Central European Journal of Energetic Materials, **2010**, *7*(2), 97-113
ISSN 1733-7178

Calculation of Combustion, Explosion and Detonation Characteristics of Energetic Materials

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Abstract: In this work, the thermodynamic code for the determination of the chemical equilibrium composition of a non-ideal heterogeneous system is presented. Computation of combustion, explosion and detonation parameters for some explosives is performed as well as isentropes of products expansion and detonation energy are estimated. Moreover, the non-equilibrium calculations are carried out, in which chemical inertness of one from the components of explosive composition as well as no heat exchange between the component and the detonation products are assumed. At the end, some calculated detonation characteristics are compared with the experimental ones.

Keywords: thermochemical codes, energetic materials, combustion, explosion, detonation

Introduction

Effective, theoretical calculations of the detonation parameters and the chemical equilibrium composition of reaction products based on physical and chemical properties of an energetic material, as its atomic composition, enthalpy of formation and density, have became possible thanks to the thermodynamic approach taking into consideration:

- the mathematical model of an ideal detonation,
- the principle of extremum of characteristic functions delineated by Gibbs,
- thermodynamic equations of state for the real gasses (reaction products) with a wide range of pressure and temperature.

Nowadays many numerical methods and programs are being used

(thermochemical codes) for carrying out thermodynamic calculations of the detonation parameters of condensed explosives, for example a BKW Fortran [1], ARPEGE [2], Ruby [3], TIGER [4], CHEETAH [5], EXPLO5 [6], MWEQ [7], BARUT-X [8]. Although in many research centers in the world thermochemical codes were worked out, access to them is difficult and, moreover, any changes in the codes aren't possible because they are made available in the compiled form. Therefore, at the Department of Explosives in the Warsaw Military University of Technology, decision has been taken to create own numerical code named ZMWNI.

In Ref. [9], the review of thermodynamic methods for determining the equilibrium composition of complex mixtures was made. These methods are used in thermochemical codes to determine the combustion and detonation parameters for energetic materials. On this base the method for the determination of the equilibrium and non-equilibrium states for ideal heterogeneous systems was proposed in Ref. [10] and the computer program called ZMWI was applied for calculation of the parameters of combustion and detonation of ideal explosives compositions.

In the work [11] the method of calculation of the equilibrium state of reacting, non-ideal mixture and ways of application of this method for estimating the parameters of combustion, explosion and detonation of energetic materials were described. In addition, procedures were proposed for calculation the JWL (Jones-Wilkins-Lee) isentrope and the detonation energy on the basis of thermochemical calculation results. Moreover, the method of non-equilibrium calculations was discussed in which the chemical inertness of one or a few components could be assumed and no heat exchange between an inert compound and reaction products could be supposed.

In the present work the thermochemical program ZMWNI is described. The code can calculate the parameters of combustion, explosion and detonation of condensed energetic materials as well as determine the curve of expansion of detonation products in the form of JWL isentrope [12] and the energy of detonation [13]. Moreover, the ZMWNI code is able to determine the non-equilibrium states for frozen composition or for different temperatures of components.

In the program ZMWNI, the method based on the minimization of chemical potential is applied to calculate the equilibrium or non-equilibrium composition of a reactive system. The final collection of components is obtained through solving the set of linear equations and the method of steepest descent ([14], [11]). Physical properties of gasses are described by the BKW equation of state (Becker, Kistiakowsky, Wilson). For condensed components the OLD equation of state, applied in the thermochemical codes TIGER and CHEETAH, is used.

To determine the equilibrium state for combustion, explosion in a fixed volume or detonation of an energetic material, the physical conditions appropriate for the given process are taken into account. These conditions are described herein.

In the work the results of exemplary calculations are also presented. To verify the ZMWNI program these results are compared with that obtained from the CHEETAH code. In particular, the outcome of determination of the adiabatic combustion temperature, JWL isentrope and detonation energy are shown. Moreover, new possibilities of the program, i.e., the non-equilibrium calculations, are demonstrated. At the end, some experimental data are confronted with the results obtained from the ZMWNI calculations.

Equilibrium calculations

Constant-volume explosion

Conservation of the internal energy is a physical condition for a constant-volume explosion. For this condition, the temperature is an unknown state parameter. The aim of calculations is determination of the composition of products, for which the principle of conservation of internal energy is fulfilled and the thermodynamic potential reaches its minimum.

