NECESSITY OF CONSIDERING CHEMICAL REACTION EQUILIBRIUM IN QUASI-STATIC PRESSURE THERMODYNAMIC MODEL FOR CONFINED TNT EXPLOSIONS

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ABSTRACT

The thermodynamic model is often used to describe the quasi-static pressure with the mass-to-volume ratio (*m/V*) in confined explosions and further derive physical quantities such as adiabatic index based on chemical components and temperature. However, there is a limited study to investigate the necessity of considering reaction equilibrium in the thermodynamic model of TNT confined explosions. This study first conducted a comparative study of thermodynamic model results with the reaction equilibrium considered or not. The results reveal that introducing reaction equilibrium causes a maximum relative difference of less than 20% in quasi-static pressure. However, the *m/V* for solid carbon generation shifts from 0.371 kg/m^3 to 3.850 kg/m^3, the *m/V* corresponding to peak temperature transitions from 0.371 kg/m^3 to 0.680 kg/m^3, and discrepancies in material components and temperature results become increasingly significant when $m/V > 0.1$ kg/m^3. Therefore, models considering reaction equilibrium are essential for calculating physical quantities related to product components and temperature. Then, a simplified calculation method for determining mole numbers of components, temperature and pressure in the quasi-static stage of TNT confined explosion was proposed, which showed good consistency with the thermodynamic model results considering reaction equilibrium. Finally, a practical solution for calculating afterburning energy in numerical models for quasi-static pressure simulation was proposed, which reached great accuracy and achieved a broader applicability range than the two existing methods. The research contributes to a theoretical understanding of the necessity for considering reaction equilibrium in the thermodynamic model, as well as achieving the rapid calculation of thermodynamic parameters in the quasi-static stage and accurate simulation of numerical models.

Keywords: chemical reaction equilibrium, confined explosion, quasi-static pressure, thermodynamic model.

1 INTRODUCTION

The explosive detonation in confined space typically exhibits shockwave convergence at space corners and significant thermal effects. Structural damage arises from both the reflected pressure during wave propagation and the quasi-static pressure after the flow field stabilizes. For negative oxygen balance explosives like TNT, detonation products can further react with oxygen in the confined space, resulting in the afterburning effect, which increases the temperature within space and the load on internal walls [1], [2]. The quasi-static stage of confined explosions is characterized by a long duration, with the quasi-static pressure being notably affected by the afterburning effect and strongly influencing the structural response [3], [4]. Therefore, accurately calculating the thermodynamic state in the quasi-static stage of confined explosions is crucial for designing structures to resist internal explosions and assessing structural damage.

Currently, TNT is widely used in structural anti-explosion research and blast-resistant engineering design. Researchers have conducted a series of experimental and numerical studies for TNT confined explosions. Existing experimental research primarily involves

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conducting explosion experiments in spherical or cylindrical fully confined containers with varying mass-to-volume ratios m/V. The explosives were mainly placed at the space centre, and piezoelectric, piezoresistive, and thermocouple sensors on internal walls were used to measure pressure and temperature during the quasi-static stage, respectively. Fig. 1 presents quasi-static pressure obtained from experiments [2], [5]–[12] in comparison with the UFC curve [13] derived from experimental fitting. The experimental results demonstrate good agreement with the UFC curve. Existing numerical studies primarily adopt combustion models [14] or incorporating afterburn energy into the equation of state [1], [15] to simulate afterburning effects and have demonstrated that numerical methods such as combustion models can effectively replicate both wall loadings and structural damage observed in experiments.

