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Determination of Detonation Parameters by coupled with considering shock compression character of aluminum in detonation reaction zone and second-order reaction theory of aluminized explosives

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Abstract

The theoretical and accurate determination of the detonation parameters of explosives is a key issue in the design of a reasonable composition of explosives.In this paper, theoretical computing method for determination of detonation parameters was established by coupled with considering shock compression character of aluminium in detonation reaction zone and second-order reaction theory of aluminized explosives.The BKW equation of state was chosen as the state equation of the detonation product, and the state equation of Cowan was applied as the state equation of condensed carbon in the detonation product. The thermodynamic state quantities of the gaseous product were determined by applying the BKW equation of state to the relational expression between the thermodynamic state quantities. In addition, the condensed phase carbon (graphite) as a solid product was considered and the Cowan equation of state was used to determine the thermodynamic state quantities of the solid product. A algorithm of the detonation parameters calculation of aluminized explosives by Gibbs free energy minimization principle was constructed, the detonation parameters were calculated and compared with the experimental values. The calculated values of detonation velocity are below 4.0% and the calculated values of detonation pressure have relative errors below 6.8% and the experimental values.

Keywords: *Aluminized explosive, Detonation parameter, Shock compression, BKW equation of state, Cowan equation of state.*

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Introduction

The detonation parameters of the explosive satisfy the fundamental equation of the detonation wave, which consist of the law of conservation of mass, momentum and energy at front of detonation wave, the CJ (Chapman-Jouget) condition and the equation of state.

$$\left.\begin{aligned} D &= v_0\sqrt{\frac{p_j - p_0}{v_0 - v_j}} \\ u_j &= (v_0 - v_j)\sqrt{\frac{p_j - p_0}{v_0 - v_j}} \\ E_j - E_0 &= \frac{1}{2}\left(p_j + p_0\right)\left(v_0 - v_j\right) + Q_v \\ -\left(\frac{\partial p}{\partial v}\right)_j &= \frac{p_j - p_0}{v_0 - v_j} \\ p_j &= f\left(v_j, T_j\right) \end{aligned}\right\}$$

Here D, u_j-Detonation velocity and velocity of product at the front of detonation wave, m/s

p_0, p_j-Initial pressure of unreacted explosive and pressure of product at the front of detonation wave, Pa

v_0, v_j - The initial specific volume of the unreacted explosive and the specific volume of the product at the front of detonation wave, m^3/kg

T_j-Temperature of the product at the front of detonation wave, K

E_0, E_j, Q_v - Internal energy of unreacted explosive and detonation product, and explosion heat, J/kg

The first and second equation of the above mentioned equation are equations of the conservation of mass and momentum respectively, and the third is the equation of the conservation of energy, called Hugoniot relational expression. The fourth is the equation for the CJ condition, and the fifth is the equation of state of the detonation product.

From the Hugoniot relational expression and the state equation of the detonation products, the possible states of the detonation products are a curve in the $p - v$ coordinate system, i.e. Hugoniot curve, and the possible states of the detonation products satisfying the conservation of mass and momentum are straight lines through $\left(p_0, v_0\right)$, i.e. Rayleigh lines.

The intersection of Rayleigh and Hugoniot curves reflects the possible detonation state, and considering the CJ condition, the point where Rayleigh and Hugoniot curves intersect is called CJ point, reflecting the steady detonation state, and determining the parameters at this point is the detonation parameter [1,2].

At present, aluminized explosive is widely used, but up to now its detonation reaction mechanism has not been perfectly explained.

Adding a certain amount of aluminum powder to high-explosives such as TNT, hexogen, octogen, etc, increases the heat of detonation and the work capacity of explosives, but decreases the detonation velocity and the detonation pressure.

Some researchers have suggested the second-order reaction theory, the inert thermal dilution theory, and the chemical thermal dilution theory of detonation reaction mechanism of aluminized explosives, have been proposed, but no theory has comprehensively analyzed the detonation reaction mechanism of aluminum-containing explosives.

Others have suggested to consider the reactivity of aluminum in the detonation reaction zone. But they haven't got enough results because influence relationship of factors on the reactivity of aluminum is very complicated. It included many factors like the characteristics of the main explosive, the particle shape and the size distribution of aluminum particle.