The results of constant-volume explosion calculations are presented in Tables 1 and 2 and they are compared with the values obtained from the CHEETAH code. The BKWC database [5] has been applied in the both programs. Calculations have been carried out for a loading density of 0.625 g/cm^3. The values of specific enthalpy, energy and entropy in Table 1 are relative given as changes from the reactants state.

Table 1. Comparison of the thermodynamic functions and parameters obtained from the ZMWNI and CHEETAH codes for the constant-volume explosion of TNT

Pressure [atm]	Specific volume [cm^3/g]	Temperature [K]	Enthalpy [cal/g]	Energy [cal/g]	Entropy [cal/K/g]	Volume of gaseous products [cm^3/g]	Code
15801	1.6	2823.2	611.99	0	1.860	1.6	ZMWNI
15806	1.6	2823.7	612.45	0	1.863	1.6	CHEETAH

Table 2. Comparison of the products compositions obtained from the ZMWNI and CHEETAH codes for the constant volume explosion of TNT

Product	Contents [mole/mole$_{Exp}$]		Product	Contents [mole/mole$_{Exp}$]	
	ZMWNI	CHEETAH		ZMWNI	CHEETAH
CO	4.239E+00	4.239E+00	CH_2O	8.209E-03	8.217E-03
N_2	1.465E+00	1.465E+00	CH_3	6.102E-03	6.111E-03
H_2	1.243E+00	1.243E+00	C_2H_2	5.529E-03	5.538E-03
H_2O	6.002E-01	6.002E-01	C_2H_6	4.846E-03	4.850E-03
CO_2	5.690E-01	5.690E-01	CH_2O_2	4.650E-03	4.655E-03
CH_4	2.541E-01	2.541E-01	CHNO	2.748E-03	2.751E-03
NH_3	4.165E-02	4.167E-02	H	1.830E-03	1.833E-03
CHN	2.584E-02	2.586E-02	CHO	1.211E-03	1.213E-03
C_2H_4	1.270E-02	1.271E-02	CH_3OH	1.157E-03	1.159E-03

From the presented data it follows that differences between the values of component quantity calculated by the both programs are less than 0.2%.

Combustion

For the adiabatic combustion at a constant-pressure state, the enthalpy of a system should be constant during the process. For an assigned pressure and enthalpy, calculations are aimed for seeking a minimum of the thermodynamic potential. In this way the so-called adiabatic combustion temperature is determined, which is often used to characterize energetic properties of materials.

The results of equilibrium calculations for exemplary mixtures containing polytetrafluoroethylene (PTFE) and powder of magnesium are presented in Tables 3 and 4. Calculations have been performed for a pressure of 1 atm. The BKWS database [15] containing compounds of fluorine and magnesium has been used. The enthalpy, energy and entropy are calculated as changes from the reactants state.

Table 3. Comparison of the thermodynamic parameters obtained from the ZMWNI and CHEETAH codes for the adiabatic combustion of the mixture containing 70% PTFE and 30% Mg

Pressure [atm]	Specific volume [cm^3/g]	Temperature [K]	Enthalpy [cal/g]	Energy [cal/g]	Entropy [cal/K/g]	Volume of gaseous products [cm^3/g]	Code
1	4919.29	3696.69	0	-119.11	1.595	4919.12	ZMWNI
1	4919.30	3696.70	0	-119.12	1.595	4919.26	CHEETAH

Table 4. Comparison of the products compositions obtained from the ZMWNI and CHEETAH codes for the adiabatic combustion of the mixture containing 70% PTFE and 30% Mg

Product	Contents [mole/mole$_{Exp}$]		Product	Contents [mole/mole$_{Exp}$]	
	ZMWNI	CHEETAH		ZMWNI	CHEETAH
F_2Mg	5.643E-01	5.643E-01	Mg	6.156E-03	6.156E-03
F	1.667E-01	1.667E-01	C_2F_2	3.755E-05	3.756E-05
CF_2	1.746E-02	1.746E-02	C_2	3.794E-03	3.794E-03
CF	4.986E-02	4.986E-02	F_2	1.524E-06	1.525E-06
FMg	6.752E-02	6.752E-02	C_5	3.511E-04	3.511E-04
CF_3	4.799E-05	4.801E-05	C_2F_4	1.524E-08	1.526E-08
CF_4	1.798E-06	1.799E-06	C_4	1.613E-04	1.613E-04
C_3	2.753E-02	2.752E-02	C_2F_6	9.929E-13	9.943E-13
F_4Mg_2	3.296E-05	3.297E-05	*C solid	4.726E-01	4.733E-01

Similarly to the constant-volume explosion, differences between the contents values calculated for the constant-pressure combustion by the use of the CHEETAH and ZMWNI codes are small and they are below 0.2%.

