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Evaluation of detonation performance of explosives ICM-101, ONC, and TNAZ based on improved VHL equation of state

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ABSTRACT

Detonation performance is crucial for evaluating the power of high explosives (HEs), and the equation of state (EOS) that accurately describes the high-temperature, high-pressure, and high-temperature, medium-pressure states of detonation products is key to assessing the damage efficiency of these energetic materials. This article examines the limitations of the VLW EOS in representing the thermodynamic states of explosive detonation gas products under high-temperature and medium-to high-pressure conditions. A new gas EOS for detonation products, called VHL (Virial-Han-Long), is proposed. The accuracy of VHL in describing gas states under high-temperature and medium-to high-pressure conditions is verified, and its performance in evaluating explosive detonation and working capabilities is explored. The results demonstrate that VHL exhibits high precision in calculating detonation performance. Subsequently, the detonation performance of three new HEs (ICM-101, ONC, and TNAZ) was calculated and compared to traditional HEs (TATB, CL-20, and HMX). The results indicate that ONC has superior detonation performance compared to the other explosives, while ICM-101 shows a detonation velocity similar to CL-20 but with slightly lower detonation pressure. The detonation characteristics of TNAZ are comparable to those of the standard HE HMX. From the perspective of products, considering the comprehensive work performance (mechanical work and detonation heat), both ONC and ICM-101 demonstrate relatively superior performance.

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1. Introduction

As metastable substances, explosives react violently to external stimuli and possess unstable chemical properties. Their high energy and suddenness of accidental reactions make them prone to high-risk safety incidents, such as explosions, which can result in significant casualties and property damage. These incidents pose a serious threat to the development of weapons and equipment, as well as to public safety [1]. Therefore, evaluating the detonation performance of explosives is crucial in preventing such safety incidents. While experimental trials are reliable for assessing the detonation performance of high explosives (HEs), the testing process is complex and dangerous. Some experiments are expensive, time-consuming, and environmentally unfriendly. Particularly for

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newly synthesized explosive materials, the laboratory yield is often around 1 g, which is insufficient for a comprehensive evaluation of detonation capability. As a result, it is vital to quantify the potential impact of an explosion using reliable theoretical simulation methods to assess the detonation performance of new formulations that have not been fully characterized experimentally. Theoretical evaluation methods include empirical formulas, machine learning, and thermodynamic evaluation. Empirical methods face challenges due to their reliance on various sets of parameters [2]. Data-driven machine learning predictions are dependent on data guality (uniform measurement standards), data quantity (limited types of explosives and few measured detonation velocity entries), and the development of dedicated models for strongly coupled energetic materials (generic models often have low accuracy) [3]. Therefore, thermodynamic evaluation software remains the most accurate tool for such assessments.

In thermodynamic calculations, the equation of state (EOS) for explosive detonation products is essential. The EOS describes the relationship between pressure, temperature, and volume of

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detonation gas products, based on experimental data or molecular dynamics theory. It forms the foundation for studying the initiation and detonation of energetic materials. The precision of the EOS in characterizing state parameters is strongly correlated with the accuracy of detonation performance predictions. Despite its importance, few state equations can adequately model the state changes of reaction products in specific weapon systems. For example, complex phenomena such as shell charging, crack propagation, deflagration-to-detonation transitions (DDT), and conditions in the medium-temperature, atmospheric-pressure, and low-pressure regions are challenging to capture with current models. The choice of a robust EOS is therefore essential for accurate predictions and safe design. Additionally, thermodynamic codes built on EOS models such as BKW [4], WCA [5] and JCZ [6], KHT [7], and VLW [8–10] are widely used to estimate detonation performance. However, those existing thermochemical approaches like BKW and others all have known deficiencies. Take the most widely used and famous BKW EOS as an example. It employs multiple sets of empirical parameters, such as α and β , which are adjusted and fitted based on impact compression data of detonation products and the detonation performance parameters of various explosives. One set of parameters cannot be accurately applied to all explosives. Although these parameters are calibrated using experimental data from existing explosives and yield satisfactory results, there are significant limitations when predicting the performance of new materials [4]. Unlike other codes, the EOS used by Fortran VLW [8–10] or our VHL code does not rely on empirical parameters, which will be detailed in the following sections. However, as a typical EOS in the virial system, it has been shown that the calculated values provided by VLW EOS for higher-order virial coefficients can differ significantly from those found in the literature. Given the current state of research, we have developed a theoretically derived virial equation based on statistical physics to describe the detonation process of energetic materials across different states.

The accuracy of an EOS becomes even more critical across a wide range of temperatures and pressures, especially in applications like underwater weapons and thermobaric explosives. In underwater weapons, explosives generate bubbles in a closed aquatic environment, and the pulsating energy of these bubbles is utilized to destroy targets. The state of detonation products evolves rapidly from high temperature and pressure to medium pressure and, eventually, to normal or even negative pressure [11,12]. Similarly, in thermobaric explosives, the detonation occurs at high temperature and medium pressure, where oxygen in the air chemically reacts with the detonation products. However, widely-used models like the JWL EOS, which assumes isentropic expansion, cannot accurately describe these reactions [13]. As the use of thermobaric explosives and underwater weapons continues in combat. an accurate EOS across varying conditions is increasingly recognized as vital for assessing their destructive efficacy. The accuracy of an EOS is closely linked to the correctness of the potential function parameters, which describe intermolecular interactions, influencing macroscopic properties like pressure, volume, and temperature. By refining these parameters, an EOS can be applied to a broader range of materials and conditions, improving its predictive capacity.

This work presents the development of a novel detonation product state equation, VHL (Virial-Han-Long), grounded in the physical principles of the virial equation and using reliable fundamental data. This new EOS is designed to accurately describe the high-temperature, medium- and high-pressure states of detonation products. Additionally, we have established a thermodynamic calculation tool capable of efficiently computing the detonation performance characteristics and the isentropic expansion processs of detonation products. Moreover, the detonation property of three new promising high explosives (HEs): ICM-101 ([2,2'-bi(1,3,4-oxadiazole)]-5,5'-dinitramide, $C_4H_2N_8O_6$), ONC (Octanitrocubane, $C_8N_8O_{16}$), and TNAZ (1,3,3-trinitroazetidine, $C_3H_4N_4O_6$) were calculated, analyzed and compared with three typical HEs: TATB (2,4,6-triamino-1,3,5-trinitrobenzene, $C_6H_6N_6O_6$), CL-20 (hexanitrohexaazaisowur-tzitane, $C_6N_{12}H_6O_{12}$), and HMX (octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, $C_4H_8N_8O_8$). Our analysis suggests that these new high-energy explosives have promising applications.

2. Theoretical foundation

2.1. Optimizing of VHL EOS

Within the framework of statistical mechanics, the equation of state (EOS) can be determined in two ways [14]. The first method derives the EOS from the interaction potential U(r) between two molecules and the radial distribution function g(r). When calculating the parameters of the detonation product mixture, it is essential to first derive the EOS of a basic medium composed of the same type of molecules, and then calculate the deviation between the parameters of the researched mixture and those of this basic medium. By combining the solution of the mixing problem based on conformal solution theory with the Lennard-Jones-Devonshire (LJD) cell theory, an example of the EOS is obtained.

The second approach to determining the EOS involves using statistical mechanics methods to calculate the statistical sum of all energy states in a system composed of N molecules. This sum is expressed as $\sum \exp(-U/(kb))$, where *U* is the energy of the *i*-th state, and $p = RT\left(\frac{d \ln z_N}{dV}\right)_{T,N}$. This method introduces a simple model of dense gas, providing the compressibility of detonation product components and offering a supplementary assumption about the mixing properties of detonation products. As the simplest model of dense gas, it is assumed that the motion of a particle in the system can be attributed to independent motion within a designated region (cell). Under high pressure, a structure with the highest packing density can be achieved, exhibiting sufficient symmetry, so the particle's motion occurs within the spherically symmetric potential field of other particles.

Both BKW EOS and VLW EOS belong to the second approach. In the following paragraph, we compare VHL EOS with VLW EOS, BKW EOS, and JCZ3 EOS. For further details on the differences among these EOS models, please refer to the Supplementary Materials. The BKW EOS approximates the second-order virial coefficients but is only accurate when βw approaching 0. The VLW EOS, which approximates from third-order virial coefficients, suggests through similarity theory that virial coefficients are similar at high temperatures, allowing higher-order virial coefficients to be solved using second-order ones. However, in practice, the calculated values provided by VLW EOS for higher-order virial coefficients significantly differ from the literature values.