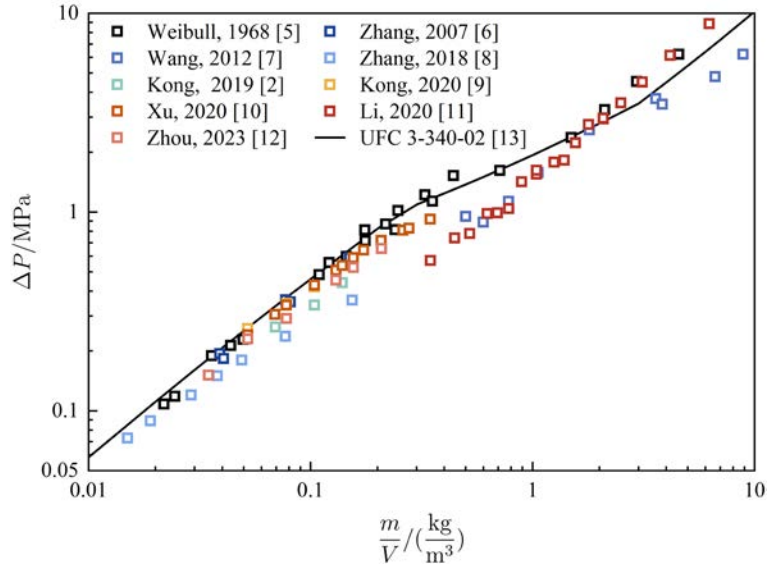


Figure 1: Quasi-static pressure from TNT confined explosion experiments and the corresponding UFC curve.

To accurately calculate the thermodynamic parameters in the quasi-static stage of confined explosions, thermodynamic models based on the assumptions of constant-volume processes and complete reactions have been proposed and widely adopted. The thermodynamic models can effectively capture actual chemical processes and calculate parameters such as mole numbers of components, temperature, pressure, and gas adiabatic index in the quasi-static stage. Kinney et al. [16] proposed a thermodynamic model that incorporates chemical reaction equilibrium, which demonstrated good agreement between the calculated pressure and experimental results. However, the model requires iteration of both temperature and mole numbers of components to ensure reaction equilibrium, and the computational stability depends on the selection of initial values, making the calculation relatively complex. Feldgun et al. [17] proposed a simplified thermodynamic model without chemical reaction equilibrium. The model also shows good agreement with experimental pressure results and only requires temperature iteration, making the solution process simpler, leading to its widespread application in determining gas adiabatic indices and energy release

parameters for theoretical and numerical simulations [15], [17]. Nevertheless, the model cannot consider the influence of temperature on reaction equilibrium.

In summary, pressure results obtained from thermodynamic models with and without the reaction equilibrium for confined TNT explosions exhibit good agreement with experiment pressure results and enable the derivation of physical parameters including chemical compositions, temperature, and adiabatic index. However, there is a limited study to conduct a systematic investigation to consider the necessity of introducing reaction equilibrium in the thermodynamic model for different physical parameters. Considering that thermal effects in confined explosions may alter reaction equilibrium, thermodynamic parameters including temperature and adiabatic coefficients from models without chemical equilibrium could deviate significantly from those obtained through reaction equilibrium analysis, thereby impeding accurate representation of real physical processes in theoretical or numerical models. This study first conducted a comparative analysis of thermodynamic model results with the reaction equilibrium considered or not to demonstrate the necessity of considering reaction equilibrium for different physical quantities. Subsequently, a simplified calculation method was proposed to determine mole numbers of product compositions, temperature, and pressure in the quasi-static stage of TNT confined explosions when reaction equilibrium is accounted for. Finally, a practical solution was proposed to determine the value of additional afterburn energy for numerical modelling, thereby achieving effective quasi-static pressure simulation.

2 THE NECESSITY OF CONSIDERING REACTION EQUILIBRIUM IN THE THERMODYNAMIC MODEL

To investigate the effect of reaction equilibrium on thermodynamic model results, the results of thermodynamic models with and without reaction equilibrium were compared based on a unified model solution framework, and then the necessity of considering reaction equilibrium was demonstrated.