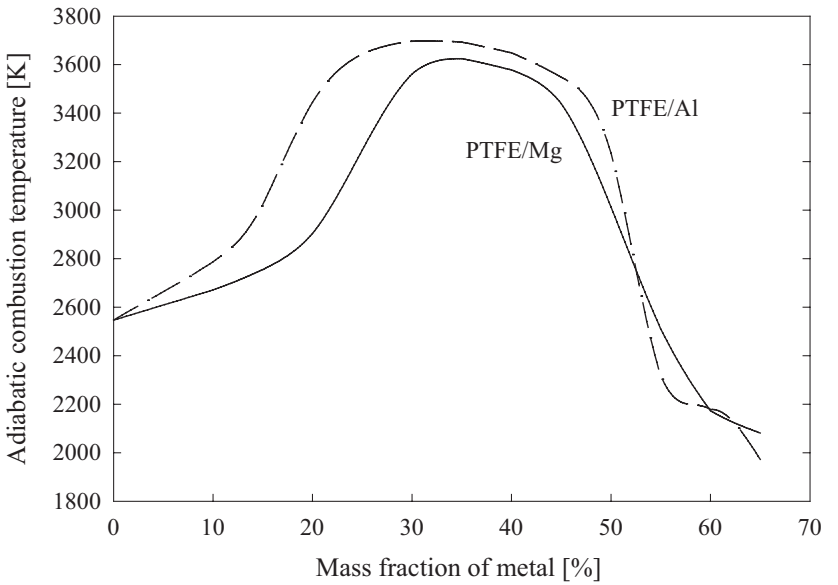

Figure 1. Dependence of the adiabatic combustion temperature on the mass fraction of metal in PTFE/Al and PTFE/Mg mixtures.

The adiabatic temperature is very often used in numerical modeling of the combustion process in solid energetic materials. The option of the constant-pressure combustion in the ZMWNI code enable us to determine this parameter for a chosen composition. For example, the dependence of the adiabatic temperature on the mass fraction of a metal is presented in Figure 1 for mixtures of PTFE with Mg or Al.

Detonation parameters and isentropes of products expansion

To determine detonation parameters the relations resulting from the ideal detonation theory are usually used. From the equations of mass and momentum conservation one can obtain the relation combining the detonation velocity, pressure and specific volume at the front of detonation wave (the so-called Rayleigh line)

$$\frac{D^2}{v_1^2} = -\frac{p_2 - p_1}{v_2 - v_1},$$

where p_1, v_1 denote the pressure and specific volume of an explosive, p_2, v_2 are the pressure and specific volume of the reacting composition at the front of detonation wave whereas D is a speed of propagation of the wave. This equation complete the equation of a detonation adiabate which connects p_2 and v_2 (the energy conservation equation). According to the Chapman-Jouguet hypothesis, the parameters p_2, v_2 at the point of tangency between the Rayleigh line and the detonation adiabate curve are corresponding to the steady-state detonation. For this point the detonation velocity D reaches a minimum. This condition and the principle of minimum of the thermodynamic potential are used to determine the detonation pressure and the products composition. After determining p_2 and v_2, other parameters of the detonation wave are calculated on the basis of commonly known relations at the Chapman-Jouguet point.

The results of exemplary calculations for RDX (density 1.63 g/cm^3) are presented in Tables 5-7.The enthalpy, energy and entropy are found as absolute values.