To effectively describe the changes in the gas components of detonation products as they transition from high temperature and high pressure to high temperature and medium pressure, the potential parameters of the detonation products must be calibrated. The published literature indicates that there is still room for improvement in the thermodynamic description of the gas components in various detonation products. Therefore, our research highlights that the accuracy of the virial coefficient is crucial. VHL thermodynamic code is used to calculate the thermodynamic properties of a mixture with a known composition ratio, which contain gases, liquids, and solids [8,15–19].The gas EOS for the VHL thermodynamic code is based on the virial equation [20], which is described as:

$$\frac{pV_m}{RT} = 1 + \frac{B(T)}{V_m} + \frac{C(T)}{V_m^2} + \frac{D(T)}{V_m^3} + \frac{E(T)}{V_m^4} + \cdots$$
(1)

where *P* is pressure, V_m is gaseous molar volume, *T* is temperature, *R* is gas constant. *B*(*T*), *C*(*T*), *D*(*T*), *E*(*T*), …, respectively, represent the second, third, fourth, fifth, …, order of virial coefficients, which are functions of intermolecular potential. Deriving from statistical physics [21], the theoretical expression of the second virial coefficient is as follows:

$$B(T) = -2\pi N \int_{0}^{\infty} \left(e^{-\frac{U(r)}{kT}} - 1 \right) r^{2} dr$$
(2)

where *N* is Avogadro's constant, U(r) is a potential function, *r* is separation distance, *K* is Boltzmann's constant. Using the Lennard-Jones (L-J) potential function(for details, see supplymentary), the analytical solutions for the dimensionless virial coefficients of second order are as follows [22]:

$$B^{*}(T^{*}) = \sum_{j=0}^{\infty} b^{(j)} T^{*-(2j+1)/4}$$
(3)

where $B = b_0 B^*(T^*)$, $b_0 = 2\pi N\sigma^3/3$, $T^* = kT/\varepsilon$ is the dimensionless temperature, ε and σ are the potential parameters of the L-J function, $b^{(j)} = -\frac{2^{j+1/2}\Gamma((2j-1)/4)}{(4j!)}$. Barker et al. [23] performed precise theoretical calculations based on the L-J potential energy function for the dimensionless third-order, fourth-order, and fifthorder coefficients of the virial equation. The results listed the coefficient values at particular temperatures in a tabular form, which is not useful for regularly research needs. Based on Barker's theory, Hu et al. [24] gave empirical equations for the fourth and fifth order virial coefficients in finite series form. Nonetheless, the computation error is comparatively high in certain non-dimensional temperature ranges; in some cases, it even approaches 20% in comparison to theoretical values. Based on the theoretical derivation of Barker et al., we optimized the third-order and fourth-order virial coefficients accordingly. The third-order and fourth-order dimensionless virial coefficients are expressed as analytical functions in this paper using nonlinear optimization techniques and findings computed using Barker theory. Eq. (4) illustrates how a simpler combination function is used to describe higher order virial coefficients. By optimizing methane molecular dynamics data and high-temperature experimental data [25,26], the combination function's coefficient values are determined.

The complete expression of VHL is:

$$\frac{pV}{RT} = 1 + wB^* + w^2C^* + w^3D^* + w^4E^* + (a + bT^*)w^f$$
(4)

$$C^* = c_1T^{*c_2} + c_3T^{*c_4} + c_5T^{*c_6} + c_7T^{*c_8} + c_9T^{*c_{10}}$$

$$D^* = d_1T^{*d_2} + d_3T^{*d_4} + d_5T^{*d_6} + d_7T^{*d_8} + d_9T^{*d_{10}}$$

$$E^* = e_1T^{*e_2} + e_3T^{*e_4}$$

$$w = \frac{b_0^2}{b_{CH_4}V}$$

where $b_{CH_4} = 67.21$, C^* , D^* , E^* represent the dimensionless virial coefficients of the third, fourth, and fifth orders, respectively. The

specific values of c_1-c_{10} , d_1-d_{10} , e_1-e_4 , a, b, f are shown in Table 1. Fig. 1 displays a comparison and percentage of error between the computed values in Ref. [23] and the fitting curves of the third and fourth order dimensionless virial coefficients. The optimized third-order and fourth-order values shown in Fig. 1 can well reproduce the relationship between the virial coefficient values and temperature. The maximum error between the calculated value and the literature value for the third-order and fourth-order dimensionless virial coefficient are 1.97% and 1.03%, respectively. Under high temperature conditions, such as condensed phase explosives and gas-phase gas explosion, the temperature range (often larger than 1000 K) is nearly error-free.

2.2. Principle of theoretical calculation for detonation performance

According to thermodynamic theory, if the independent variables are temperature T, specific volume V, and the number of moles of the *i*th product x_i , all thermodynamic functions can be deduced from free energy F. For an ideal gas, Gibbs free energy F is represented by:

$$p = -\left(\frac{\partial F}{\partial V}\right)_{T,x_i} \tag{5}$$

internal energy E is:

$$E = -T^2 \frac{\partial(F/T)}{\partial T} \tag{6}$$

entropy S is derived from F:

$$S = -\left(\frac{\partial F}{\partial T}\right)_{V,x_i} \tag{7}$$

By simultaneously solving Eqs. (4) and (5), a partial differential equation for F respecting V.

$$-\left(\frac{\partial F}{\partial V}\right) = \frac{\overline{x}RT}{V} \left(1 + wB^* + w^2C^* + w^3D^* + w^4E^* + (a + bT^*)w^{3.608}\right)$$
(8)

If we assume that gas is regarded as ideal gas $V \rightarrow \infty$ or $\omega \rightarrow 0$, a mathematical expression for the thermodynamic free energy function *F* can be obtained.

$$F = \sum_{i} x_{i} RT \left(\phi_{i} - 1 + \ln \frac{x_{i} RT}{V} \right) + \overline{x} RT \left(wB^{*} + \frac{w^{2}}{2} C^{*} + \frac{w^{3}}{3} D^{*} + \frac{w^{4}}{4} E^{*} + \frac{w^{3.608}}{3.608} (a + bT^{*}) \right)$$
(9)

where $\phi_i = \frac{\mu_i}{RT} = \frac{1}{RT} [(G^0 - H^0_{298})_i + (H^0_{298})_i]$, $\mu_i = \frac{\partial F}{\partial x_i}$, μ_i is the chemical potential of the detonation product components. Therefore, the internal energy of 1 mol of gas can be obtained as:

$$\widetilde{E} = E\overline{x} = \sum \frac{x_i}{\overline{x}} \left[\left(H^0 - H^0_{298} \right)_i - RT + \left(H^0_{298} \right) \right] -RTw \left(T^* \frac{\partial B^*}{\partial T^*} + \frac{w}{2} T^* \frac{\partial C^*}{\partial T^*} + \frac{w^2}{3} T^* \frac{\partial D^*}{\partial T^*} + \frac{w^3}{4} T^* \frac{\partial E^*}{\partial T^*} + \frac{bw^{2.608}}{3.608} T^* \right)$$
(10)

The entropy of 1mol gas is:

Table 1 The constant of the fitting equation for the dimensionless Virial coefficients for each order

| <i>c</i> ₁ | <i>c</i> ₂ | C3 | <i>C</i> ₄ | <i>C</i> ₅ | <i>c</i> ₆ | C ₇ | <i>C</i> ₈ | C9 | <i>c</i> ₁₀ |
|-----------------------------------|--|--|-------------------------------|--------------------------------------|--|--------------------------------------|---------------------------------------|-------------------------------|--|
| -0.96665 d_1 -2.31154 | -4.51039 d ₂ -7.49608 | –2.58733 d ₃ –2.56864 | -0.85487 d_4 -1.14947 | 2.08033 d ₅ 2.09534 | -0.51631 d ₆ -0.84757 | 2.02825 d ₇ 2.81486 | -2.15543 d ₈ -4.4448 | -0.12489 d_9 -0.30669 | -7.65161 d ₁₀ -11.36945 |
| <i>e</i> ₁ -2.15701 | e ₂ -2.52736 | <i>e</i> ₃ 0.2708 | e ₄ -1.0019 | a -0.002431 | b 0.0001776 | f 3.608 | | | |



Fig. 1. Comparison between calculated values and experimental values of the third and fourth dimensional coefficients.