In addition, quantitative considerations of the acceleration and heating of aluminum particles in the detonation reaction zone have been attempted to calculate the detonation parameters, but not satisfactory results [3-7].

It is very difficult to consider quantitatively the factors such as the aluminium particle shape and particle size distribution characteristics, the reactivity, acceleration and heating of aluminium at the detonation reaction zone. So they didn’t calculate the detonation parameters of aluminized explosives.

Since it is very difficult to quantitatively consider the particle shape and size distribution characteristics of aluminum in aluminized explosive, the reactivity of aluminum in the detonation reaction zone, acceleration and heating, the detonation parameters of aluminized explosive are not theoretically calculated based on the basic relations of detonation waves, but by semi-empirical equations obtained based on experimental data.

The detonation reaction time for high explosive is very short. It is only 0.5 μs. In contrast, the reaction of aluminum occurs after 5-100 μs at the back of detonation wave.

This shows that the second-order reaction theory about detonation reaction mechanism of aluminized explosive, in which aluminum does not take part in the detonation reaction and acts as an inert additive in the detonation reaction zone, has some validity.

However, in the detonation reaction zone, no method has been proposed to calculate the detonation parameters by considering aluminum as an inert additive and taking into account its shock compression properties quantitatively.

2. Theoretical part

2.1 Calculation of the equilibrium composition of detonation products

The calculation of the detonation parameters entails the calculation of the composition of the detonation product.

The composition calculations of detonation products are generally processed by empirical method, equilibrium constant method, and free energy minimization principle [8-10].

The empirical and equilibrium constant methods have the disadvantage of being unable to calculate the product composition if the accuracy of the calculation is low and the equilibrium constants of the elementary reactions are not given.

Therefore, it is reasonable to proceed on the basis of Gibbs free energy minimization principle to calculate the composition of the detonation products.

As the detonation reaction proceeds, the temperature and pressure of the system are changed. The composition of the detonation product is also changed and the system reaches a chemical equilibrium state. The change process of coposition satisfies the law of conservation of mass and the free energy of the system at equilibrium state is minimized.

Assume that the detonation reaction is carried out in a l chemical explosive to produce NS gaseous and condensed phase products, gas products from 1 to 1~N_G and condensed phase products from N_G+1~N_S.

At this time, the total number of moles of the gaseous product is.

$$n = \sum_{j=1}^{N_G} n_j \qquad (1)$$

Here, n - Total number of moles of gaseous products, mol

n_j -Number of moles of jth product component

N_G –Number of gaseous product components

N_S –Number of product components

The Gibbs free energy in a system consisting of N_S product is,

$$g = \sum_{j=1}^{N_S} \mu_j n_j \qquad (2)$$

Here, μ_j - chemical potential per mole of the jth product, J/mol

The chemical equilibrium condition is minimizaion of the Gibbs free energy at equilibrium state.

On the other hand, the detonation reaction of the explosive satisfies the law of conservation of mass.

$$\sum_{j=1}^{N_S} a_{ij} n_j - b_i^0 = 0 \quad (i = 1, \cdots l) \qquad (3)$$

Here, a_{ij} -Number of atoms of i[th] element in 1mol of j[th] product

l -Total number of elements

b_i^0 -Number of atoms of i[th] element in explosive

The problem of calculation of equilibrium composition is changed to find the conditional extremum of a function. So from the indeterminate multipliers method of Lagrange, the system of equations for calculating equilibrium composition is

$$\begin{cases} \mu_j + \sum_{i=1}^{l} \lambda_i a_{ij} = 0 \quad (j = 1, \cdots, N_S) \\ \sum_{j=1}^{N_S} a_{ij} n_j - b_i^0 = 0 \quad (i = 1, \cdots l) \end{cases}$$

(4)

The thermodynamic state of the system is uniquely determined by two thermodynamic quantities of state such as temperature and pressure, enthalpy and pressure, entropy and pressure etc.

Since the equation of state of an ideal gas is generally not applicable in the detonation state, a reasonable equation of state corresponding to the detonation state must be chosen. The chemical potential and entropy of the product are then varied.

The equilibrium composition of the detonation products is calculated by Newton - Raphson method.

2.2. Equation of state and thermodynamic quantities of state of detonation products

2.2.1. Equation of state of detonation products

To calculate the detonation parameters of the explosive and to solve accurately numerically the expansion of the detonation products, the equation of state of the detonation products must be considered.