2.1 The framework for solving thermodynamic models

Fig. 2 shows the framework for solving thermodynamic models in this study. The solution framework was utilized to ensure that the differences between two model results are solely attributed to the consideration of reaction equilibrium or not. The initial step for solving models involves inputting the m/V and setting the initial value of the adiabatic combustion temperature T_{ad}. For the thermodynamic model without considering reaction equilibrium, the number of moles of the product can be calculated directly based on the chemical reaction equation, where elemental mass conservation is inherently satisfied. The mass conservation equation for element e can be expressed as:

$$\sum_k x_k l_{e,k} = \sum_j x_j l_{e,j}. \tag{1}$$

$l_{e,k}$ and $l_{e,j}$ represent the numbers of element e atoms in the kth reactant and jth product component, respectively, while x_k and x_j denote the molar coefficients of the kth reactant and jth product in the equation. For the thermodynamic model considering chemical equilibrium, initial mole numbers n_i for each product i were first estimated. Then, the equilibrium constant K_p at temperature T_{ad} was calculated. The residuals of the mass conservation equations were computed, and n_i were iteratively adjusted until the mass conservation equations converge. After the mole numbers of products are determined, T_{ad} was iterated based on energy conservation until energy convergence was achieved:

$$H_{\mathrm{reac}} - H_{\mathrm{prod}} - R\left(n_{\mathrm{reac}}T_{\mathrm{init}} - n_{\mathrm{prod}}T_{\mathrm{ad}}\right) = 0. \tag{2}$$

H_{reac} and H_{prod} are the standard formation enthalpies of the reactants and products, respectively, while n_{reac} and n_{prod} denote the total molar amounts of gaseous reactants and products. After T_{ad} was determined, the confined-space overpressure was calculated using the ideal gas law:

$$\Delta p = \frac{n_{\mathrm{prod}}RT_{\mathrm{ad}}}{1\ \mathrm{mol} \cdot V_{\mathrm{prod,gas}}} - p_0. \tag{3}$$

In the above equation, p_0 denotes the initial atmospheric pressure, and $V_{\mathrm{prod,gas}}$ represents the spatial volume occupied by the gaseous products after the reaction is completed.

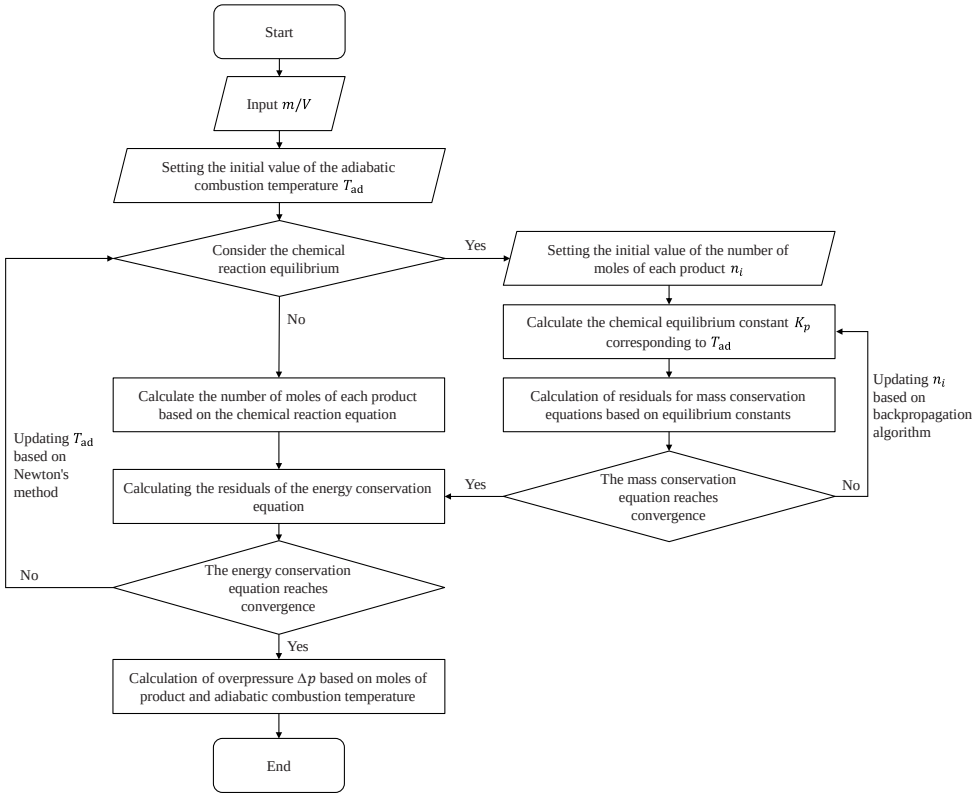


Figure 2: The solution framework of thermodynamic models.

