure and detonation velocity.

Keywords: explosive, modeling, finite elements, detonation velocity, detonation pressure

1. INTRODUCTION

Today, in the front of structural engineers, many challenges exist, among these, protecting of the civilian buildings and device structures against the terrorist activities has a great importance. This type of protection need a very good understanding of the explosion phenomena, starting with what is and what happens in an explosive by burning initiation and finishing with studding the interaction between blast waves and structures. This paper presents some researching results of authors regarding fundamentals of detonation phenomena, its numerical modeling and how the detonation parameters are determined by the specific properties of an explosive.

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. Our paper is referring only to third type, namely, to chemical explosion. This explosion type is most used by terrorists for bomb manufacturing or other explosive devices.

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. Exothermically reacting shock waves are classified into two types: detonation waves and deflagration waves. Detonation waves are supersonic and compressive and deflagration waves are subsonic and expansive. 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.

For majority high explosives, detonation velocity range is from 5,000 to 8,000 meters per second. The detonation wave converts the solid or liquid explosive into a very hot, dense, high-pressure gas. The volume of this gas, which had been the explosive material, is then the source of strong blast waves in air, acting upon different structures, human being and others. Pressures, immediately behind the detonation wave front, usually run from 18,000 to 35,000 MPa. Only about one-third of the total chemical energy is released in the detonation process; the remaining two-thirds are released more slowly, in explosions in air as the detonation products mixed with air and burn results.

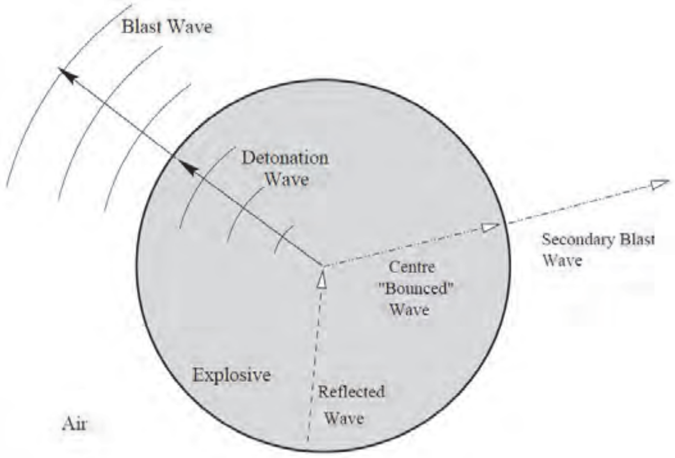


Fig. 1. Types of explosion waves.

2. THEORY OF DETONATION FUNDAMENTALS

The roots of detonation theory we can find in France, in 1880 year, when were made the first experimental observations. After only 20 years the first mathematical approaches had appeared, when Chapman and Jouguet, independently mathematically formulated the detonation process in gases.

Chapman-Jouguet (C-J) theory idealizes detonation as a planar mathematical discontinuity that propagates steadily. The passage of discontinuity leads to a complete release of the stored chemical energy.

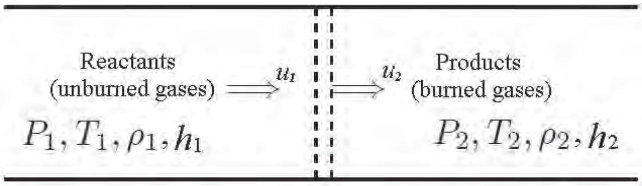


Fig. 2. Shock wave passage in explosive.

For the theoretical approaches, a remark has to be underlined: the structure of detonation wave is highly three-dimensional, but for avoinding the complexity of such phenomena, until now all the specialists consider an available gain by carring out a one-dimensional analysis of a detonation wave (theoretical model presented in Figure 2).

The detonation front, this shock (Figure 2) separates the unburned explosive, with known parameters and the burned products which are going to be known. Across the shock the ***Rankine-Hugoniot conditions*** must be fullfiled: mass conservation, momentum conservation and energy conservation (relations (1)...(3)).