Table 5. Comparison of the RDX detonation parameters obtained from the ZMWNI and CHEETAH codes

Detonation velocity [m/s]	Mass velocity [m/s]	Isentrope exponent	Code
8267	2004	3.125	ZMWNI
8266	2005	3.123	CHEETAH

Table 6. Comparison of the thermodynamic detonation parameters obtained from the ZMWNI and CHEETAH codes for RDX

Pressure [atm]	Specific volume [cm^3/g]	Temperature [K]	Enthalpy [cal/g]	Energy [cal/g]	Entropy [cal/K/g]	Volume of gaseos products [cm^3/g]	Code
266513.7	0.465	4259.9	3546.33	546.65	1.73	0.465	ZMWNI
266578.7	0.465	4259.2	3546.64	546.52	1.73	0.465	CHEETAH

Table 7. Comparison of the products compositions obtained from ZMWNI and CHEETAH codes for RDX

Product	Contents [mole/$mole_{Exp}$]		Product	Contents [mole/$mole_{Exp}$]	
	ZMWNI	CHEETAH		ZMWNI	CHEETAH
N_2	2.84E+00	2.84E+00	CNN	6.15E-11	6.12E-11
CO_2	1.98E+00	1.98E+00	N_2O_3	1.68E-11	1.68E-11
H_2O	1.09E+00	1.09E+00	C_3O_2	7.21E-12	7.16E-12
CH_2O_2	4.22E-01	4.22E-01	C_3	1.07E-12	1.06E-12
NH_3	2.97E-01	2.97E-01	N_2O_5	7.49E-15	7.50E-15
CH_4	1.97E-01	1.97E-01	C_4	6.87E-21	6.78E-21
C_2H_6	1.45E-01	1.45E-01	C_4N_2	1.98E-27	1.95E-27
H_2	8.95E-02	8.93E-02	C_5	4.84E-30	4.75E-30
CO	4.48E-02	4.47E-02	*C solid	4.89E-03	4.86E-03

Differences between values of product contents calculated by the both programs remain small (below 1.5%).

If the detonation parameters of an explosive are determined then calculation of the isentrope of expanding products is possible. Every point on the isentrope must fulfill a condition of constant entropy, i.e., $S = const$.

The expansion isentrope for the detonation products of RDX from the pressure at the CJ point to the atmospheric one was calculated. It was assumed that the composition of products is frozen when their temperature lowers to 1800 K. This value of the "frozen" temperature results from the theoretical and experimental data presented in work [16]. The results of calculation of the isentrope are presented in Table 8. Differences between the values calculated by the ZMWNI and CHEETAH codes are below 0.1%.

Table 8. Comparison of the pressure values calculated in chosen points of the isentrope of RDX detonation products by the use of the ZMWNI and CHEETAH codes

v/v_0	p [atm]	
	ZMWNI	CHEETAH
0.76	266513.70	266578.70
1.00	115775.30	115748.20
2.20	13642.10	13637.60
2.41	10943.00	10951.60
4.10	3380.70	3379.60
6.50	1408.80	1408.30
10.00	675.70	675.50
20.00	231.10	231.10
40.00	85.30	85.30
80.00	32.60	32.60
160.00	12.60	12.60

To solve a problem connected with the interaction of the explosion on the surroundings (expansion of the explosion products into air, the explosion in water or ground, reflection of a detonation waves at a boundary with solids, throwing fragments, forming a cumulative jet) a knowledge of the equation of state for the detonation products is necessary. Universally used equation of this type was suggested by Jones, Wilkins and Lee (JWL) [12].

The JWL equation is obtained from the expansion of internal energy in the neighbourhood of an isentrope of the detonation products. This isentrope has the following form on the plain (v, p)

$$p_s = Ae^{-R_1 V} + Be^{-R_2 V} + CV^{(-1-\omega)}, \tag{1}$$

where $V = v/v_0$.

Constants A, B, C, R_1, R_2 and ω are most often determined empirically. A cylindrical test, described in detail in Ref. [18], is one of essential methods of appointing them. These constants can also be determined on the basis of thermochemically calculated expansion isentrope. The second option was applied in the CHEETAH code [5] and in the ZMWNI code as well.

In the calculation algorithm of the JWL isentrope constants in the ZMWNI code, an assumption has been made that the JWL curve and the curve of the constant entropy obtained from thermochemical calculations have the same values at the CJ point and their derivates are equal also at this point. This condition

means, that isentrope exponent defined in the following way

$$\gamma \equiv -\left(\frac{\partial \ln p}{\partial \ln v}\right)_S = -\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_S, \tag{2}$$

takes the same values at the CJ point for both curves. The way of calculation of the JWL constants in the ZMWNI program was described precisely in work [11].