During the solving process, Newton's method was used to solve T_{ad} until the residual remained below 0.1 K, while the backpropagation algorithm was employed to iterate n_i until its residual remained below 10^{-6} mol. By initializing the temperature at 500 K and using the n_i values from the non-equilibrium model as initial values for the model with chemical equilibrium, the stability of both algorithms can be effectively ensured.

2.2 The thermodynamic model without reaction equilibrium

The thermodynamic model without reaction equilibrium employs a simplified model proposed by Feldgun et al. [17] with several modifications. Define Φ as the molar number of air per unit mole of TNT:

$$\Phi\left(\frac{m}{V}\right)=\frac{n_{\mathrm{Air}}}{n_{\mathrm{TNT}}}=\frac{p_0 M_{\mathrm{TNT}}}{RT_{\mathrm{init}}}\left(\frac{1}{m/V}-\frac{1}{\rho_{\mathrm{TNT}}}\right)=9.284\left(\frac{1}{m/V}-\frac{1}{1630}\right). \tag{4}$$

In the above equation, n_{Air} and n_{TNT} represent the molar quantities of air and TNT, respectively. M_{TNT}= 0.227 kg/mol denotes the molar mass of TNT, and ρ_{TNT} = 1630 kg/m^3 is the density of TNT. Since the complete combustion of one mole of TNT requires 5.25 moles of oxygen, the condition for achieving stoichiometric combustion using ambient air (where oxygen constitutes 21% by volume) is expressed as 0.21Φ = 5.25. Solving this equation yields the transitional mass-to-volume ratio $(m/V)_{\mathrm{trans},1}$ = 0.371 kg/m^3. In this way, the reaction equation for confined explosion can be derived. When m/V < 0.371 kg/m^3, it is assumed that the explosive undergoes complete reaction, leading to the following expression:

$$\begin{gathered}\mathrm{C_7H_5N_3O_6}+\Phi(\,0.21\mathrm{O_2}+0.79\mathrm{N_2})\\(0.79\Phi+1.5)\mathrm{N_2}+(0.21\Phi-5.25)\mathrm{O_2}+2.5\mathrm{H_2O}+7\mathrm{CO_2}.\end{gathered} \tag{5}$$

When $m/V \geq$ 0.371 kg/m^3, under the assumption that all oxygen participates in the combustion process, the proportion of explosive undergoing complete combustion is given by $\mu = 0.21\Phi/5.25 = \Phi/25$, while the remaining fraction undergoes no-afterburning detonation. The reaction equations can be expressed as:

$$\begin{gathered}\mathrm{C_7H_5N_3O_6}+\Phi(\,0.21\mathrm{O_2}+0.79\mathrm{N_2})\\(0.79\Phi+1.5)\mathrm{N_2}+2.5\mathrm{H_2O}+7\mu\mathrm{CO_2}+3.5(1-\mu)\mathrm{CO}+3.5(1-\mu)\mathrm{C}.\end{gathered} \tag{6}$$

By incorporating eqns (5) and (6) into the solution framework introduced in Section 2.1, the model without reaction equilibrium can be solved.

2.3 The thermodynamic model with reaction equilibrium

The thermodynamic model with reaction equilibrium mainly employs the model proposed by Kinney et al. [16]. Assuming that the reaction products from confined TNT detonation comprise carbon (C), seven gaseous molecular species (CO, CO_2, O_2, H_2, H_2O, N_2, NO), and four free radical species (OH, H, O, N). The reaction equations can be expressed as

$$\begin{gathered}\mathrm{C_7H_5N_3O_6}+\Phi(\,0.21\mathrm{O_2}+0.79\mathrm{N_2})\\n_{\mathrm{C}}\mathrm{C}+n_{\mathrm{CO}}\mathrm{CO}+n_{\mathrm{CO_2}}\mathrm{CO_2}+n_{\mathrm{O_2}}\mathrm{O_2}+n_{\mathrm{H_2}}\mathrm{H_2}+n_{\mathrm{H_2O}}\mathrm{H_2O}+n_{\mathrm{N_2}}\mathrm{N_2}+n_{\mathrm{NO}}\mathrm{NO}\\+n_{\mathrm{OH}}\mathrm{OH}+n_{\mathrm{H}}\mathrm{H}+n_{\mathrm{O}}\mathrm{O}+n_{\mathrm{N}}\mathrm{N}.\end{gathered} \tag{7}$$