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

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

$$h_1 + \frac{u_1^2}{2} = h_2 + \frac{u_2^2}{2} \tag{3}$$

By combination of equations (1) and (2), a line equation is obtained – ***Rayleigh line*** (4):

$$\frac{P_2 - P_1}{\frac{1}{\rho_2} - \frac{1}{\rho_1}} = \frac{P_2 - P_1}{V_2 - V_1} = -m^2 \tag{4}$$

For a fixed flow rate *m*, plotting P versus $1/\rho$, Rayleigh line is represented. For a given values of P_1 and ρ_1, Rayleigh line equation is written:

$$P = a\left(\frac{1}{\rho_2}\right) + b \tag{5}$$

where $a = -m^2$ is the slope and $b = P_1 + m^2 V_1$ is the interception of P axe.

Analyzing relations (1) and (2) leads us to possible domains for accepted solutions of the equations. These domains are represented in the Figure 3. By combination of equations (1), (2) and (3), in an ideal gas conditions ($\gamma = c_p / c_v$) and taking into account the energy (q) added by explosive burning, equation (6) of ***Rankine-Hugoniot curve*** is obtained:

$$\frac{\gamma}{\gamma - 1}\left(P_2 V_2 - P_1 V_1\right) - \frac{1}{2}\left(P_2 - P_1\right)\left(V_1 + V_2\right) - q = 0 \tag{6}$$

The fix point $\left(P_1, V_1\right)$, representing the initial state, is known as the origin of the Rankine-Hugoniot curve, which does not pass through the origin of axes system $P - V$.

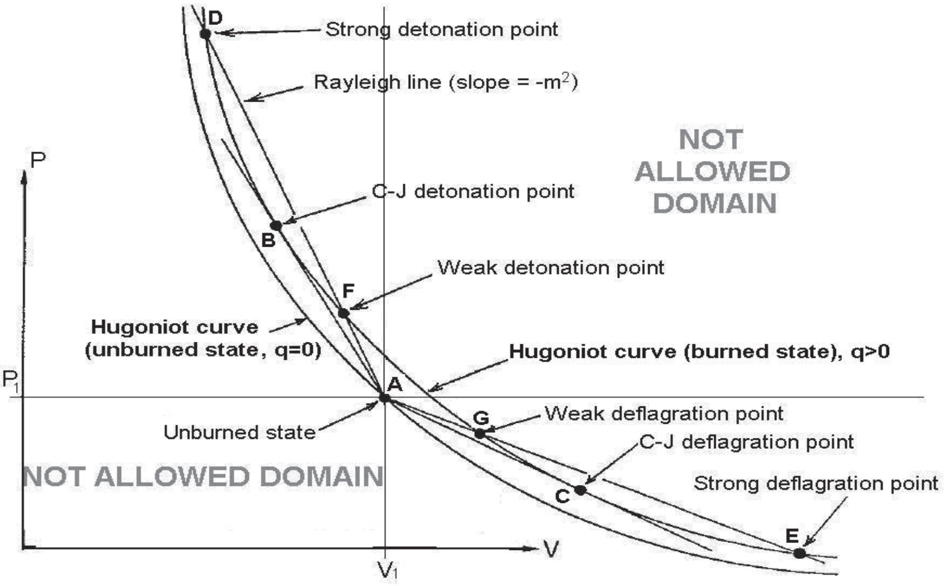


Fig. 3. Rayleigh lines and Hugoniot curves in pressure-specific volume axes.

Figure 3 presents the Rayleigh lines and Rankine-Hugoniot curves together with points representing characteristic states. These points have those coordinates representing the solutions of equations (1)...(3). Among these points, Chapman-Jouguet (C-J) points are most important. There is such a point in deflagration domain and other in detonation domain.

This point (C-J) is a characteristic of the energetic material (explosive). Chapman-Jouguet characteristics (velocity, pressure, etc.) are those which make difference between different explosives. The characteristics strong or weak, for detonation and for deflagration respectively, are referring to the values comparatively with C-J points of the domains. C-J points are certain equilibrium points, others (strong or weak) can be or not, does or does not occur.