$$\widetilde{S} = \frac{S}{\overline{x}} = \sum \frac{x_i}{\overline{x}} \left(S_i^0 - R \ln \frac{x_i R T}{V} \right) - Rw + \left[\left(T^* \frac{\partial B^*}{\partial T^*} + B^* \right) \right]$$
$$+ \frac{w}{2} \left(T^* \frac{\partial C^*}{\partial T^*} + C^* \right) + \frac{w^2}{3} \left(T^* \frac{\partial D^*}{\partial T^*} + D^* \right) + \frac{w^3}{4} \left(T^* \frac{\partial E^*}{\partial T^*} + E^* \right)$$
$$+ \frac{w^{2.608}}{3.608} \left(bT^* + (a + bT^*) \right)$$
(11)

The chemical potential is:

$$\mu_{i} = \left[\left(G^{0} - H_{298}^{0} \right)_{i} + \left(H_{298}^{0} \right)_{i} + RT \ln \frac{x_{i}RT}{V} \right] + RTB^{*} \left[\frac{2(b_{0})_{i}}{V_{CH_{4}}} \right] + RTC^{*} w \left[\frac{2(b_{0})_{i}}{V_{CH_{4}}} - \frac{w}{2} \right] + RTD^{*} w^{2} \left[\frac{2(b_{0})_{i}}{V_{CH_{4}}} - \frac{2w}{3} \right] + RTE^{*} w^{3} \left[\frac{2(b_{0})_{i}}{V_{CH_{4}}} - \frac{3w}{4} \right] + RT(a + bT^{*}) w^{2.608} \left[\frac{2(b_{0})_{i}}{V_{CH_{4}}} - \frac{2.608w}{3.608} \right]$$
(12)

For solid carbon in detonation products, Cowan EOS [27] or VINET EOS [28] is used to get the free energy values. Then the internal energy *E*, entropy *S*, and chemical potential μ_i can be obtained from Eqs. (10)–(12). The free energy of possible products is computed for different components using the minimal free energy theory, and the mixed component x_i is discovered when the free energy is minimum. The matching values of *P*, *T*, *S*, *V*, and *E* are then ascertained. The mass, momentum, and energy conservation equations on either side prior to and behind the detonation wavefront are as follows, in accordance with the CJ theory:

$$D_{\rm CJ}^2 = \frac{V_0^2}{V_0 - V_{\rm CJ}} \left(P_{\rm CJ} - P_0 \right) \tag{13}$$

$$U_{\rm pCJ} = \sqrt{(P_{\rm CJ} - P_0)(V_0 - V_{\rm CJ})}$$
(14)

$$E_{\rm CJ} - E_0 = (P_{\rm CJ} + P_0) (V_0 - V_{\rm CJ}) / 2 + Q$$
(15)

where *D* is detonation velocity, U_p is particle velocity, *Q* is a heat of reaction, subscript 0 and CJ represents the initial state and the CJ state, respectively. Hence, the values of *D*, *P*, *T*, U_p , *V*, and *E* at CJ point can be determined.

In the calculation of the isentropic expansion zone, the pressure value of the detonation product was adjusted based on the isentropic condition and the minimum free energy condition of the detonation product, and the volume, temperature and internal energy that satisfies the condition is calculated according to the VHL gas product EOS and the solid Cowan EOS or VINET EOS. By concurrent solving Eqs. (4), (9), (10) and (15), the product Hugoniot curve can be obtained. Thus, the isentropic curve passing through any point on the product Hugoniot curve can be calculated by combining Eq. (11) with dS = 0.

3. Results and discussion

3.1. Model validation

3.1.1. Verification of the accuracy in describing gas states under high temperature and medium to high pressure conditions

To verify the validity and limitations of this novel model, we describe the states of high-temperature, medium, and highpressure gases using the VHL EOS. Non-polar and weakly polar gases detonation product (CH₄, CO₂, CO, O₂, N₂ and H₂) have constant potential characteristics that do not change with temperature. This article applies a complex optimization method [29] to optimize the high-order virial coefficient constants of the VHL EOS and the LJ potential parameter values of methane relying on hightemperature experimental data and molecular dynamics data [25,26]. For CO₂ [30], CO and O₂, this article uses molecular dynamics calculation data from Belonoshko et al. [26], with temperature ranges of 718-4978 K, 725.1-4286 K, 707.7-4067 K, and pressure ranges of 0.5116-111.078 GPa, 0.5416-113.04 GPa, and 0.329–111.5 GPa, respectively. For N₂ and H₂, the NIST database [31] is utilized, with a temperature range of 1000K-2000K and a pressure range of 0.1–2.0 GPa. For highly polar molecule H₂O, the hydrogen bond that binds water molecules together makes the phase diagram of water incredibly rich and multifaceted. Due to a dearth of experimental data in a pertinent region, the majority of EOS characterizing water are consequently restricted to a specific temperature and pressure range [32]. Therefore, additional highpressure and high-temperature experimental data are required to fully characterize the EOS of water. According to the literature research results, the potential energy function of water molecules varies with temperature in high-temperature situations [33]. For the potential characteristics of water, this article employs the leastsquare method [34] to produce the water potential energy function that fluctuates with temperature. The particular form can be found in Eqs. (16) and (17).

$$\varepsilon_T = \varepsilon_0 (1 + a / T) \tag{16}$$

$$b_T = b_0 + b \exp(-T/c)$$
 (17)

By fitting it's obtained that $\varepsilon_0 = 229.61778$, a = 1188.7, $b_0 = 45.0936$, b = -70.86645, c = 352.45852. It has been demonstrated that it can accurately characterize the thermodynamic state of water in both the low-temperature, medium-pressure and high-temperature, high-pressure sections. Table 2 presents a comparison between the values found in the literature and the potential parameter values optimized using the complex optimization

Table 2

The potential parameter values of methane, CO_2 , CO, O_2 , N_2 , H_2 , NH_3 , NO, HCI, CI_2 , CF_4 , and HF used in this article are compared to those reported in the literature.

| ε/ k | $b_0/(ml \cdot mol^{-1})$ | Ref. |
|---|--|--|
| Methane 154.0 140.94 147.5 139.571 147.94 149.0 | 63.40 64.72 64.43 65.17 65.43 67.21 | [35] [26] [36] [37] [38] This Paper |
| CO ₂ 247.0 205.0 181.8 | 63.37 85.05 67.30 | [33] VLW [39] This Paper |
| CO 98.0 100.2 109.3 | 63.37 67.22 65.53 | [33] VLW [39] This Paper |
| O ₂ 106.7 117.5 129.3 | 52.45 57.75 57.36 | [35] VLW [39] This Paper |
| N ₂ 96.0 95.05 120.5 | 62.34 63.78 64.32 | [33] VLW [39] This Paper |
| H ₂ 34.60 29.20 39.35 | 30.44 29.76 45.61 | [40] VLW [39] This Paper |
| NH₃ 138.0 150.0 | 70.0 60.0 | VLW [39] This Paper |
| NO 131.0 112.0 | 40.0 56.34 | VLW [39] This Paper |
| HCI 393.3 | 44.12 | This Paper |
| Cl₂ 152.0 | 131.0 | This Paper |
| CF ₄ 198.4 | 71.45 | This Paper |
| HF 346.7 | 151.19 | This Paper |

method used in this work.