The coefficients of the JWL isentrope for RDX were determined on the basis of the values of pressure and the specific volume along the isentrope obtained from thermochemical calculations. The values of the constants determined by the ZMWNI program and by the CHEETAH code are given in Table 9. The expansion isentropes calculated by the use the thermochemical codes are compared in Figures 2 and 3 with the JWL curves.

Table 9. Sets of the JWL coefficients calculated by the ZMWNI and CHEETAH codes for RDX detonation products

A [GPa]	B [GPa]	C [GPa]	R_1	R_2	ω	Code
989.0848	11.11902	1.514244	5.166874	1.045774	0.396143	ZMWNI
828.1	10.527	1.499	4.844	1.066	0.395	CHEETAH

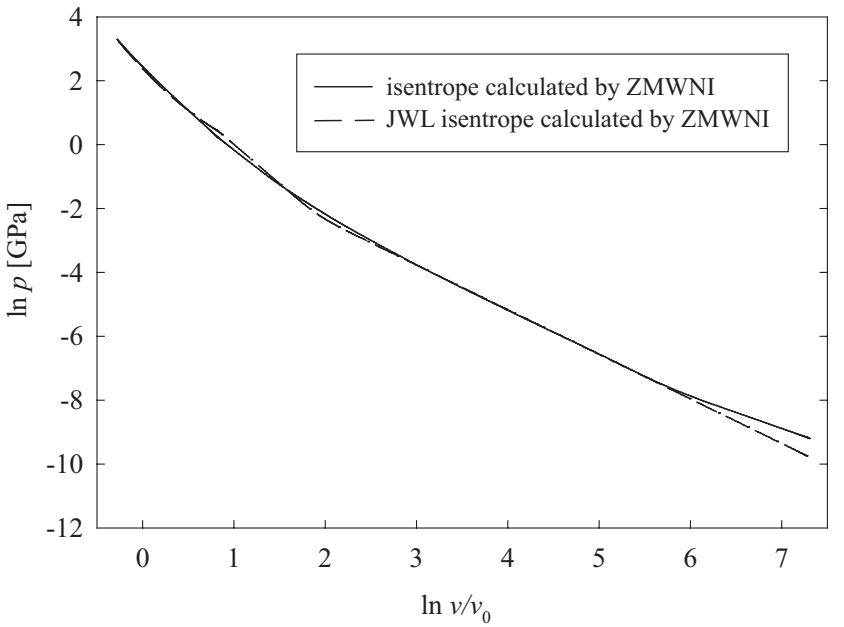

Figure 2. Comparison of the isentrope calculated by the use of the ZMWNI code with the JWL isentrope obtained from this code.

The methods of the JWL coefficients determination applied in the both codes are different. The conditions of the equality of the functions $p = p(v)$ and their derivates at the CJ point are not be presumed in the CHEETAH code. However, relatively large differences are observed along the calculated isentrope and its JWL approximation for the both codes. It concerns especially pressures of about 1000 atm, where the differences are up to 15% and small pressures of about few atmospheres, for which the differences in the pressures achieve even 45%. It may indicate inapplicability of the JWL isentrope equation to the curve of the constant entropy obtained from thermochemical calculations.

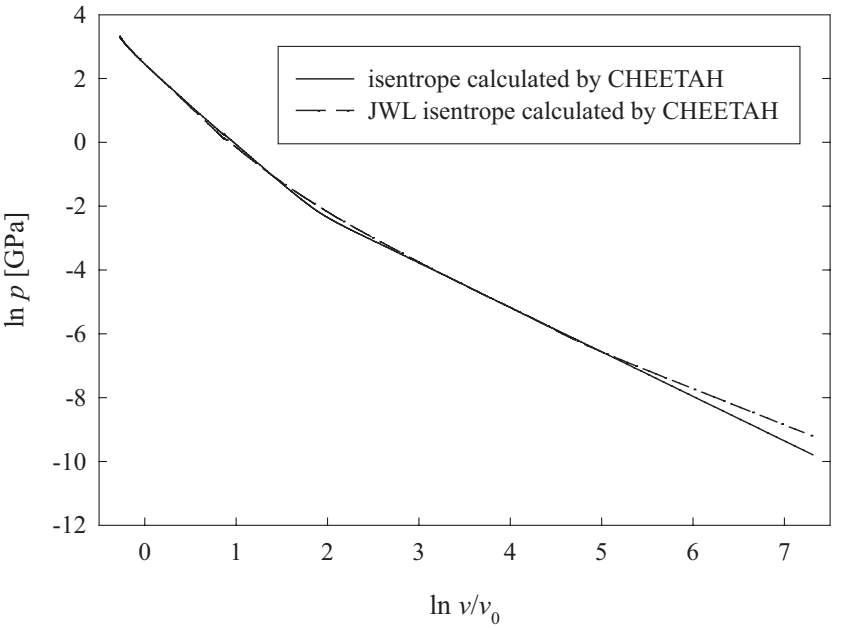

Figure 3. Comparison of the isentrope calculated by the use of the CHEETAH code with the JWL isentrope obtained from this code.