As it can be noticed in the Figure 1, detonation waves go beyond the explosive border, going on as blast waves. These waves are those which interact with structures or any other objects. The knowing of C-J characteristics is a subject of researching in the explosive field. Knowing of the explosive characteristics (physical, detonation, chemical etc.) is the first step in evaluations of explosive effects.

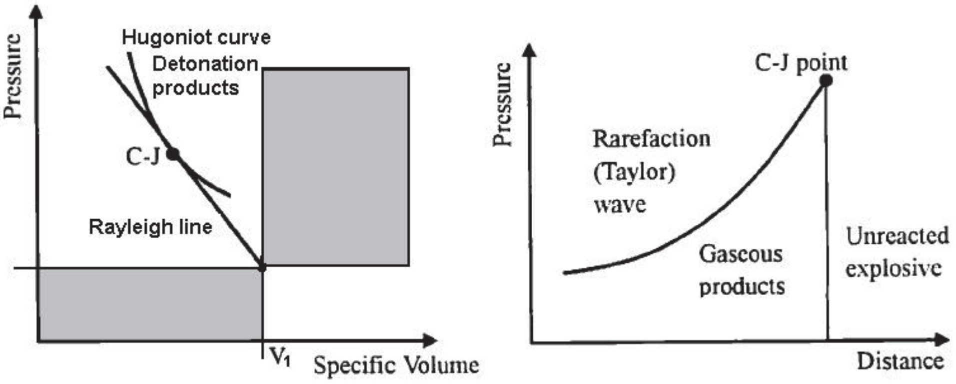
Researching of detonation phenomena is made experimentally and by numerical method - most used method being finite element method and in last time, free particle methods (smoothed particle hydrodynamics) are also used. Nowadays, two main theories are large accepted for explications and for modeling of the detonation phenomena: Chapman-Jouguet (C-J) theory and Zeldovich, von Neumann and Doering (ZND) theory.

2.1. Chapman-Jouguet Theory

In according with this 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.

Chapman-Jouguet (C-J) theory is based on some assumptions: shock wave move at a speed of local sonic velocity, as the particles behind the shock front are concerned. In equilibrium conditions, the moving velocity of the shock front has a minimum value. This velocity value is called detonation velocity or Chapman-Jouguet velocity. So, the state behind the shock front is characterized by the Chapman-Jouguet state. All the variables of C-J state satisfy the Hugoniot jump conditions, described by equations (1)...(3).

In Chapman-Jouguet conditions, a complete release of the stored chemical energy occurs. The above considerations are included in what is named Chapman-Jouguet model and are synthesized graphically, in the Figure 4.



a) Pressure versus specific volume **b)** Pressure versus distance

Fig. 4. Pressure variation in C-J model.

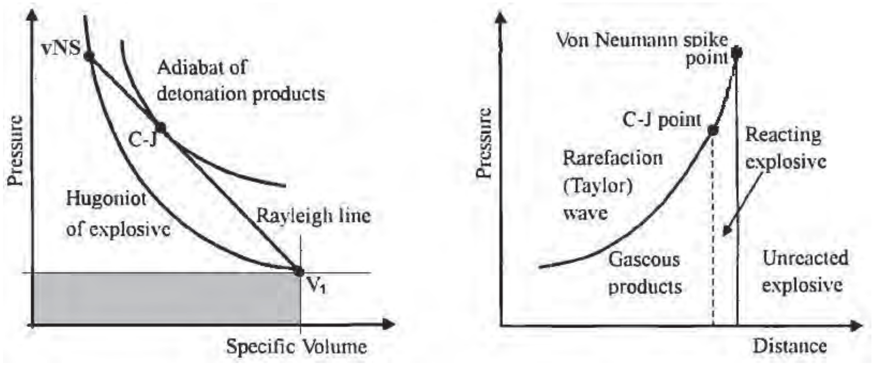
2.2. Zeldovich-von Neumann-Doering Theory

Zeldovich-von Neumann-Doering (ZND) model is a result of Chapman-Jouguet theory developing, obtained by each of them independently. 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 still remains 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 Chapman-Jouguet point, reaching the equilibrium. The detonation products expand backward. These concepts are graphically illustrated in the Figure 5.