The PVT relationship of high-temperature methane is determined by applying the VHL EOS, as indicated in Supplementary Table S1. Volume is the dependent variable in the computation, temperature and pressure are the independent variables to compare with the state equations of DMW and BS. For 112 data points, the computed AAD% is 1%, AAD is defined in Eq. (18). When the temperature is 1116.6 K and the pressure is 0.14953 GPa, the estimated volume has a maximum variation of 3.28%. Table S1 shows the calculation results for both the DMW and BS state equations. The data in Table S1 show that DMW is suitable for representing the thermodynamic state of methane at low pressures. Under high pressures, such as those above 10 GPa, volume calculation deviates significantly, with no viable answer. When the temperature is 2304.4 K and the pressure is 184.188 GPa, the computed volume inaccuracy is 76%. At high pressures, the thermodynamic state of methane can be well described by the BS EOS. There is a significant discrepancy in the volume computation when the pressure is low, like at 100 MPa, with an AAD% of 9.4% for 112 data points. The largest inaccuracy is 116.8% when the temperature is 1128.6 K and the pressure is 0.02819 GPa. This indicates that the VHL EOS performs noticeably better than the DMW and BS EOS in representing the thermodynamic state of high-temperature methane gas over a broad pressure range. Fig. 2 depicts a twodimensional plane diagram with pressure and temperature as independent variables and volume deviation as the dependent variable. At lower pressures, the VHL state equation explains methane gas with a specific deviation. For example, at 1116.6 K and 0.14953 GPa, the predicted volume variation is 3.28%. Compared to similar state equations such as BS, DMW, and so on, VHL remains more accurate. At explosive atmosphere (0.1-50 GPa), the average deviation of the VHL EOS characterizing the thermodynamic state of methane is significantly less than 1%. When the pressure exceeds 100 GPa, the VHL EOS maintains acceptable predictive accuracy (Fig. 2). This article calculates the PVT relationship of CO₂ using VHL and VLW EOS and compares the obtained molecular dynamics values, which are provided in Table S2. The deviation of CO₂ volume calculation under different temperatures or pressures is shown in Fig. 2. The average absolute deviation computed using the VHL EOS is 0.971%, with a maximum deviation of 4.04%. This is significantly lower than the average absolute deviation of 20.2% and maximum deviation of 87.149% calculated using the VLW EOS. At the same time, it is significantly lower than the maximum error of 22.82% estimated by Belonoshko et al. [26] with polynomial state equations. This leads to the conclusion that by optimizing the CO₂ potential energy parameters alone, the VHL equation of state may adequately characterize the high temperature, medium, and high pressure states of CO₂. The PVT correlations for CO, O₂, H₂, and N₂ are listed in Tables S3-S6 along with a comparison to values from the literature. Fig. 2 displays the variation in volume calculation under various pressures or temperatures. The maximum deviations are 3.4%, 8.680%, 1.593%, and -0.708%, respectively, and the average absolute deviations are calculated using the VHL state equation as 0.764%, 1.244%, 0.698%, and 0.369%. These values are significantly lower than the maximum deviations (30.556%, 35.988%, 18.514%, -11.182%) and average absolute deviations (12.289%, 10.091%, 6.698%, 6.318%) calculated using the VLW EOS. Therefore, the VHL derived from the virial theory can better describe the hightemperature, medium and high-pressure states of gas components found in detonation products.

$$AAD\% = \frac{1}{N} \sum_{i=1}^{N} \left| \left(V_{\text{HL}} - V_{\text{ref}} \right) / V_{\text{ref}} \right| \times 100$$
(18)



Fig. 2. The volume deviation of CH₄, CO₂, CO, O₂, H₂ and N₂ under various pressure circumstances is explained using the VHL EOS.

3.1.2. Verification of detonation performance assessment

The detonation performance of explosives varies with their density, meaning their CJ detonation temperature and pressure differ, corresponding to distinct pressure and temperature ranges for the explosive detonation products. Therefore, an effective method for evaluating the accuracy of high-temperature and high-pressure state equations is to precisely calculate the detonation performance characteristics of CHNO explosives at varying densities. We computed the detonation parameters of numerous known explosives and their binder mixes, which provides valuable insights into the broader performance of the new VHL code. The explosive properties, specifically detonation velocity (D) and detonation pressure (P), calculated using VHL, BKW [41,42], and CHEETAH [41,42], are listed in Tables 3–5. For comparison, experimental data from published studies is also included. For different types of explosives, the components we consider include CH₄, CO₂,

CO, O₂, N₂, H₂, NH₃, NO, solid carbon (C), HCl, Cl₂, CF₄, and HF, specific parameters can be found in Table 2.

The accuracy of measuring explosive pressure and detonation velocity is influenced by several factors, including the uniformity and purity of the explosive, the precision of testing equipment and instruments, environmental conditions (such as temperature, humidity, and atmospheric pressure), the form of the explosive charge, the selection of testing methods, and the operators' adherence to protocols. Additionally, experimental values are not perfect CJ values due to the diameter effect; however, when the charge diameter is sufficiently large—for example, 20 mm for ideal explosives—these values are very close to the ideal CJ values. It should be noted that the computed values correspond to the CJ state [43,44].

Tables 3–5 demonstrate that the new model performs well in predicting the detonation characteristics for a wide range of

Table 3

| Calculated detonation | parameters | of the | common | homogeneous | solid | explosives |
|-----------------------|------------|--------|--------|-------------|-------|------------|
|-----------------------|------------|--------|--------|-------------|-------|------------|

| Explosive | Formula | $ ho/(g \cdot cm^{-3})$ | $D/(\mathbf{m} \cdot \mathbf{s}^{-1})$ | | | | <i>P</i> /GPa | | | | |
|-----------|--|---|--|--|--|--|--|--|---|--|--|
| | | | Exp [42]. | VHL | BKW [42] | CHEETAH [45] | Exp [42]. | VHL | BKW [42] | CHEETAH [45] | |
| RDX | C ₃ H ₆ N ₆ O ₆ | 1.8 1.72 1.6 1.2 0.95 0.56 | 8750 8460 8130 6770 5800 4050 | 8860 8500 7996 6603 5720 4300 7030 | 8960 8630 8150 6790 6060 4720 7190 | 8780 8480 8040 6690 5850 4170 7030 | 34.1 31.3 26.3 15.2 9.6 3.2 21 | 33.1 29.3 27.7 13.8 8.5 3.2 18.6 | 33.4 30.2 26 15.2 10 3.8 20 3 | 34.7 30.9 26.1 14.3 9 2.8 | |
| | | 1.45 1.36 1.0 0.8 | 6500 6200 5000 4340 | 6522 6178 4988 4400 | 6510 6220 5210 4740 | 6370 6090 5060 4450 | 14.4 12.4 6.7 3.7 | 14.6 12.4 6.7 4.3 | 15.3 13.4 7.7 5.3 | 14.7 12.8 7 4.3 | |
| PETN | C ₅ H ₈ N ₄ O ₁₂ | 1.76 1.45 1.23 0.99 0.48 | 8270 7180 6370 5480 3600 | 8276 7254 6474 5575 3660 | 8680 7480 6760 5990 4120 | 8400 7170 6380 5580 3500 | 33.7 20.8 13.9 8.7 2.4 | 31.6 19.8 13.5 8.4 2.1 | 31.2 20.8 15.3 10 2.6 | 29.6 18.7 13.3 8.5 1.8 | |
| ТАТВ | C ₆ H ₆ N ₆ O ₆ | 1.88 1.85 | 7760 7660 | 8200 8070 | 8190 8070 | 8230 8100 | 25.9 | 28.4 26.9 | 28.5 27.3 | 30.8 29.1 | |
| TETRYL | $C_7H_5N_5O_8$ | 1.73 1.68 1.61 1.36 | 7850 7500 7580 6680 | 7630 7440 7373 6480 | 7810 7630 7380 6590 | 7720 7550 7320 6540 | 23.9 22.6 14.2 | 24.3 22.4 20.8 14.5 | 25.5 23.9 21.8 15.7 | 25.7 23.9 21.7 15.2 | |
| НМХ | C ₄ H ₈ N ₈ O ₈ | 1.89 1.6 1.2 0.75 | 9110 7910 6580 4880 | 9160 7995 6540 4990 | 9350 8140 6780 5420 | 9110 8040 6680 5060 | 39 28 16 6 | 39.79 27.69 13.8 5.3 | 37.4 25.9 15.1 6.4 | 39.9 26 14.3 5.2 | |

Table 4

Calculated detonation parameters of some liquid explosives.

| Explosive | Formula | $\rho/(g \cdot cm^{-3})$ | $D/(\mathbf{m} \cdot \mathbf{s}^{-1})$ | | P/GPa | | | |
|--|---|--------------------------|--|------|----------|-----------|-------|----------|
| | | | Exp [41]. | VHL | BKW [41] | Exp [41]. | VHL | BKW [41] |
| Nitroglycerine | C ₃ H ₅ N ₃ O ₉ | 1.59 | 7580 | 7469 | 7700 | | 21.52 | 24.6 |
| Liquid TNT | $C_7H_5N_3O_6$ | 1.477 | 6580 | 6446 | 6556 | 17.2 | 17.2 | 16.0 |
| Nitromethane | $C_1H_3N_1O_2$ | 1.128 | 6290 | 6318 | 6463 | 14.1 | 11.52 | 13.0 |
| 1/1.25 mol Acrylonitrile/Tetranitromethane | $C_{4,25}H_3N_6O_{10}$ | 1.380 | 6710 | 6745 | 7074 | 15.6 | 16.35 | 19.2 |
| 1/1.29 mol Benzene Tetranitromethane | C _{7.29} H ₆ N _{5.16} O _{10.32} | 1.362 | 6850 | 6882 | 6960 | | 17.27 | 18.1 |
| 1/0.25 mol Nitromethane/Tetranitromethane | $C_{1,25}H_3N_2O_4$ | 1.31 | 6880 | 6762 | 7094 | 15.6 | 15.3 | 18.1 |
| 14.5/85.5 Toluene/Nitromethane | $C_{2.503}H_{5.461}N_{1.4006}O_{2.8013}$ | 1.088 | 5840 | 6079 | 5945 | 10 | 10.24 | 10.6 |