An important problem in using the equation of state of a detonation product is to use it to determine the thermodynamic parameters accurately.

In the previous calculations, we used only the relationship between pressure, volume and temperature, although we considered the equation of state, and used simple thermodynamic parameters obtained by the ideal gas equation of state, without considering the thermodynamic parameters such as energy, entropy, and free energy by the equation of state.

In this paper, we have chosen the BKW equation of state as the state equation of the detonation product, based on which the thermodynamic parameters are determined and

used for the calculation of the detonation parameters.

2.2.1.1. BKW equation of state

BKW equation of state is [11, 12].

$$\frac{PV_g}{RT} = 1 + xe^{\beta x} = F(x) \qquad (5)$$

$$x = \frac{\kappa k}{V_g (T + \Theta)^{\alpha}}$$

$$k = \sum_g x_i k_i$$

$$x_i = n_i / n_g$$

Here, P –Pressure, MPa

V_g -Molar volume of gaseous product, cm^3/mol

T –Temperature, K

R –Gas constant, J/(mol·K)

x_i is the mole fraction of ith gas component and k_i is the value characterizing the covolume of ith component. The subscript g indicates the gaseous product.

α, β, κ, Θ are regulation parameters. The quantity Θ is the value received to prevent the pressure divergence when the temperature approaches to zero.

Regulation parameters of BKW equation of state are.

Group of Hexogen: $\alpha = 0.54$, $\beta = 0.181$, $\kappa = 14.15$, $\Theta = 400$

Group of Trotyl: $\alpha = 0.5$, $\beta = 0.09585$, $\kappa = 12.685$, $\Theta = 400$

Group of hexogens is selected for explosives that form a small amount of condensed carbon during detonation. In contrast, group of trotyl is selected for the explosives that form a large amount of condensed-phase carbon. The quantitative selection criteria of these groups are as follow.

$$G = NM \qquad (6)$$

Here, N – The number of moles of gaseous products formed when explosive of 1g is explosived, mol/g

M – Average molar mass of gaseous product, g/mol

Select the hexogen group in the case of $G \geq 0.82$. In the opposite case, the trotyl group is selected.

2.2.1.2. Equation of state of condensed-phase carbon

The detonation products include condensed-phase carbon such as graphite and diamond.

Several equations of state have been suggested to describe the state of condensed-phase carbon in detonation products. Among them the equation of state of Cowan is widely used [13].

The equation of state proposed by Cowan which condensed-phase carbon in the detonation product consider graphite, is as follows..

$$p = p_1(\eta) + a(\eta)T_s + b(\eta)T_s^2 \quad (7)$$

$$p_1(\eta) = -2.4673 + 6.7692\eta - 6.9555\eta^2 + 3.0405\eta^3 - 0.3869\eta^4$$

$$a(\eta) = -0.2267 + 0.2712\eta$$

$$b(\eta) = 0.08316 - 0.07804\eta^{-1} + 0.03068\eta^{-2}$$

$$T_s = \frac{T}{11605.6}$$

$$\eta = \frac{\rho}{\rho_0}$$

Here, p –Pressure, 10^5 MPa

T -Temperature, K

ρ_0 -Crystal density of condensed-phase carbon (graphite 2.25g/cm^3), g/cm^3

ρ -Density of condensed-phase carbon of each temperature and pressure

The coverage of this equation of state is $0 < T_s < 2$, $0.95 < \eta < 2.5$.

2.2.2. Thermodynamic quantity of state of the detonation products

Generally, the detonation product is mixture of gaseous and solid products. The thermodynamic quantity of state of the mixture is

$$G = n_g G_g + n_s G_s \quad (8)$$

Here, G -Thermodynamic quantity of state per unit mass of mixture

G_g, G_s - Thermodynamic quantity of state per mole of gas and solid

n_g, n_s - Molar mass of gases and solids per unit mass of mixture, mol

The relationship between thermodynamic quantities of state is

$$\left(\frac{\partial E}{\partial V}\right)_T = T\left(\frac{\partial P}{\partial T}\right)_V - P \quad (9)$$

$$\left(\frac{\partial S}{\partial P}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_P \quad (10)$$

$$\frac{E}{RT} - \frac{S}{R} = \frac{F}{RT} - 1 \quad (11)$$

T, P, V, E, S, F are the temperature, pressure, volume, internal energy, entropy, and Gibbs free energy.