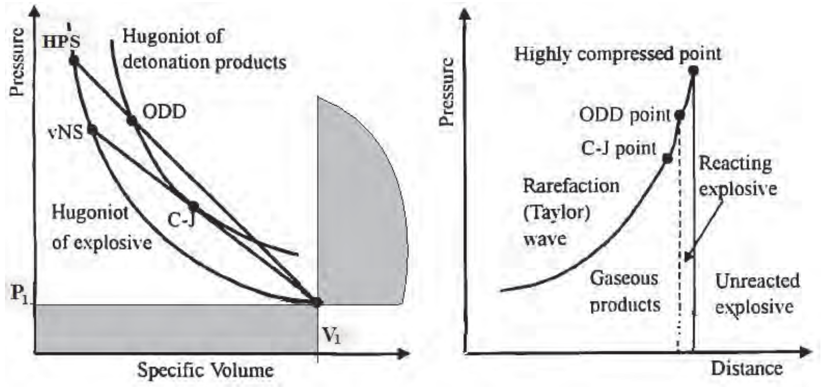
2.3. Overdriven Detonation

In some conditions (different explosives etc.), the detonation wave with its shock front 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).



a) Pressure versus specific volume **b)** Pressure versus distance

Fig. 5. Pressure variation in ZND model.



a) Pressure versus specific volume **b)** Pressure versus distance

Fig. 6. Pressure variation in overdriven pattern.

Analyzing the Figures 5 and 6, we can notice that in the case of ZND model the reaction starts at vNS pressure. In the case of overdriven model, the reaction starts at HPS pressure.

This reaction comes an end in ODD point, on Hugoniot curve of detonation products. Other aspect has to be noticed: in the C-J and ZND models (theories), the propagation of detonation is viewed as a steady process, while in overdriven model (theory), the propagation of detonation is an unsteady process. The sound speed and other parameters, in overdriven detonation is greater than in C-J or ZND detonation.

3. NUMERICAL ANALYSIS OF DETONATION

Analytical study of detonation process, for any adopted model, remains a very difficult problem. So, like in many other engineering studies the numerical calculus is a proper, efficient and even fast way. Finite element method and newer free particle method (specially smoothed particle hydrodynamics) are the best methods. If the general theory of FEM is available in detonation study, two new aspects must be understood and correctly used: adequate material model and equation of state (EOS) attached to this. Some essentials about these subjects are presented below.

3.1. Material Models

There are some professional programs which have in their material library dedicated material models for explosives. For instance, Ls-Dyna code - one of the famous professional program - has such material model named MAT_HIGH_EXPLOSIVE_BURN. This material model, like others, uses an EOS and can simulate detonation by release controlling of the chemical energy. So, firstly, in the initialization phase, a lighting time t_1 is computed for each element by dividing the distance from the detonation point to the center of the element by the detonation velocity *D*. The burn fraction F is the maximum of values F_1 or F_2:

$$F_1 = \begin{cases} \dfrac{2(t-t_1)\cdot D \cdot A_{e\max}}{3v_e} & t > t_1 \\ 0 & t \le t_1 \end{cases} \quad ; \quad F_2 = \frac{1-V}{1-V_{CJ}} \tag{7}$$

If F exceeds 1, it is reset to 1 and it is held constant. In the relation (7), t is the current time, V is the current volume, V_{CJ} is the Chapman-Jouguet relative volume. The pressure in a high explosive FE is:

$$p = F \cdot p_{EOS}(V, h) \tag{8}$$

where p_{EOS} is the pressure calculated by adopted EOS, V is the relative volume and h is the internal energy density per unit initial volume. Once the explosive material detonates, the material behaves like a gas and the deviatoric trial stress (s_{ij}) is set zero.