As it has been noticed, the JWL equation is often used in the computer simulations of explosion phenomena. The equation has rather a simple form and it can be easily applied in numerical algorithms. However, the differences between the curves obtained from thermochemical calculations and the JWL approximations noticed above ordered us to examine the JWL isentropes more precisely. To this purpose the isentrope exponent (2) was determined as a function of volume of the RDX detonation products. In the case of JWL isentrope its values were calculated from the relation (2) by differentiation of the

function (1). The isentrope obtained from the ZMWNI code were interpolated with the spline functions (the third step polynomials) and the exponent was calculated. The results of calculations are presented in Figure 4. The expansion isentrope estimated from the CHEETAH code is omitted, because it agrees with the ZMWNI curve in the scale of the picture.

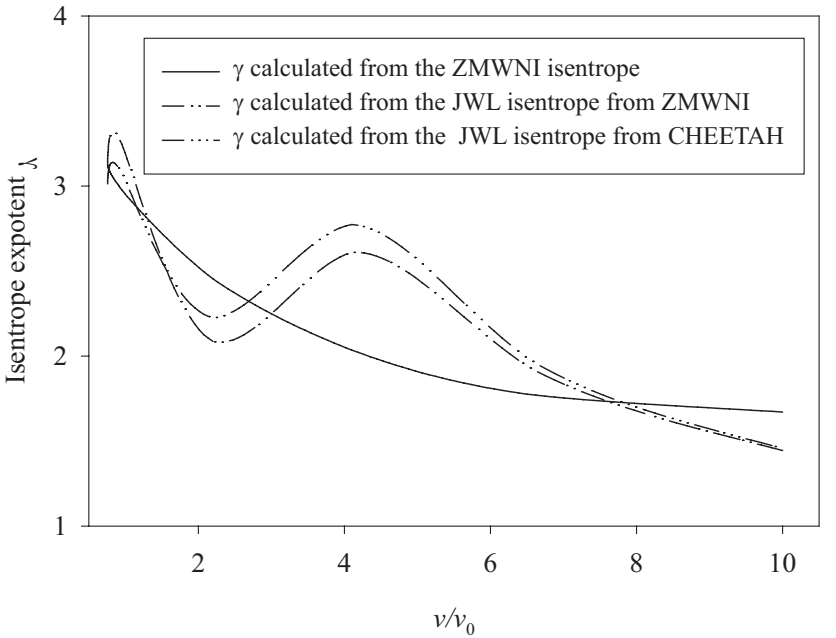

Figure 4. Dependence of the isentrope exponent on the relative volume of the RDX detonation products obtained by different methods.

The course of the curves obtained from the JWL equation is different from that calculated directly from the thermochemical code ZMWNI. In our opinion, this difference results from the fact, that the JWL isentrope is described by a three term function. The observed great changeability of the isentrope exponent may influence essentially the results of modeling of gasdynamical processes, because a speed of sound in the detonation products is connected with the value of the exponent.

Knowledge of the expansion isentrope enables us to calculate the so-called detonation energy. The detonation energy is defined as the maximum expansion work done by the detonation products during their expansion from the CJ point to infinitive volume minus the compression energy of an explosive [16]. According to the Jacobs concept, the detonation energy can be divided into two parts. The

mechanical part, $W(v_x)$, is the expansion work done by the detonation products from the CJ pressure to the initial pressure p_0 and the corresponding volume v_x of the products. The thermal one, Q_h, is defined as the heat extracted by cooling the detonation products at constant pressure to the initial temperature. After calculation of the JWL coefficients it is relatively easy to estimate the mechanical and thermal parts of the detonation energy. The way of appointing the detonation energy by the use of the ZMWNI code is described in Ref. [11].