2.2.2.1. Thermodynamic quantity of state of the gaseous product

The BKW equation of state was applied to the relationship between thermodynamic parameters to determine the thermodynamic parameters of the gaseous products.

The internal energy of the gaseous product is

$$\frac{E_g}{RT}=\sum_i x_i\frac{\left(E_T{}^0-H_0^0\right)_i}{RT}+\sum_i x_i\frac{\left(H_0^0\right)_i}{RT}+\frac{\alpha T}{T+\Theta}\left(F(x)-1\right) \quad (12)$$

Here, E_g -Internal energy of gaseous product, J/mol

E_T^0 -Standard internal energy of the product at temperature T, J/mol

H_0^0 -Standard enthalpy of formation of products, J/mol

Entropy of the gaseous product is

$$\frac{S_g}{R}=\sum_i x_i\frac{\left(S_T{}^0\right)_i}{R}-\sum_i x_i\ln x_i-\ln\frac{P}{P^0}+\ln F(x)-\frac{e^{\beta x}-1}{\beta}+\frac{\alpha T}{T+\Theta}\left(F(x)-1\right) \quad (13)$$

Here, S_g -Internal energy of gaseous product, J/mol

S_T^0 -Standard Entropy of the gas component at temperature T and atmospheric pressure P^0, J/(mol·K)

P^0 - Atmospheric pressure, MPa

The chemical potential μ_i of the ith gaseous product is

$$\mu_i=\left(\frac{\partial(nF)}{\partial n_i}\right)_{T,P,n_j} \quad (14)$$

Here, F – Gibbs molar free energy, J/mol

n_j - All other components except n_i

From above, the chemical potential of the ith gaseous product is

$$\frac{\mu_i}{RT}=\frac{\left(F^0-H_0^0\right)_i}{RT}+\frac{\left(H_0^0\right)_i}{RT}+\ln\frac{x_iP}{P^0}+\frac{e^{\beta x}-1}{\beta}-\ln F(x)+\frac{k}{l} \quad (15)$$

2.2.2.2. Thermodynamic quantity of state of the solid product

The condensed-phase carbon (graphite) is considered to the solid product and the thermodynamic quantity of state was determined using its equation of state.

The internal energy of the condensed-phase carbon is

$$E_s=\left(H_T^0-H_0^0\right)_s+\left(H_0^0\right)_s-P^0V_s^0+\int_{V_s^0}^{V_s}\left[b(V)T^2-p_1(V)\right]dV \quad (16)$$

Here, E_s -Internal energy of the solid product, J/mol

V_s -Molar volume of the solid product, cm^3/mol

V_s^0 - Molar volume of the solid component at temperature T and atmospheric pressure P^0

H_T^0 -Standard enthalpy of the solid component at temperature T, J/mol

The entropy of the condensed-phase carbon is

$$\frac{S_s}{R}=\frac{\left(S_T{}^0\right)_s}{R}+\frac{1}{R}\int_{V_s^0}^{V_s}\left[a(V)+2b(V)T\right]dV$$

(17)

The chemical potential of the condensed-phase carbon is

$$\frac{\mu_s}{RT}=\frac{\left(F^0-H_0^0\right)_s}{RT}+\frac{\left(H_0^0\right)_s}{RT}+\frac{F_s'}{RT}$$

(18)

$$\frac{F_s'}{RT}=\frac{PV_s-P^0V_0^0}{RT}-\frac{1}{RT}\int_{V_s^0}^{V_s}\left[p_1(V)+a(V)T+b(V)T^2\right]dV$$

(19)

2.2.3. Thermodynamic data

To determine the thermodynamic state of a detonation product, its thermodynamic data must be given.

The standard enthalpy of formation $H^0(298.15)$ for different products and $\left[H^0(T)-H^0(298.15)\right]$, $\left[G^0(T)-H^0(298.15)\right]$, $C_p{}^0(T)$, $S^0(T)$ at 100 K intervals in the temperature range of 0-6000 K are given in [14].

To use thermodynamic functions in the calculation program of composition, it is convenient to convert the data given with discrete type to temperature into the functional form.