3.2. Equations of State

For explosive materials some equations of state (EOS) are available: polytrophic (γ- law) EOS, Jones-Wilkins-Lee (JWL) EOS, Jones-Wilkins-Lee-Baker (JWLB) and Becker-Kistiakowsky-Wilson (BKW) EOS etc. The most used EOS are JWL and JWLB. The JWL equation of state (9) defines pressure as a function of relative volume, V, and internal energy per initial volume, h, as:

$$p = A\left(1 - \frac{\omega}{R_1 V}\right)e^{-R_1 V} + B\left(1 - \frac{\omega}{R_2 V}\right)e^{-R_2 V} + \frac{\omega h}{V} \tag{9}$$

where ω, *A*, *B*, R_1 and R_2 are user defined input parameters. The JWL equation of state is used for determining the pressure of the detonation products of high explosives. In the same aim, JWLB equation of state (10) is used, but the pressure of the detonation products of high explosives is:

$$p = \sum_{i=1}^{5} A_i \left(1 - \frac{\lambda}{R_i V}\right)\cdot e^{-R_i V} + \frac{\lambda h}{V} + C\left(1 - \frac{\lambda}{\omega}\right)\cdot V^{-(\omega+1)} \tag{10}$$

$$\lambda = \sum_{i=1}^{5} A_i \left(A_{\lambda i} V + B_{\lambda i}\right)\cdot e^{-R_{\lambda i} V} + \omega \tag{11}$$

where A_i, R_i, $A_{\lambda i}$, $B_{\lambda i}$, $R_{\lambda i}$, C, and ω are input constants defined for each explosive.

3.3. Illustrative examples

Based on above theoretical fundamentals, using Ls-Dyna program and more explosive types, we researched the influence of different parameters (EOS, mesh size, explosive type) upon detonation process. A quantity of explosive ($\approx 1\ kg$) with the same geometry (a sphere with $R \approx 5\ cm$), placed somewhere in space, without any restriction was considered for simulation of detonation process (what happen inside of explosive). The initiation point of detonation was considered just in the sphere center.

The finite element (FE) model was a plane (2D) one, axis-symmetric; three mesh sizes were considered (Fig. 7), the maximum FE dimension being 2 mm, 1 mm and 0.50 mm. Two explosive types were used: TNT and PETN, having the characteristics presented in the Table nr. 1. Other parameters used in this study were taken from literature and own experience.

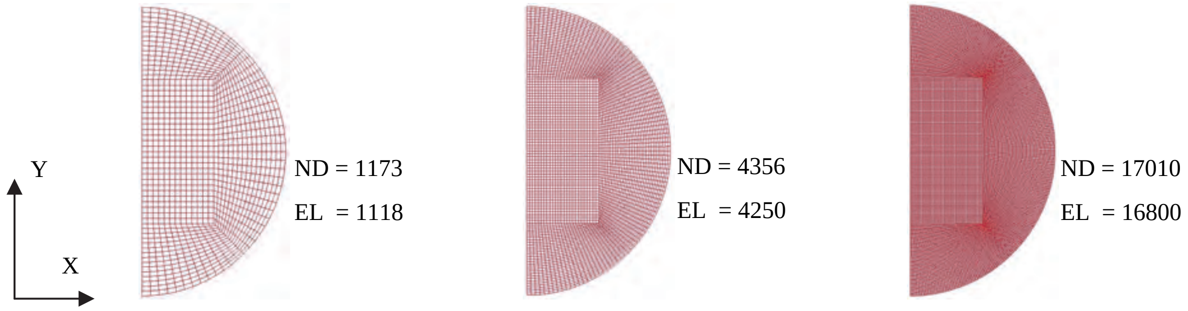


Fig. 7. Finite element meshes used in numerical analysis.

Table 1. **Explosive characteristics**

Parameter	ρ	P_{CJ}	D_{CJ}	h	ω
Measure unit	kg/m^3	Pa	m/s	$Pa \equiv J/m^3$	---
TNT	1630	2.10e10	6930	7.0e9	0.300
PETN	1700	2.55e10	7530	8.1e9	0.350

The influence of the mesh dimension is a very important one, because there is a great variation in time and in space. As the detonation velocity is concerned (FED = finite element dimension), mesh size influence is quantitatively illustrated by the Figure 8.