The equation system contains 12 variables, thus requiring 12 independent equations for solution. Based on the mass conservation, four governing equations can be established:

$$\begin{cases} n_{\mathrm{C}} + n_{\mathrm{CO}} + n_{\mathrm{CO_2}} = 7 \\ 2n_{\mathrm{H_2}} + 2n_{\mathrm{H_2O}} + n_{\mathrm{OH}} + n_{\mathrm{H}} = 5 \\ 2n_{\mathrm{N_2}} + n_{\mathrm{NO}} + n_{\mathrm{N}} = 3 + 2 \cdot 0.79\Phi \\ n_{\mathrm{CO}} + 2n_{\mathrm{CO_2}} + 2n_{\mathrm{O_2}} + n_{\mathrm{H_2O}} + n_{\mathrm{NO}} + n_{\mathrm{OH}} + n_{\mathrm{O}} = 6 + 2 \cdot 0.21\Phi. \end{cases} \tag{8}$$

The remaining eight equations are established based on chemical equilibrium principles. Assuming that the following eight chemical reactions occur during the combustion process, and all components reach equilibrium upon completion of the reactions:

$$\mathrm{H_2} \rightleftharpoons 2\mathrm{H}, \qquad K_1 = \frac{p_{\mathrm{H}}^2}{p_{\mathrm{H_2}}}. \tag{9}$$

$$\mathrm{O_2} \rightleftharpoons 2\mathrm{O}, \qquad K_2 = \frac{p_{\mathrm{O}}^2}{p_{\mathrm{O_2}}}. \tag{10}$$

$$\mathrm{N_2} \rightleftharpoons 2\mathrm{N}, \qquad K_3 = \frac{p_{\mathrm{N}}^2}{p_{\mathrm{N_2}}}. \tag{11}$$

$$\mathrm{H_2O} \rightleftharpoons \mathrm{H_2} + 0.5\mathrm{O_2}, \qquad K_4 = \frac{p_{\mathrm{H_2}}^2 p_{\mathrm{O_2}}^{0.5}}{p_{\mathrm{H_2O}}}. \tag{12}$$

$$\mathrm{H_2O} \rightleftharpoons \mathrm{OH} + 0.5\mathrm{H_2}, \qquad K_5 = \frac{p_{\mathrm{OH}} p_{\mathrm{H_2}}^{0.5}}{p_{\mathrm{H_2O}}}. \tag{13}$$

$$\mathrm{H_2O} + 0.5\mathrm{N_2} \rightleftharpoons \mathrm{H_2} + \mathrm{NO}, \qquad K_6 = \frac{p_{\mathrm{H_2}} p_{\mathrm{NO}}}{p_{\mathrm{H_2O}} p_{\mathrm{N_2}}^{0.5}}. \tag{14}$$

$$\mathrm{CO_2} \rightleftharpoons \mathrm{CO} + 0.5\mathrm{O_2}, \qquad K_7 = \frac{p_{\mathrm{CO}} p_{\mathrm{O_2}}^{0.5}}{p_{\mathrm{CO_2}}}. \tag{15}$$