Thermodynamic functions are determined with polynomial according for temperature.

$$\frac{C_p{}^0(T)}{R}=a_1+a_2T+a_3T^2+a_4T^3+a_5T^4$$

$$\frac{H^0(T)}{RT}=a_1+\frac{a_2}{2}T+\frac{a_3}{3}T^2+\frac{a_4}{4}T^3+\frac{a_5}{5}T^4+\frac{a_6}{T}$$

$$\frac{S^0(T)}{R}=a_1\ln T+a_2T+\frac{a_3}{2}T^2+\frac{a_4}{3}T^3+\frac{a_5}{4}T^4+a_7$$

$$\frac{G^0(T)}{RT}=a_1(1-\ln T)-\frac{a_2}{2}T-\frac{a_3}{6}T^2-\frac{a_4}{12}T^3-\frac{a_5}{20}T^4+$$

Coefficients $a_1 \sim a_7$ .are determined using the method of least squares.

2.3. Calculation method of detonation parameters of aluminized explosives

To calculate the detonation parameters of aluminized explosives, assume the following assumptions.

First, aluminum particles are equally distributed in the main explosive.

Second, the aluminum particles do not participate in the detonation reaction and are subjected to a sudden shock compression in the detonation reaction zone, resulting in a pressure balance between the detonation product and the aluminum particles.

Third, there is no heat exchange between detonation products and aluminum particles.

From this assumption, the detonation parameters can be calculated by considering the inert additive uniformly dispersed in the main explosive phase and its shock compression properties in the detonation reaction zone

When an aluminum-containing explosive is detonationd, the detonation reaction zone becomes a mixed state of aluminum particles with the detonation products of the main explosive, with specific volume and internal energy as follows:

$$v_j = \alpha_1 v_1 + \alpha_2 v_2 \qquad (20)$$

$$E_j = \alpha_1 E_1 + \alpha_2 E_2 \qquad (21)$$

Here, α_1, α_2 - Mass fraction of main explosive and aluminum

v_1 , v_2 - Specific volume of detonation products and aluminum, m^3/kg

E_1, E_2 - Internal energy of detonation products and aluminum, J/kg

From the law of conservation of mass, the following relation is given:

$$\alpha_1 + \alpha_2 = 1 \qquad (22)$$

In the initial state of the composite explosive, the specific volume of composite explosive is calculated as follows:

$$v_0 = \alpha_1 v_{01} + \alpha_2 v_{02} \qquad (23)$$

$$v_0 = \frac{1}{\rho_0}, \quad v_{01} = \frac{1}{\rho_{01}}, \quad v_{02} = \frac{1}{\rho_{02}}$$

Here, v_{01}, v_{02} - Initial specific volume of main explosive and aluminum, m^3/kg

ρ_0, ρ_{01}, ρ_{02} - Initial density of the composite explosive, the main explosives and aluminum kg/m^3

From Eqs. 22 and 23, initial specific volume of main explosive is determined as follows:

$$v_{01} = \frac{1}{\rho_{01}} = \frac{v_0 - \alpha_2 v_{02}}{\alpha_1} = \frac{1}{1-\alpha_2}\left(\frac{1}{\rho_0} - \frac{\alpha_2}{\rho_{02}}\right) \qquad (24)$$

From Eq. 24, the initial specific volume of the main explosive can be calculated when the mass fraction of aluminum and the initial density of the composite explosive are given.

The equation of conservation of energy for the composite explosive is as follows:

$$E_j - E_0 = 0.5(p_j + p_0)(v_0 - v_j) + \alpha_1 Q_1 \qquad (25)$$

Here, Q_1 - Explosion heat of main explosive, J/kg

When aluminum is shock-compressed to pressure p_j, the equation of conservation of energy is as follows:

$$E_2 - E_{02} = 0.5(p_j + p_0)(v_{02} - v_2)$$

(26)

Here, E_{02} -Initial internal energy of aluminum, J/kg

On the other hand, when the shock adiabatic equation of aluminum is considered to $D_2 = a + \lambda u$, and using the fundamental equation of shock wave ($p_j = \rho_{02} D_2 u$, $D_2 = v_{02}\sqrt{\frac{p_j}{v_{02} - v_2}}$), specific volume of aluminum can be determined as follows:

$$v_2 = v_{02}\left(1 - \frac{1}{\lambda}\frac{\sqrt{1 + 4\lambda p_j v_{02}/a^2} - 1}{\sqrt{1 + 4\lambda p_j v_{02}/a^2} + 1}\right)$$