Table 5

Calculated detonation parameters of some heterogeneous solid explosives.

| Explosive | Formula | $\rho/(g \cdot cm^{-3})$ | $\frac{D}{(m \cdot s^{-1})}$ | | | P/GPa | | |
|---|---|--------------------------|------------------------------|------|-------------|--------------|-------|-------------|
| | | | Exp [41,42]. | VHL | BKW [41,42] | Exp [41,42]. | VHL | BKW [41,42] |
| Composition B 64/36 RDX/TNT | C _{6.851} H _{8.75} N _{7.650} O _{9.3} | 1.713 | 8030 | 7978 | 8084 | 29.4 | 29 | 28.4 |
| Octol 76.3/23.7 HMX/TNT | $C_{6.835}H_{10.025}N_{9.215}O_{10.43}$ | 1.809 | 8476 | 8487 | 8555 | 34.3 | 34.23 | 33.3 |
| Cyclotol 77/23 RDX/TNT | $C_{5.045}H_{7.461}N_{6.876}O_{7.753}$ | 1.743 | 8250 | 8257 | 8311 | 31.3 | 31.45 | 30.5 |
| LX-14 95/5 HMX/Estane | $C_{4.8}H_{9.1365}N_{8.024}O_{8.2811}$ | 1.81 | 8760 | 8890 | 9749 | | 31.55 | 34.8 |
| PBX-9011, 90/10 HMX/Estane | $C_{5.696}H_{10.476}N_{8.062}O_{8.589}$ | 1.767 | 8500 | 8554 | 8496 | 29.8 | 28.28 | 31.9 |
| EDC-11, 64/4/30/1/1 HMX/RDX/TNT/Wax/Trylene | $C_{1.986}H_{2.7825}N_{2.233}O_{2.6293}$ | 1.782 | 8213 | 8345 | 8384 | 31.5 | 33.2 | 31.5 |
| HMX_based | $C_{1.61}H_{2.59}N_{2.54}O_{2.567}F_{0.053}Cl_{0.0145}$ | 1.845 | 8669 | 8773 | | 34.5 | 32.32 | |
| 9159 | $C_{1.45}H_{2.73}N_{2.6}O_{2.65}F_{0.04}Cl_{0.01}$ | 1.863 | 8870 | 8896 | | 36.8 | 37.8 | |
| LX-15-0 (HNS/Kel-F) | C13.675 H5.783N5.675O11.35 F0.596Cl0.163 | 1.58 | 6840 | 6732 | 6730 | | 16.34 | 18.1 |
| LX-17-0 (TATB/Kel-F) | C _{6.096} H _{5.807} N _{5.711} O _{5.711} F _{0.53} Cl _{0.145} | 1.91 | 7630 | 7678 | 8080 | | 20.02 | 28.9 |
| PBX-9407 | C _{1.41} H _{2.66} N _{2.54} O _{2.69} F _{0.09} Cl _{0.07} | 1.6 | 7910 | 7974 | 7920 | 28.7 | 27.23 | 24.8 |
| LLM105/F2314/W = 95.2/4/0.8 | $C_{1.90}H_{1.778}N_{2.644}O_{2.204}F_{0.106}Cl_{0.03}$ | 1.848 | 8042 | 8067 | | | 26.27 | |
| 21/79 Hydrazine/Hydrazine Nitrate | H _{8.154} N _{4.577} O ₃ | 1.4418 | 8600 | 8775 | 8682 | | 24.35 | 26.5 |
| 70/30 Hydrazine/Hydrazine Nitrate | H _{32.685} N _{16.843} O ₃ | 1.14 | 8025 | 8038 | 9393 | | 17.95 | 22.7 |

available explosive molecules and their variations. To provide a clearer view of the calculation error, Fig. 3 presents the relative errors of the calculation results among VHL EOS, BKW EOS, and

CHEETAH EOS. The versions of the BKW EOS used include BKWS, RDX Param BKW, and TNT Param BKW, while CHEETAH is based on the JCZ3 EOS. It is evident that, for all types of explosives—liquid, homogeneous, and heterogeneous-regardless of density, the new model's calculations are as reliable as, if not slightly more so than, those of BKW. The error analysis in Tables 3-5 is summarized in Table 6, the maximum and minimum errors of detonation velocity for VHL are 6.17% and 0.073% for RDX of 0.56 g/cm³ and PETN of 1.76 g/cm^3 respectively, for detonation pressure the maximum and minimum errors are 18.3% and 0.0% for Nitromethane of 1.128 g/ cm^3 and some explosives respectively. We also calculated the MPE (mean percentage error) and RMSE (root mean square error) for different explosives. For detonation velocity, the MPE of VHL is 1.5% and BKW is 4.03%, while for detonation pressure, the MPE of VHL is 5.33% and BKW is 7.97%, which indicates that the VHL is slightly inferior to BKW in detonation velocity and detonation pressure calculation. Meanwhile, the RMSE also demonstrated that the VHL lower the dispersion for the detonation velocity and detonation pressure.

3.1.3. Validation of assessing the working capacity of explosives

An important use of the thermodynamic EOS for detonation products is not only in calculating the detonation performance parameters of explosives, but also in characterizing the explosives' working capacity through the isentropic expansion process of detonation products. The underwater test and the cylindrical test are the two most often used experimental techniques for determining the explosive force of explosives. Using thermodynamic relationships, the entropy value of the CI state of the explosive is computed. Based on the detonation product's isentropic expansion calculation, the PV curve of the detonation product is then determined. Finally, the dynamic state equation-JWL is derived through fitting, which is then used in numerical simulations of cylindrical and underwater experiments [46-49]. The TNT explosive densities used in this research are 1.580 g/cm³ for underwater shock wave trajectory testing and 1.634 g/cm³ for cylindrical tests, respectively [50]. The density of HMX-based explosives is 1.863 g/cm³, which is consistent with underwater detonation products and water interface expansion trajectory investigations. The computed isentropic expansion curve of detonation products is given in Fig. 4.

For the pressure *P*-volume *V* relationship in the expansion zone, the JWL EOS is fitted from the P-V relationship. The Supplementary contains a detailed introduction to JWL EOS. Table 7 displays the parameter values of the JWL state equation for the detonation products of TNT and HMX based explosives, which are fitted using the computed isentropic expansion curve. The parameter values for the JWL state equation provided in pertinent literature are also listed in Table 7.

Based on the input parameters of the JWL EOS obtained by calculation, the LS-DYNA hydrodynamic code was used to numerically simulate the cylinder and underwater test of TNT and HMX- based PBX explosive. In both cylinder tests and underwater tests, the corresponding models exhibit highly complex degrees of freedom. The state equations and constitutive models for materials such as copper pipes, water, and the explosive itself are typically drawn from Refs. [54-57]. These simulation parameters are generally fixed, leaving the IWL (Iones-Wilkins-Lee) parameters as the primary variables in simulations concerning work capacity. Accurately describing the thermodynamic relationships in the expansion zone of explosive detonation products is critical for the precision of the JWL equation of state (EOS). This, in turn, directly impacts the reliability of the work capacity predictions. The cylinder is an axisymmetric structure, and an axisymmetric calculation model can be established in the cylindrical coordinate system, as shown in Fig. 5. In Fig. 5, the ABEF zone is the part of explosive in the cylinder, which adopts the point initiation and detonates directly at point A, and the CDFG zone is the copper tube part. CF denotes the cylinder length, EF and EG is the inner diameter and outer diameter of the copper pipe. The high explosive burn model was used for explosives, and the red copper uses the John-cook material model [54], the state equation uses the Gruneisen state equation [55]. The calculated values of cylinder wall velocity at the expansion distance $R - R_0 = 19$ mm are shown in Table 8 for comparison with the experimental values [58].