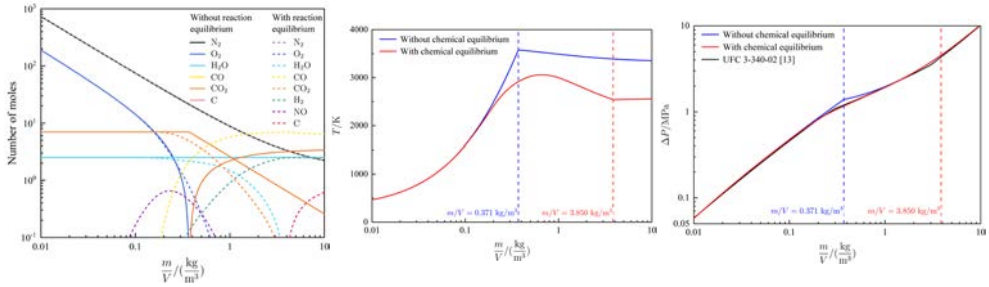
$$\mathrm{CO} \rightleftharpoons \mathrm{C} + 0.5\mathrm{O_2}, \qquad K_8 = \frac{p_{\mathrm{O_2}}^{0.5}}{p_{\mathrm{CO}}}. \tag{16}$$

In the above equations, p_i represents the dimensionless partial pressure of product i, and K_1–K_8 represent the equilibrium constants for the respective reactions, which can be calculated based on the chemical kinetics database [18]. By solving eqns (8)–(16) and incorporating eqn (7) into the solution framework introduced in Section 2.1, the model with reaction equilibrium can be solved. The carbon generation point of the model can be determined to be 3.850 kg/m^3 using the bisection method.

2.4 Result comparison of the models

Fig. 3 compares the results of product components, temperature, and pressure derived from the two models within 0.01 kg/m^3 ≤ m/V ≤ 10 kg/m^3. Figs 3(a) and 3(b) indicate that discrepancies in components and temperature emerge when m/V > 0.1 kg/m^3 and become pronounced with increasing m/V. The introduction of reaction equilibrium shifts the m/V for carbon generation from 0.371 kg/m^3 to 3.850 kg/m^3, reduces the peak adiabatic flame temperature from 3578 K to 3060 K, and alters the m/V corresponding to maximum temperature from 0.371 kg/m^3 to 0.680 kg/m^3. Fig. 3(c) shows that pressure differences between models remain insignificant when m/V < 0.1 kg/m^3 or m/V > 1 kg/m^3. At

m/V = 0.371 kg/m^3, the model results without reaction equilibrium (1.394 MPa) exhibit a maximum relative error of 19.3% compared to the results from the reaction equilibrium model (1.168 MPa).



(a) (b) (c)

Figure 3: Model results comparison. (a) Product components; (b) Temperature; (c) Pressure.

The main reason for differences between two model results in product components and temperature is that as the m/V ratio increases, the elevated T_{ad} drives the dissociation reactions of CO_2 and H_2O toward the forward direction. Consequently, the m/V corresponding to CO generation occurs earlier than the thermodynamic model without reaction equilibrium, while the m/V corresponding to O_2 depletion is delayed. Concurrently, the dissociation reactions also increase the proportion of partially combusted products such as CO and H_2 in space. However, since the overpressure is proportional to both n_{prod} and T_{ad}, the influence of product components and temperature is not significantly reflected in the pressure result. Given that the components and temperature in model results exhibit significant differences when m/V > 0.1 kg/m^3, the model considering reaction equilibrium is a more rational choice for calculating physical quantities directly related to components and temperature.

3 A SIMPLIFIED CALCULATION METHOD FOR DETERMINING COMPONENTS, TEMPERATURE, AND PRESSURE

To facilitate engineering application of the thermodynamical model with reaction equilibrium, this section presents a simplified method for determining the mole numbers of product composition, temperature, and pressure in the quasi-static stage of TNT confined explosions based on the thermodynamic model result and symbolic regression technique.

3.1 Components

Neglecting the free radical and NO terms in chemical reaction products, list the mass conservation equations of CHON elements for the remaining seven products (C, CO, CO_2, O_2, H_2, H_2O, N_2):

$$\begin{cases} 2n_{\mathrm{N_2}} = 3 + 2 \cdot 0.79\Phi \\ n_{\mathrm{C}} + n_{\mathrm{CO}} + n_{\mathrm{CO_2}} = 7 \\ 2n_{\mathrm{H_2}} + 2n_{\mathrm{H_2O}} = 5 \\ n_{\mathrm{CO}} + 2n_{\mathrm{CO_2}} + 2n_{\mathrm{O_2}} + n_{\mathrm{H_2O}} = 6 + 2 \cdot 0.21\Phi. \end{cases} \tag{17}$$