(27)

Here, D_2, u -Shock velocity and the velocity of the medium in aluminum, m/s

a -Constant, m/s

λ - Reactivity coefficient

Substitution of eqs. 20, 21, and 23 into eq. 25 derived eq. 28 as follows:

$$\alpha_1(E_1 - E_{01} - Q_1) + \alpha_2(E_2 - E_{02}) = 0.5(p_j + p_0)[\alpha_1(v_{01} - v_1) + \alpha_2(v_{02} - v_2)]$$

(28)

And then, the following relation is satisfied:

$$E_1 - E_{01} - Q_1 = (H_1 - p_j v_1) - (H_0 - p_0 v_{01}) - (H_f - H_0)$$
$$= H_1 - H_f - p_j v_1 + p_0 v_{01}$$

(29)

Here, H_0, H_1 - Enthalpy of detonation product of the main explosive at initial temperature and detonation temperature, J/kg

H_f -Enthalpy of formation of the main explosive, J/kg

Substitution of eqs. 26 and 29 into eq. 28 derived eq. 30 as follows:

$$H_1 - H_f = 0.5(p_j - p_0)(v_{01} + v_1)$$

(30)

Equation 30 is equivalent to the equation of energy conservation in the primary explosive as a result of the equation of energy conservation in the mixed explosive.

It can be concluded that the equations of energy conservation in the detonation products and aluminum of the main explosive can be considered independently of each other and that the specific volume of the main explosive detonation products and the specific volume of aluminum can be added to determine the specific volume in the detonation reaction zone.

The detonation wave parameters satisfy the fundamental equations of the detonation wave, which consist of the equations of the conservation of mass, momentum and energy in the detonation reaction zone, the equation of state, and the CJ condition.

The system reaches chemical equilibrium immediately under the condition that

temperature and pressure of the system are given, and the state of the system is determined from Gibbs free energy minimization principle. When the temperature and the pressure of the system are given and from them the composition of the product, which satisfies the equation of the conservation of mass, is calculated, the state of the system is determined uniquely and also thermodynamic quantities of state of the system are determined.

When the pressure of the system is set, it is determined temperature of the system that the free energy of the system is minimized, satisfies the equations of the conservation of mass, momentum and energy. The specific volume of the product is determined from the equation of state when the temperature and the pressure of the system are given, and determining the specific volume according to various pressure changes results in a one set of Hugoniot curves.

From the obtained Hugoniot curve, it is found that the point that satisfies the CJ condition, i.e., the point that gives the minimum detonation velocity, is the CJ point, and the detonation parameters are determined at this point.

The algorithm for calculating detonation parameters of aluminized explosives from Gibbs free energy minimization principle is as follows.

Enter the composition of explosive, the density of charge, the density of aluminum and the shock adiabatic equation.

Calculate the mass fraction α_1, α_2 of the main explosive and aluminum.

Read the thermodynamic data of the main explosive components from the database and calculate the conditional molecular formula and the enthalpy of formation of the main explosive.

Find the possible detonation products of the main explosive and read thermodynamic data from the database.

Set the pressure of the detonation product.

Set the temperature of the detonation product.

Based on the equation of state of the detonation product and the Gibbs free energy minimization principle, calculate the equilibrium composition of the detonation product at a given pressure and temperature.

On the equilibrium composition at a given pressure and temperature, determine whether Eq. 12 is satisfied, if not, then go to ⑥ and repeat.

Calculate the specific volume v_1 of the detonation product using the equation of state of the detonation product.

Calculate the specific volume of aluminum using eq.9.

Calculate the specific volume using eq.2.

Decide whether the specific volume calculated according to different pressures (100 MPa to 60 GPa) is full (Hugoniot curve obtained) and if not satisfied, go to ⑤ and repeat the process.

From the Hugoniot curve, find the CJ point by considering the CJ condition. It is determined quantities of state such as p_j, v_j, T_j at CJ point.

Calculate remaining parameters D, u_j using the fundamental equation of the detonation wave. Record results and then finish.

The algorithm for calculating the detonation parameters of aluminized explosives from Gibbs free energy minimization principle is shown in Fig.1.