Table 8 shows that there is a 2.58%, 3.65%, and 9.46% difference, respectively, between the experimental data and the computed cylinder wall expansion velocity using the JWL state equation parameters derived from VHL, VLW, and BKW. The velocity value of the cylinder wall expansion to the characteristic distance in cylindrical tests can be estimated more accurately by the VHL thermodynamic code. Although a calibrated JWL model can be used to estimate the expansion velocity of a cylinder with high accuracy, VHL EOS is an excellent prediction tool for novel explosives, which can control the model accuracy threshold within 5%. When designing novel explosives or explosives that have not undergone a cylindrical test, the ability to efficiently assess an explosive's working capacity is crucial. This can be achieved with the combination of the VHL thermodynamic code and the hydrodynamic code LS-DYNA.

In this paper, the underwater shock wave trajectory test of TNT explosives was further simulated numerically. The particular experimental configuration and outcomes are displayed in Ref. [131]. The relationship curve of the shock wave trajectory with time is given in the literature as follows:

$$\frac{x}{D} = \sum_{i=1}^{n} A_i [1 - \exp(-B_i t)] + \frac{c_0}{D} t$$
(19)





Fig. 3. The relative error results of detonation velocity (a) and detonation pressure (b).

Table 6

Error analysis of calculation results.

| Error type (100%) | Detonation parameters | BKW | VHL |
|---|-----------------------|----------|------------|
| Minimum error ^a | Р | 0 | 0 |
| | D | 0.047 | 0.073 |
| Maximum error ^b | Р | 43.24 | 18.3 |
| | D | 17.05 | 6.17 |
| MPE (mean percentage error) ^c | Р | 7.97 | 5.33 |
| | D | 4.03 | 1.5 |
| RMSE(root mean square error) ^d | Р | 1.47 GPa | 1.22 GPa |
| | D | 370 m/s | 138.19 m/s |

^a The minimum error is defined as:min((cal.-exp.)/exp.*100 %).

^b The maximum error is defined as:max((cal.-exp.)/exp.*100 %).

^c MPE: $\frac{100\%}{n} \sum_{i=1}^{n} \frac{\text{cal.} - \text{exp.}}{\text{exp.}}$ ^d RSME: $\sqrt{\frac{\sum_{i=1}^{n} (\text{cal.} - \text{exp.})^2}{2}}$



Fig. 4. Calculation results of isentropic expansion curves for detonation products of TNT and HMX based explosives.

 $A_1 = 7.174$, $B_1 = 0.07521$, $A_2 = 4.892 \times 10^{10}$, $B_2 = 7.793 \times 10^{-13}$, $c_0 = 1.46$, *D* is the explosive detonation velocity, 6.844 mm/µs. This article offers a geometric model for the underwater shock wave trajectory test of TNT explosives, as demonstrated in the lower right corner of Fig. 6, with reference to the experimental setup. The detonation point is the center of the top end of the TNT explosive. Since the water medium is equal to an infinite medium within the effective range of experimental observation, the modeling does not take the water-filled optical glass box into account. The thermodynamic code VHL was used to compute the parameters of the JWL

state equation, and Fig. 6 depicts the relationship between the displacement and time of shock wave propagation along the axial direction of TNT explosives. The figure additionally showcased the experimental values obtained by Zhao et al. [59]. The computed values demonstrated a strong correlation with the experimental values, suggesting that the thermodynamic code VHL is capable of accurately describing the thermodynamic state of TNT explosive detonation products in water.

Additionally, this article performed numerical simulations of underwater tests using HMX-based explosive, the specifics of these experiments are included in the supplementary section. As mentioned earlier, the optical glass box housing the water is not taken into account during modeling. Look at the dimensions marked in Fig. 7, where EFGH is ϕ 25.4 mm \times 240 mm HMX-based explosive, ABCD is water. The detonation point is located in the center of the HMX-based explosive's top end, and the high-energy explosive combustion model is used for HMX-based explosive. Fig. 7 depicts the experimental values and calculation results of the applied thermodynamic codes VLW and BKW. The VHL calculation results diverge greatly from experimental values during the initial expansion stage of HMX-based explosives. This could be due to the influence of shock wave propagation in water during the initial expansion stage, which makes it difficult to obtain a clear trajectory of the interface between HMX-based explosives and water on the film, resulting in a significant error in the interpretation of experimental data during the initial expansion stage of detonation products. As time passes, the difference between the calculated and experimental values gradually decreases. In the later stages of explosive product expansion, the computed results are consistent with the experimental values. The results show that VHL can precisely replicate the radial expansion displacement of HMX-based explosive detonation products in water. It is intuitive to conclude

Table 7

The parameters of the JWL equation of state for the detonation products of TNT and HMX based explosives.

| ···· F ··· ··· ··· ··· ··· ··· ··· ··· | | | | | | | | | |
|--|--------------------------|---------|----------|-----------------------|-----------------------|------|--------------------------|-------------------|------------|
| Explosive | $\rho/(g \cdot cm^{-3})$ | A/MPa | B/MPa | <i>R</i> ₁ | <i>R</i> ₂ | w | $E_0/(kJ \cdot cm^{-3})$ | Algorithm | Source |
| TNT | 1.634 | 12.157 | 0.44165 | 6.3199 | 2.5858 | 0.3 | 9.166 | VHL | This paper |
| | | 2.14714 | 0.10337 | 3.9608 | 1.4034 | 0.5 | 8.417 | BKW | [39] |
| | | 3.33259 | 0.24058 | 4.6137 | 1.9583 | 0.5 | 6.873 | VLW | |
| | | 3.738 | 0.375 | 4.15 | 0.9 | 0.35 | 7.0 | EXP. ^a | [51] |
| | 1.580 | 31.7306 | 0.46026 | 7.9265 | 2.5529 | 0.3 | 8.559 | VHL | This paper |
| | | 3.07 | 0.39 | 4.485 | 0.79 | 0.3 | 6.62 | EXP. ^b | [52] |
| HMX-based(HMX: binder: | 1.863 | 14.7289 | 0.458834 | 5.3673 | 2.2245 | 0.3 | 12.647 | VHL | This paper |
| Insensitive agent $= 95:4.3:0.7$) | | 19.6493 | 0.91377 | 6.14608 | 2.509 | 0.3 | 14.42 | VLW | This paper |
| | | 3.0751 | 0.11244 | 3.4917 | 1.1304 | 0.5 | 13.28 | BKW | [39] |
| | | 9.859 | 0.2054 | 4.8 | 1.15 | 0.29 | 9.8 | EXP. ^c | [53] |

^a The density corresponding to the experimental value provided here is 1.63 g/cm³.

^b The density corresponding to the experimental value provided here is 1.583 g/cm³.

^c The density corresponding to the experimental value provided here is 1.844 g/cm³.



Fig. 5. Model sketch of calculation.

that the VHL thermodynamic code is superior at representing the thermodynamic state of detonation product expansion in the intermediate and later periods when comparing the calculation results of many thermodynamic codes.

It might be concluded that the proposed model can describe gases ranging from highly compressed to ideal gas states. It is trustworthy for assessing the detonation performance of both homogeneous and heterogeneous explosives with initial density in the order of $10^{-3}-2$ g/cm³. Compared to correlation coefficients in BKW and EXPLO5, which are based on macroscopic detonation experiments to fit empirical parameters, our state equation begins with the physical meaning of the virial equation and can better describe the basic state relationship of specific products in high temperature, medium, and high pressure states.

3.2. Prediction of detonation performance

In this section, the quantitative detonation parameters (including detonation velocity *D*, detonation pressure *P*, detonation heat, specifific kinetic energy and the moles of detonation products) of three relatively new explosives ICM-101, ONC, and TNAZ were calculated at varying densities. For comparison, TATB, HMX, and CL-20, the three typical representatives of HEs in existence,

Table 8

Comparison of the wall velocity of TNT explosives at the typical location of cylinder wall expansion between calculated and experimental values.

| Parameter | EXP. | VHL | VLW | BKW |
|--|-------|-------|-------|-------|
| The expansion velocity of cylinder wall <i>U</i> /(mm•µs ⁻¹) | 1.396 | 1.432 | 1.447 | 1.582 |
| Velocity Deviation 100% × (CalExp.)/Exp. | 0 | 2.58 | 3.65 | 9.46 |



Fig. 6. The displacement and time relationship of shock wave propagation along the axial direction of TNT explosives in underwater experiments.

were also calculated as reference. Over the last few decades, energetic materials utilized in both military and civilian industries have sparked global interest as a significant material for economic and weaponry development [60]. Traditional energetic compounds, such as trinitrotoluene (TNT) [61], hexogen (RDX), octogen (HMX) [62], and hexanitrohexaazaisowurtzitane (CL-20) [63], cannot meet the requirements of the rapidly developing military and space industries; additionally, some of these compounds continue to face several issues, such as high cost [64], high toxicity [65], and contamination [66]. As a result, finding new high-energy materials is vital for advancing both the armament business and social development. ICM-101 exhibits a remarkably high density $(1.99 \text{ g cm}^{-3} \text{ at } 298 \text{ K})$, poor solubility in water and most organic solvents, decent thermal stability, a positive heat of formation, and excellent detonation properties. The combination of favorable physical properties and detonation performance, along with its straightforward preparation, underscores its potential as a highenergy density material (HEDM) [67]. With an estimated density of $1.9-2.2 \text{ g/cm}^3$, a positive heat of formation ranging from 81 to 144 kcal/mol, and energy output exceeding that of CL-20, ONC is



Fig. 7. The link between the radial expansion displacement of the center point on the side of an HMX-based explosive and time.