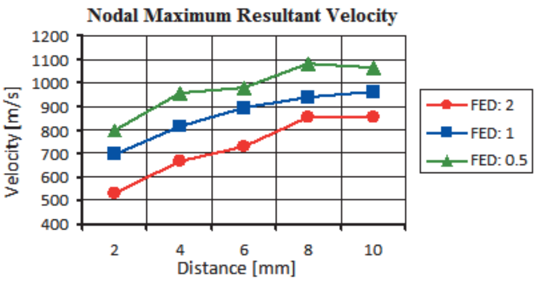


Fig. 8. The influence of the mesh size

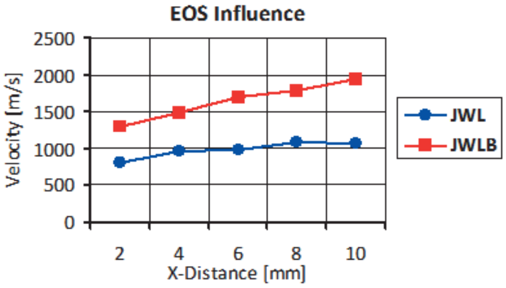


Fig. 9. EOS influence upon velocity

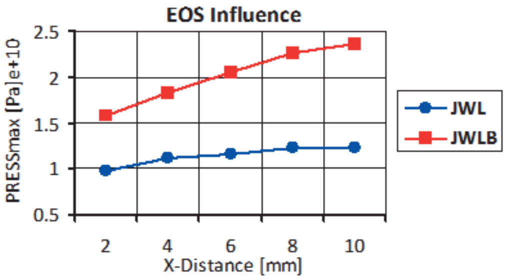


Fig. 10. EOS influence upon pressure

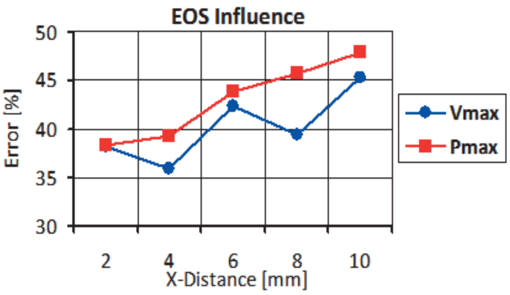


Fig. 11. Errors JWL versus FWLB

In the Figures 9 and 10 the influence of the adopted EOS is illustrated, regarding to detonation velocity and pressure respectively. As we can see, the values of the detonation parameters are strongly determined by the EOS type. Experimentally, we found that JWLB EOS using leads to a closer results with the reality. The calculus errors of detonation parameters using JWL EOS, comparatively with JWLB EOS, are graphically represented in the Figure 11.

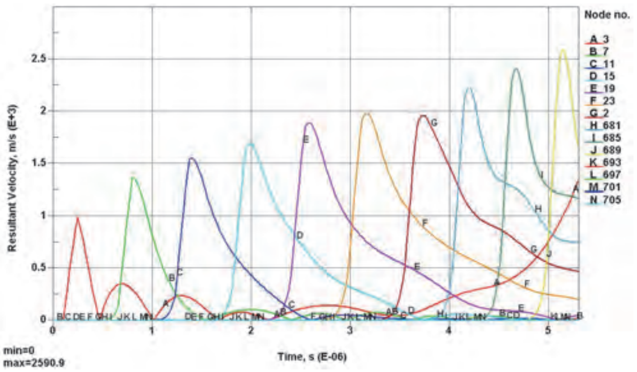


Fig. 12. Nodal resultant velocity in time

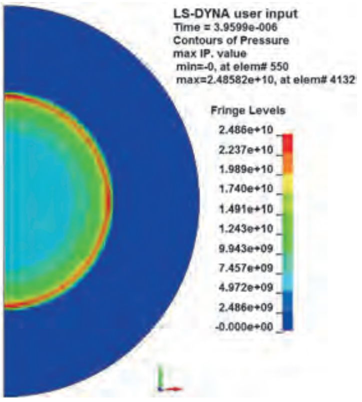


Fig. 13. Nodal pressure field

Table 2. **Influence of D_{CJ} on the nodal wave velocity and pressure**

D_{CJ} [m/s]	**Distance [mm]**	**2**	**4**	**6**	**8**	**10**
6000	Velocity [m/s]	784	968	1139	1214	1367
6930		694	815	892	941	961
7500		608	718	814	773	830
6000	Pressure [Pa]e+10	0.912	1.164	1.286	1.465	1.625
6930		0.892	1.024	1.099	1.158	1.199
7500		0.863	0.950	1.001	1.078	1.093