As it can be seen from Fig.1, the calculation of detonation parameters from Gibbs free energy minimization principle involves the calculation of the equilibrium composition of state which pressure and temperature are given.

The algorithm for calculation of the equilibrium composition of state which pressure and temperature of detonation products is as follows.

Input the data – pressure and temperature, the thermodynamic function data, composition of the detonation product, and conditional molecular formular of the explosive.

Set the initial composition of the detonation product.

Calculate the chemical potential of components of the detonation product under the given pressure and temperature.

Calculate the Gibbs free energy g_0 corresponding to the initial composition.

Obtain new composition using Newton-Raphson method.

Calculate the chemical potential of compositions of the detonation product under the given pressure and temperature.

Calculate the Gibbs free energy g_1 corresponding for new composition.

$|g_1 - g_0|$ satisfies the error limit, and then if does not satisfy, set $g_0 = g_1$ and go to ⑤, repeat the process.

Calculate the internal energy and entropy of the product.

Save the product composition, its internal energy, entropy and Gibbs free energy, and finish.

3. Results and discussion

Density of aluminium is 2.71g/cm^3, the shock adiabatic equation is $D_2 = 5330 + 1.35u$.

The detonation parameters of typical aluminum-containing explosives are calculated and the results of a comparison of the main parameters, detonation velocity and detonation pressure, with experimental values reported in the literature [15-18], are presented in Table 1.

As can be seen from Table 1, the calculated values of detonation velocity are below 4.0% and the calculated values of detonation pressure have relative errors below 6.8% and the experimental values.

Thus, calculation results have high accurate and the calculation method established for detonation parameters of aluminized explosive is valid.(Thus, the calculation results are found to be highly accurate and the established method of the detonation parameters calculation of aluminized explosive is valid.)