Table 9

Detonation performance of the six explosives from calculation and literature.

| Explosive | Formula | $\rho/(g \cdot cm^{-3})$ | OB ^a | $D/(m \cdot s^{-1})$ | P/GPa | $D_r/(m \cdot s^{-1})$ | P _r /GPa | Ref. |
|-----------|---|--------------------------|-----------------|----------------------|-------|------------------------|---------------------|------------------------|
| ICM-101 | C ₄ H ₂ N ₈ O ₆ | 1.99 | -18.6 | 9394 | 44 | 9481 | 41.9 | [67] (EXPLO5) |
| ONC | C ₈ N ₈ O ₁₆ | 2.065 | 0 | 9963 | 52.7 | 9830 | | [72] (ab initio) |
| | | 1.974 | | 9607 | 47.9 | 9600 | 43.17 | [73] (DFT) |
| | | 1.971 | | 9595 | 47.8 | 9570 | | [72] (ab initio) |
| | | 1.954 | | 9530 | 47.0 | 9510 | | [72] (ab initio) |
| | | 1.932 | | 9447 | 45.9 | 9450 | | [72] (ab initio) |
| | | 1.930 | | 9440 | 45.8 | 9450 | | [72] (ab initio) |
| TNAZ | $C_3H_4N_4O_6$ | 1.84 | -16.7 | 8766 | 35.7 | 8730 | 37.2 | [74] (DFT) |
| TATB | C ₆ H ₆ N ₆ O ₆ | 1.895 | -55.8 | 8272 | 30.7 | 7860 | 31.5 | [41] (Exp.) |
| | | | | | | 8411 | 32.6 | [41] (Exp.) |
| | | | | | | 8365 | 32.5 | [75] (SDA) |
| | | 1.85 | | 8090 | 28.1 | 7660 | 25.9 | [76] (Exp.) |
| | | 1.80 | | 7878 | 25.4 | 7472 | 26.5 | [77] (Exp.) |
| | | | | | | 7658 | 25.94 | [78] (Exp.) |
| | | | | | | 7860 | | [39] (Exp.) |
| CL-20 | C ₆ H ₆ N ₁₂ O ₁₂ | 2.035 | -10.95 | 9777 | 47 | 9445 | 46.7 | [79] (EXPLO5) |
| | | | | | | 9637 | 45 | [79] (Kamlet & Jacobs) |
| | | | | | | 9455 | 46.7 | [80] (EXPLO5.05) |
| | | 1.96 | | 9451 | 42.6 | 9440 | | [81] (Exp.) |
| | | | | | | 9372 | 40.16 | [81] (CHEETAH) |
| | | | | | | 9191 | 40.64 | [81] (EXPLO5) |
| HMX | $C_4H_8N_8O_8$ | 1.9 | -21.6 | 9203 | 40.3 | 9221 | 41.5 | [67] (Exp.) |
| | | 1.89 | | 9160 | 39.8 | 9110 | 39 | [76] (Exp.) |
| | | 1.6 | | 7995 | 27.7 | 7910 | 28 | [76] (Exp.) |
| | | 1.4 | | 7336 | 20.58 | 7300 | 21 | [76] (Exp.) |
| | | | | | | | | |

^a OB: oxygen balance, which indicates the difference between the explosive's actual oxygen content and the quantity of oxygen needed for the explosive's complete oxidation of its hydrogen and carbon.

classified as a "super explosive" in the United States. It is an environmentally benign high-energy explosive, free of hydrogen and halogens, with low characteristic signals and insensitivity to impact. Unfortunately, the applicability of this compound is limited by its low yield and the laborious nature of its current synthesis process [68]. In 1990, Archibald and colleagues synthesized TNAZ for the first time [69]. Its density and detonation characteristics closely match those of the standard HE HMX [70], and at approximately 100 °C, it undergoes a melting transition without decomposition, allowing for melt casting [71]. The aforementioned novel HEs are considered some of the most promising candidates for advanced HEs. However, there is currently no comprehensive literature comparing their detonation performance.

Whether an energetic compound can be widely used as an explosive or propellant depends on key molecular characteristics, including detonation velocity, detonation pressure, explosion heat, and material density. The detonation performance of ICM-101, ONC, TNAZ, TATB, CL-20, and HMX was calculated using the VHL code, as listed in Table 9. Here, D and P represent the calculated values from this study, while D_r and P_r are reference values quoted from the literature. It is noteworthy that the discrepancy between the

computed and reference values of detonation velocity is less than 2%, as determined by calculating the relative errors of the results in Table 9. Except for TATB, which has a density of 1.85 g/cm³, the reference data is also a calculated value, so it cannot definitively confirm the accuracy of our calculation. The difference in detonation pressure is within acceptable limits, demonstrating that the calculated results are reasonably consistent with experimental data. Therefore, it is reliable to use VHL EOS calculation results to analyze the detonation performance of ICM-101, ONC, TNAZ, TATB, HMX, and CL-20. The detonation velocities (*D*) and pressures (*P*) at varying densities (ρ) were calculated and depicted as lines in Fig. 8, which also includes data from the literature.

In Fig. 8(a), ONC has the highest predicted detonation velocities compared to CL-20, ICM-101, HMX, TNAZ, and TATB. ONC's detonation velocity is approximately 1.9% higher than that of CL-20, 6.1% higher than ICM-101, 8.3% higher than HMX, 13.7% higher than TNAZ, and 20.4% higher than TATB. Additionally, the values for both ICM-101 and TNAZ fall between those for HMX and TATB. Specifically, the detonation velocity of ICM-101 is approximately 7.2% and 13.6% higher than that of TNAZ and TATB, respectively. In terms of detonation pressures at a specific density (Fig. 8(b)), ONC



Fig. 8. Comparing the detonation performance of predicted molecules with varying densities.



outperforms the other explosives, indicating that ONC provides the best detonation performance under identical conditions. The detonation pressures of ICM-101 and CL-20 are comparable.

The equilibrium compositions of the explosives ICM-101, ONC, TNAZ, TATB, CL-20, and HMX were compared using different methods, as shown in Fig. 9(a). For the experimental data, which were obtained from the literature, the compositions were determined using calorimetric measurements. For the calculation codes, the minimal free energy theory was employed, ensuring that the product components met the minimum Gibbs free energy and mass conservation requirements. The predicted chemical equilibrium corresponds to the CJ (Chapman-Jouguet) state. The results indicate that the primary product compositions of each explosive computed in this study are consistent with those obtained through other approaches. Table 10 presents the predicted CJ equilibrium compositions of the detonation products of these six explosives, alongside the experimental data.

To provide a concise summary of the explosives' working ability, this study thoroughly analyzes the composition data. The proportions of gas, specific kinetic energy, detonation heat, gas volume, and moles of gas are shown in Fig. 9(b). The working capability is a critical aspect of evaluating energetic materials. An explosive's working capability is primarily related to its chemical reaction, which releases a large amount of gas and heat in a very short period, achieving extremely high temperatures and pressures that propel ammunition and destroy targets effectively [82]. Consequently, the working capability of an explosive is positively correlated with the mechanical work of the compressed gas product and the heat generated during detonation. The analysis of detonation products may explain the differences in working capability. The ranking of specific kinetic energy is ONC > ICM-101 > CL-20 > HMX > TNAZ > TATB, where specific kinetic energy refers to the work performed by compressing the medium with explosives. Although CL-20 has the highest gas content, mechanical work also considers pressure and gas content. Thus, relying solely on gas volume does not accurately reflect the work performed by compressing the medium with explosives. ONC ranks first in terms of explosive heat, followed by ICM-101, TNAZ, CL-20, HMX, and TATB. Given the overall work capacity of explosives, both ONC and ICM-101 perform exceptionally well. The proportions of specific gas products are shown in Fig. 9(c). The primary detonation products are N₂, H₂O, C, and CO₂. The small amount of H₂O in ONC may explain its exceptionally high detonation performance, including detonation pressure, detonation velocity, and working ability. H₂O generation has a suppressive influence on detonation performance, and ICM-101's gas detonation product also contains a minimal amount of H₂O. When combined with the explosive's oxygen balance, ONC exhibits zero oxygen balance, with its elemental carbon largely transformed into CO₂ and a comparatively low solid C concentration. The higher the CO₂ generated, the greater the detonation heat produced, which also influences its specific kinetic energy. However, since ONC can only be produced in small quantities in laboratories at present, conducting performance studies on it is challenging, and most current ONC performance characteristics are estimated values [73].