Comparison of calculated results for TNT of a density 1.63 g/cm^3 and RDX of a density 1.59 g/cm^3 is presented in Table 10. Differences between the values obtained from the ZMWNI and CHEETAH codes result from the adopted method of calculation of the JWL coefficients. The differences are less than 4%.

Table 10. Detonation energy and its components, thermal ($Q_h \cdot \rho_0$) and mechanical ($W(v_x)$), calculated by the ZMWNI and CHEETAH codes

Explosive	$Q_h \cdot \rho_0$ [kJ/cm^3]	$W(v_x)$ [kJ/cm^3]	E_0 [kJ/cm^3]	Code
RDX	0.0	9.4170	9.4170	ZMWNI
	0.0	9.3570	9.3570	CHEETAH
TNT	0.0945	6.8173	6.9118	ZMWNI
	0.0950	7.0740	7.1690	CHEETAH

Non-equilibrium calculations

The ZMWNI program can carry out two variants of non-equilibrium calculations. In the first option, the chemical inertness of particles of a chosen solid component and thermal equilibrium between the particles and the reaction products are assumed. Different temperatures for the solid particles and the products are estimated in the second variant of calculations. Only the first option is available in the CHEETAH code.

As an example, the detonation parameters were calculated for the composition containing NM (nitromethan), PMMA (polymethylmethacrylate), magnesium and aluminium powders (81.6/3.6/7.5/7.5 %wt.). It was assumed that particles of aluminium and magnesium were chemically inert. However, they were in the thermal equilibrium. The results were compared with that obtained in the CHEETAH program (Tables 11-12). They are in a good agreement.

Table 11. Detonation parameters of the NM-based composition obtained from the ZMWNI and CHEETAH codes

Detonation velocity [m/s]	Mass velocity [m/s]	Isentrope exponent	Code
6109	1489	3.102	ZMWNI
6108	1489	3.101	CHEETAH

Table 12. Thermodynamic detonation parameters of the NM-based composition obtained from the ZMWNI and CHEETAH codes

Pressure [atm]	Specific volume [cm^3/g]	Temperature [K]	Enthalpy [cal/g]	Energy [cal/g]	Entropy [cal/K/g]	Volume of gas products [cm^3/g]	Code
104160.2	0.6519	3089.8	1513.41	-130.98	1.792	0.5676	ZMWNI
104147.3	0.6519	3089.3	1512.96	-131.21	1.792	0.5676	CHEETAH

In the ZMWNI code, the shock adiabate of the particle material and the relation between a specific heat capacity and temperature are used in a method of temperature estimation of solid particles highly compressed at the detonation wave front. Details of the method are described in Ref. [11]. The results of calculations with assumption of the thermal non-equilibrium at the CJ point are presented in Tables 13 and 14 for the NM-based mixture. The hypothesis of the lack of heat exchange between the detonation products and metal particles causes an increase in temperature and pressure of the gaseous products.

Table 13. Detonation parameters of the NM-based composition obtained from ZMWNI code with assumption of the thermal non-equilibrium between solid and gaseous components

Detonation velocity [m/s]	Mass velocity [m/s]	Isentrope exponent
6204	1593	2.9

Table 14. Detonation thermodynamic parameters of the NM-based composition obtained from ZMWNI code with assumption of the thermal non-equilibrium between solid and gaseous components

Pressure [atm]	Specific volume [cm^3/g]	Gas products temperature [K]	Addition temperature [K]	Enthalpy [cal/g]	Energy [cal/g]	Entropy [cal/K/g]	Volume of gas products [cm^3/g]
113125	0.6407	3464.8	369.04	1662.5	-92.85	1.73	0.5785

In the real detonation process the outside layer of metal particles is heated by the hot gaseous products in the chemical reaction zone to a some level. Calculations carried out with assumption of thermal equilibrium or its lack enable us to estimate the "upper" and "lower" values of detonation parameters. Finally, experiment verifies results of calculations.

Comparison with experimental data

New options of the program are demonstrated by comparing results of calculations with experimental data. The detonation parameters and characteristics of blast waves were measured in work [19] for heterogeneous thermobaric mixtures. Their main components were NM and an alloy of magnesium with aluminium PAM (Mg/Al ~50/50). On the basis of the measured detonation parameters and the results of a cylindrical test authors tried to determine the model of detonation for tested mixtures. In theoretical analysis the following assumptions were assumed:

- reactivity of the solid element (PAM) in the chemical reaction zone of detonation wave (thermal equilibrium of the detonation products);
- chemical inertness of the solid addition in the reaction zone and thermal equilibrium of this component and the products;
- chemical inertness of the solid addition and lacking of the thermal equilibrium between the addition particles and detonation products.