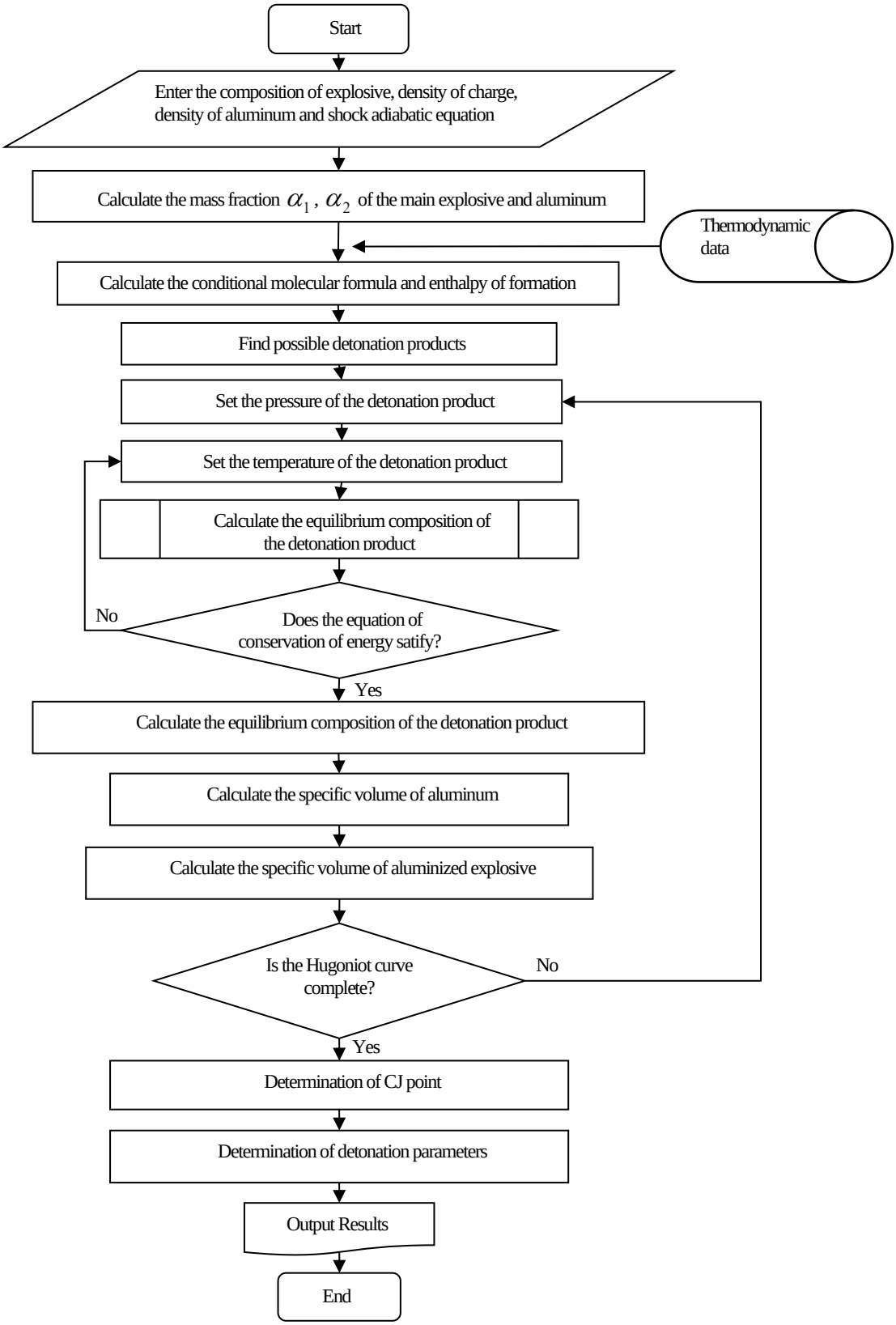

Fig.1. Calculation algorithm for detonation parameters of aluminized explosives by Gibbs free energy minimization principle

Table 1. Theoretical calculation results of detonation parameters of typical aluminized explosives

Composition	Density, g/cm³	Detonation velocity, m/s			Detonation pressure, GPa		
		Experimental results	Calculation value	Relative errors, %	Experimental results	Calculation value	Relative errors, %
80TNT/20Al	1.72	6475	6531	0.9	19.1	17.8	6.8
80TNT/20Al	1.41	5389	5566	3.3	-	11.3	-
90RDX/10Al	1.68	8030	7884	1.8	24.6	26.0	5.7
80RDX/20Al	1.73	7770	7633	1.8	-	24.6	-
70RDX/30Al	1.79	7580	7396	2.4	-	23.1	-
60RDX/40Al	1.84	7200	7088	1.6	21.1	20.9	0.9
50RDX/50Al	1.89	6810	6735	1.1	-	18.6	-
90HMX/10Al	1.76	8300	8196	1.3	-	28.8	-
70HMX/30Al	1.86	8000	7680	4.0	-	25.3	-
80RDX/5Al/15HTPB	1.594	7530	7311	2.9	22.9	21.9	4.4
42RDX/40TNT/18Al	1.81	7495	7641	1.9	23.8	24.7	3.8
41RDX/20Al/20AP/19HTPB	1.64	6724	6802	1.2	-	19.2	-
44RDX/32.2TNT/19.8Al/4WAX	1.8	7530	7268	3.5	23.0	23.2	0.9
37.4RDX/27.8TNT/30.8Al/WAX	1.88	7300	7109	2.6	21.5	22.2	3.3
40RDX/38TNT/17Al/5WAX	1.72	7220	7055	2.3	22	21.1	4.1
45RDX/30TNT/20Al/5WAX	1.71	7194	6965	3.2	-	20.6	-

4. CONCLUSIONS

Base on the second-order reaction theory about the detonation reaction mechanism of aluminized explosive, aluminum particles have been considered to the inert additive at the detonation reaction zone. And also its shock compression character has been considered.

Detonation parameters of different aluminized explosives were calculated by using Gibbs free energy minimization principle.

The equation of state of Cowan has been used to the equation of state of condensed-phase carbon in the detonation product, and the thermodynamic quantity of state of the solid product has been determined from the equation of state of Cowan.

The calculated detonation velocity for different kinds of aluminized explosives is less than 4.0% and the calculated detonation pressure is less than 6.8% relative error with the experimental value, so the calculation results are of high accuracy and the established calculation method is valid.

CRediT authorship contribution statement

***Ho Rim*:** Conceptualization, Investigation, Visualization, Writing-original draft, Writing - review & editing.

Jin Guk Pak: Conceptualization, Methodology, Investigation, Writing - original draft, Writing - review & editing, Visualization, Supervision, Project administration.

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***Jong Ju Kang*:** Conceptualization, Validation, Writing – review & editing.

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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