In summary, by analyzing the detonation performance in terms of detonation velocity, detonation pressure, detonation heat, specific kinetic energy, and detonation products, it is evident that ONC and ICM-101 exhibit superior detonation performance compared to HMX, making them potential alternatives to traditional high

Fig. 9. (a) Comparison of equilibrium compositions at CJ state for ICM-101, ONC, TNAZ, TATB, CL-20, and HMX; (b) The rank of proportion of gas, specifific kinetic energy, detonation heat, volume of the gas, moles of gas; (c) Proportion of individual gaseous detonation products.

Table 10

The calculated composition of detonation products at CJ state.

| | | | ICM-101 | ONC | | TNAZ | TATB | С | L-20 | HMX |
|--|--|--|--|--------------------------------|---|---|--|---|--|---|
| Density/(g·cm ⁻³) Specifific kinetic energy/(cal·g ⁻¹) Detonation heat/(J·g ⁻¹) Detonation heat/(J·g ⁻¹) ^{exp} Volume of the gas/(cm ³ ·mol ⁻¹) moles of gas Proportion of gas | | 1.99 662.81 7960 13.71 7.51 83.63% | 2.065 783.84 8121 8183.6 [73] 14.05 12.06 98.09% | | 1.84 584.22 6893 6954 [74] 14.48 6.00 87.93% | 1.87 458.75 3998 4241.23 [83] 14.31 7.48 62.79% | 1 6 6 1 1 9 | .965 33.00 730 690 [84] 3.80 3.50 0.61% | 1.89 631.17 6115 6185 [85] 13.44 9.85 90.7% | |
| | VHL | VHL | VHL | EXP [70]. | VHL | EXP [83]. | VHL | EXP [86]. | VHL | EXP [87]. |
| C_2H_6 HCN H_2 NH_3 CH_4 O_2 NO CO CO_2 | 5.26e ⁻⁴ 1.69e ⁻² 9.56e ⁻⁵ 7.83e ⁻⁵ 8.49e ⁻⁴ 0.031 2.50 | $1.00e^{-8}$ $1.00e^{-8}$ $1.00e^{-8}$ $2.30e^{-1}$ $1.35e^{-1}$ $1.26e^{-1}$ 7.64 | 2.59e ⁻³ 0.14 0.02 3.01e ⁻⁷ 8.27e ⁻⁵ 6.68e ⁻² 2.09 | 0.017 0.25 0.14 0.015 | $1.27e^{-4}$ 0.083 $1.01e^{-3}$ $1.00e^{-8}$ $1.39e^{-7}$ $1.62e^{-3}$ 1.56 | 0.014 0.086 0.11 0.026 0.4 1.95 | 1.72e ⁻³ 0.088 1.35e ⁻³ 5.24e ⁻⁵ 7.55e ⁻⁴ 6.28e ⁻² 4.54 | 0.002 0.032 0.27 0.166 0.013 2.02 3.6 | 3.17e ⁻⁴ 0.64 0.25 1.00e ⁻⁸ 1.21e ⁻⁷ 9.72e ⁻³ 2.72 | 0.001 0.008 0.3 0.395 0.039 1.06 1.92 |
| C(s) H ₂ O N ₂ | 1.47 0.97 3.99 | 2.35e ⁻¹ 6.55e ⁻⁷ 3.93 | 8.23e ⁻¹ 1.75 1.93 | Trace present 1.54 1.88 | 4.43 2.87 2.96 | 3.61 2.08 2.34 | 1.40 2.86 5.96 | No trace 2.31 5.61 | 1.01 2.54 3.68 | 0.97 3.18 3.68 |

explosives like HMX. However, the laboratory synthesis of ONC and ICM-101 remains limited due to complexity, high costs, and safety concerns. Future research will focus on optimizing the process and increasing production capacity. TNAZ, whose detonation characteristics are comparable to those of HMX, has a greater oxygen balance, leading to higher detonation products and heat. These characteristics, along with its acceptable thermal stability and sensitivity, suggest that TNAZ could be a viable replacement for HMX. Moreover, TNAZ offers several advantages over well-known explosives. Unlike HMX, TNAZ is compatible with brass, aluminum, steel, and glass, and is soluble in molten TNT. Thus, there remains a promising outlook for its future applications. By analyzing the primary components, specific kinetic energy, detonation heat, gas volume, and moles of gas, it is clear that the main components and the percentage of explosive products are key factors determining an explosive's working ability.

4. Conclusions

This article proposes a novel state equation, VHL, for detonation products. The second-order dimensionless virial coefficients of this equation are derived from the Lennard-Jones potential function theory, while the third and fourth-order dimensionless virial coefficients are calculated based on Baker's theoretical values and obtained through least squares fitting. The higher-order coefficients were optimized using 112 thermodynamic parameters (pressure range: 0.028 GPa-187.26 GPa. temperature range: 1008.1 K-4369.3 K) of the non-polar molecule CH₄ above 1000 K. The VHL state equation provides a reliable and effective analytical tool for accurately describing the high-temperature, medium- and high-pressure thermodynamic states of detonation product gases. The main conclusions are as follows:

- (i) The VHL EOS reliably describes the high-temperature, medium-, and high-pressure states of gas components (CH₄, CO₂, CO, O₂, N₂, H₂, H₂O) in detonation products. Its application in evaluating explosive detonation performance and work capacity demonstrates its broad reliability in thermodynamic analysis.
- (ii) Using the VHL EOS, we predicted the detonation performance of three new explosives (ICM-101, ONC, and TNAZ) and compared it with three typical high explosives (TATB, CL-

20, and HMX) in terms of detonation velocity, detonation pressure, and detonation product composition. Among them, ONC exhibited superior detonation velocity and pressure, outperforming the other explosives. ICM-101's detonation velocity is comparable to that of CL-20, though its detonation pressure is slightly lower. TNAZ's detonation characteristics are similar to those of standard high explosive HMX, but it has a higher oxygen balance, resulting in higher detonation products and heat output.

(iii) The work performed by compressing the medium with explosives, which is denoted by specific kinetic energy. In terms of products, the order of specific kinetic energy is ONC > ICM-101 > CL-20 > HMX > TNAZ > TATB. CL-20 has the biggest share in terms of gas content, whereas mechanical work takes into account both pressure and gas content. As a result, relying just on gas volume cannot accurately reflect the work performed by compressing the medium with explosives. When considering the comprehensive working capacity (mechanical work and detonation heat) of explosives, both ONC and ICM-101 have comparably superior performance.

Currently, our thermodynamic code performs well in predicting the detonation characteristics of CHNOFCl explosives. Future development will expand its applicability, increasing the variety of products and intermediates based on current components and calibrating their state data. We aim to present gas product state equation parameters that can describe a broader temperature range (from several hundred K to several thousand K) and pressure range (from MPa to tens of GPa). However, VHL is a thermochemical code without kinetics, meaning it can only determine detonation performance but not the temporal variation of detonation parameters. The next step will involve creating a database of critical thermodynamic state variables using thermodynamic codes, thereby establishing a thermodynamic-hydrodynamic parameter transfer link.

CRediT authorship contribution statement

Yong Han: Writing – original draft, Methodology, Investigation, Formal analysis, Data curation. **Qin Liu:** Writing – review & editing, Supervision, Resources, Methodology, Conceptualization. **Yingliang Duan:** Writing – review & editing, Software, Funding acquisition, Conceptualization. **Yaqi Zhao:** Supervision, Data curation. **Xinping Long:** Writing – review & editing, Supervision, Project administration, Funding acquisition, Data curation.

Declaration of competing interest

All authors disclosed no relevant relationships.

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Appendix A. Supplementary data

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