From eqn (17), the expression for $n_{\mathrm{N_2}}$ can be derived:

$$n_{\mathrm{N_2}}/\mathrm{mol} = 1.5 + 0.79\Phi \approx \frac{7.34}{m/V} + 1.50. \tag{18}$$

The mass conservation equations for elements C, H, and O involve six unknowns. To make the equations solvable, the molar quantities of at least three products must be known. By applying symbolic regression algorithm to fit the thermodynamic model results and incorporating eqns (5) and (6), the following formula can be derived:

$$n_{\mathrm{C}}/\mathrm{mol} = \begin{cases} 0, & 0.01\ \mathrm{kg/m^3} \le m/V < 3.85\ \mathrm{kg/m^3} \\ 1 - \frac{3.85}{m/V}, & 3.85\ \mathrm{kg/m^3} \le m/V \le 10\ \mathrm{kg/m^3} \end{cases}. \tag{19}$$

$$n_{\mathrm{H_2}}/\mathrm{mol} = \begin{cases} 3.41 \cdot \exp\left(-\frac{1.28}{m/V}\right), & 0.01\ \mathrm{kg/m^3} \le m/V < 3.85\ \mathrm{kg/m^3} \\ 2.5, & 3.85\ \mathrm{kg/m^3} \le m/V \le 10\ \mathrm{kg/m^3} \end{cases}. \tag{20}$$

$$n_{\mathrm{O_2}}/\mathrm{mol} = \begin{cases} \frac{1.95}{m/V} - 5.25, & 0.01\ \mathrm{kg/m^3} \le m/V < 0.25\ \mathrm{kg/m^3} \\ 2.97 \cdot \frac{0.0018^{m/V}}{m/V}, & 0.25\ \mathrm{kg/m^3} \le m/V < 0.64\ \mathrm{kg/m^3} \\ 0, & 0.64\ \mathrm{kg/m^3} \le m/V \le 10\ \mathrm{kg/m^3} \end{cases}. \tag{21}$$

After n_{C}, $n_{\mathrm{H_2}}$, $n_{\mathrm{O_2}}$ are determined, the expressions for the mole numbers of H_2O, O, O_2 can be derived using eqn (17):

$$n_{\mathrm{H_2O}}/\mathrm{mol} = 2.5 - n_{\mathrm{H_2}}. \tag{22}$$

$$n_{\mathrm{CO_2}}/\mathrm{mol} = \frac{3.90}{m/V} - 1 + n_{\mathrm{C}} - n_{\mathrm{H_2O}} - 2n_{\mathrm{O_2}}. \tag{23}$$

$$n_{\mathrm{CO}}/\mathrm{mol} = -\frac{3.90}{m/V} + 8 - 2n_{\mathrm{C}} + n_{\mathrm{H_2O}} + 2n_{\mathrm{O_2}}. \tag{24}$$

Eqn (24) shows a relatively significant cumulative error than eqns (22) and (23) compared with the thermodynamic mode result. To address this problem, n_{CO} was refitted with piecewise functions and symbolic regression:

$$n_{\mathrm{CO}}/\mathrm{mol} = \begin{cases} 0, & 0.01\ \mathrm{kg/m^3} \le m/V < 0.18\ \mathrm{kg/m^3} \\ \exp[1.97 - (2.39 \cdot m/V)^{-1.7}], & 0.18\ \mathrm{kg/m^3} \le m/V < 3.85\ \mathrm{kg/m^3} \\ 7, & 3.85\ \mathrm{kg/m^3} \le m/V \le 10\ \mathrm{kg/m^3} \end{cases}. \tag{25}$$

Comparison with thermodynamic model results shows that the relative error of the proposed eqns (18)–(23) and (25) for calculating the number of moles of each component is less than 15% when the molar quantities exceed 0.7 mol.

3.2 Temperature

T_{ad} was fitted using symbolic regression:

$$T_{\mathrm{ad}}/\mathrm{K} = 2541 + \frac{1045.5}{2.22^{m/V}} - \frac{3304.3}{292.3^{m/V}}. \tag{26}$$

The relative error of eqn (26) to the thermodynamic model result is less than 3% in 0.01 kg/m^3 ≤ *m*/*V* ≤ 10 kg/m^3.