Figure 12 presents nodal resultant velocity of some points placed on OX axis, for TNT explosive. Curve allures are in a very good concordance with the theory. In the Table nr. 2, the influence of the D_{CJ} input parameter is reflected, as the velocity and the pressure are concerned. By post-processing the results, the field of nodal pressure is presented in the Figure 13, for the same explosive. For PETN explosive, the results differs only by numerical values.

4. CONCLUSIONS

The knowing of the detonation parameters, for any explosive, has a great importance in evaluation of the explosive power and first of all in evaluation of the following developing of the explosive waves, when the shock front is going to propagate in air, or to act upon a closing box.

Numerical simulation for determination of the influence of any input parameters has also a great importance, because sometimes the right input parameter value is unknown or uncertain and an evaluation by comparing or a chosen value is necessary to be made. Like those presented above, our research was made in connection with many other parameters. The above presented detonation models are implemented in professional numerical codes and these are able to simulate in an adequate way the detonation process.

REFERENCES

[1] Kingery, C.N., Bulmash, G, *Air-Blast Parameters from TNT Spherical Air Burst and Hemispherical Surface Burst*, ARBRL-TR-02555, U.S. Army Ballistic Research Laboratory, Aberdeen Proving Ground, MD, 1984.
[2] Sachdev, PL., *Shock waves and Explosions*. Chapman & HaIVCRC, New York (2000).
[3] Silde, A., Lindholm, I., *On Detonation Dynamics in Hydrogen-Air-Steam Mixtures: Theory and Application to Olkiluoto Reactor Building*, VTT Energy, Espoo, Finland, February 2000.
[4] * * * *LS-DYNA Keyword User's Manual*, Version 971/Rev 5, Livermore Software Technology.
[5] Corporation (LSTC), May 2010.

ASUPRA CALCULULUI ANALITIC ŞI NUMERIC AL PRINCIPALILOR PARAMETRI AI PROCESULUI DE DETONAŢIE

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Rezumat: Lucrarea prezintă unele rezultate ale cercetării ştiinţifice întreprinse de autori, privind modelarea numerică a procesului de detonaţie, atât prin Metoda Elementelor Finite (MEF), cât şi prin metoda particulelor libere, în varianta SPH (Smoothed Particle Hydrodynamics). După o sintetică prezentare a detonaţiei ca parte a unui proces exploziv a cărui parametri şi efecte trebuie cunoscute, autorii descriu fundamentele calculului analitic şi modul de abordare al calculului numeric. Astfel, sunt prezentate succesiv, relaţiile Rankine-Hugoniot, teoriile Chapman-Jouguet şi Zeldovich-von Neumann-Doering, precum şi ecuaţiile de stare ale explozivilor pe timpul procesului de transformare energetică. Lucrarea continuă cu modelarea numerică folosind MEF, în mai multe variante de discretizare, folosind mai multe ecuaţii de stare şi variind o serie de parametri caracteristici în cadrul datelor iniţiale ale explozivilor. Exemplele concrete au în vedere doi explozivi: trotilul (TNT) şi pentolita (PETN). Principalii parametrii analizaţi sunt preziunea şi viteza de detonaţie, împreună cu modul de variaţie al acestora în timp şi în spaţiu. Analiza parametrilor de mai sus este realizată în contextul unor date de intrare esenţiale ale procesului de detonaţie, cu o preocupare specială a influenţei asupra presiunii şi vitezei de detonaţie a unor mărimi, precum presiunea şi viteza în punctul de echilibru Chapman-Jouguet şi energia internă specifică a explozivului. Lucrarea este utilă celor care sunt interesaţi în modelarea numerică a exploziilor, atât în scopul determinării caracteristicilor acestora cât şi în scopul determinării efectelor acestora supra structurilor de orice fel.