In the last case a theoretical model was used in which the JWL equation of state for gaseous products was obtained from the CHEETAH code. The analysis of experimental data and results of calculations leads to the conclusion that the solid addition is chemically inert and the heat flow from the detonation products to particles of the addition in the reaction zone of detonation wave is small [19].

In this work, thermochemical calculations were performed for three options listed above by the use of the ZMWNI program. Detonation velocities were calculated and compared with the measured values presented in Ref. [19]. The comparison is presented in Figure 5.

Interpretation of curves on Figure 5 is very difficult since the measured detonation velocity of pure NM (without PAM addition) is about 150 m/s lower than the calculated one. However, taking into consideration a rate of reduction in the detonation velocity with the increase of PAM contents, we can find that the experimental curve is most similar to that obtained from calculations performed with assumption of the chemical inertness of the solid PAM and no heat exchange between particles of PAM and the detonation products of NM. This observation

confirms the conclusion taken out in work [19].

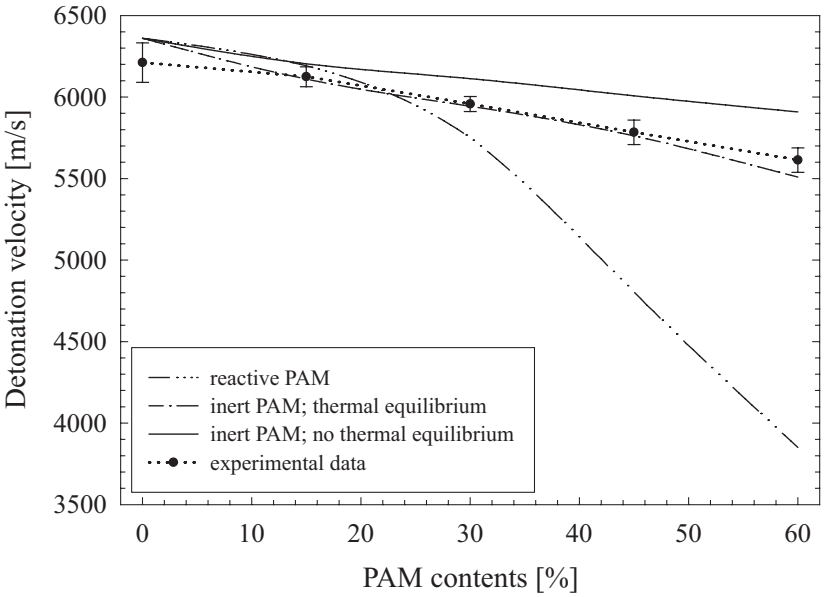

Figure 5. Detonation velocity of mixtures of NM with PAM versus PAM contents (results of calculations from the ZMWNI code).

Summary

In the work the thermochemical program ZMWNI is presented. The code can calculate the parameters of combustion, explosion and detonation of condensed energetic materials as well as the determination of the curve of expansion of detonation products in the form of JWL isentrope and the energy of detonation is possible in the program. Moreover, the ZMWNI code is able to determine the non-equilibrium states for frozen composition or for different temperatures of components.

The results of exemplary calculations are presented to verify the ZMWNI program. The results are compared with that obtained from the CHEETAH code. In particular, the calculated adiabatic combustion temperature, JWL isentrope and detonation energy are shown. Moreover, new possibilities of the program, i.e., the non-equilibrium calculations, are demonstrated. Finally, some experimental data are confronted with the results obtained from the ZMWNI calculations.

In the last years some European standards have been implemented in Poland

and they are recommended for determination of explosion and combustion parameters. However, their usage needs an application of computational procedures in thermodynamic modeling. The standards propose to develop these procedures in existing or own numerical codes. Presented program enable us to calculate combustion, explosion and detonation characteristics and it can be modified according to the procedures described in the standards.

Acknowledgements

This work was supported by the Polish Ministry of Science and Higher Education through Military University of Technology in 2009-2010 years, Project No. O N204 011036.

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