3.3 Pressure

To calculate the quasi-static pressure, assuming the volume occupied by solid carbon in the products is negligible, the expression for $V_{\text{prod,gas}}$ can be simplified to:

$$V_{\text{prod,gas}}/(\text{m}^3/\text{mol}) \approx \frac{M_{\text{TNT}}}{m/V} = \frac{0.227}{m/V}. \tag{27}$$

n_{prod} can be expressed as

$$n_{\text{prod,gas}}/\text{mol} \approx n_{\text{CO}} + n_{\text{CO}_2} + n_{\text{H}_2} + n_{\text{H}_2\text{O}} + n_{\text{N}_2} + n_{\text{O}_2} \approx \frac{7.34}{m/V} + 11 - n_{\text{C}} + n_{\text{O}_2}. \tag{28}$$

Based on the expressions for n_C and n_{O_2}, n_{prod} can be determined. After obtaining $V_{\text{prod,gas}}$, n_{prod}, and T_{ad}, the quasi-static pressure can be calculated using eqn (3). The calculated values exhibit relative errors of less than 4% compared to thermodynamic model results and less than 8% relative to UFC specification curves within 0.01 kg/m^3 ≤ *m*/*V* ≤ 10 kg/m^3.

Finally, the limitations of the simplified method should also be noted. The algorithm accounts for only a limited number of chemical species, so the results should be treated as approximate for actual product compositions within the studied component range. Additionally, while the framework is theoretically applicable to other explosives, the current formulations are validated only for TNT.

4 A PRACTICAL SOLUTION FOR QUASI-STATIC PRESSURE SIMULATION CONSIDERING AFTERBURNING ENERGY

By incorporating afterburn energy into the equation of state for detonation products, the afterburning process in confined explosions can be effectively simulated without directly resolving chemical reactions, thereby significantly reducing the computational costs of numerical simulations. The magnitude of the afterburn energy directly determines the quasi-static pressure in the numerical model. Consequently, this section proposes a theoretical and practical method for determining the afterburn energy in confined explosion simulations.

4.1 Determination of the afterburning energy

In current numerical simulations of confined explosions, the air is typically modelled with the ideal gas equation of state:

$$p = (\gamma - 1)\rho_{\text{Air}} e_{\text{Air}}. \tag{29}$$

In eqn (29), γ denotes the adiabatic index, ρ_{Air} denotes the density of the air, and e_{Air} is the internal energy of the air per unit mass. The explosive materials are generally simulated with the JWL equation:

$$p = A\left(1 - \frac{\omega}{R_1\theta}\right)\exp(-R_1\theta) + B\left(1 - \frac{\omega}{R_2\theta}\right)\exp(-R_2\theta) + \omega\rho e_{\text{explosive}}. \tag{30}$$

In eqn (30), $\theta = \rho_{\text{explosive}}/\rho$, $\rho_{\text{explosive}}$ is the initial density of the explosive, ρ is the density of the detonation products, A, B, R_1, R_2, ω are constants related to the explosive material, and $e_{\text{explosive}}$ is the internal energy of the explosive per unit mass. To simulate the development of

afterburning energy, $e_{\text{explosive}}$ can be decomposed into the internal energy induced by detonation e_{det} and augmented by afterburning e_{ab}. The afterburning-induced internal energy increases gradually over time and eventually reaches a steady-state value E_{ab} that represents the afterburning energy per unit mass of the explosive [1], [15], [20]. The JWL equation considering the afterburning energy can be written as:

$$p = A\left(1 - \frac{\omega}{R_1\theta}\right)\exp(-R_1\theta) + B\left(1 - \frac{\omega}{R_2\theta}\right)\exp(-R_2\theta) + \omega\rho(e_{\text{det}} + e_{\text{ab}}). \quad (31)$$

To facilitate the derivation of E_{ab} under a given quasi-static pressure, assuming that the afterburn energy is instantaneously released in the numerical model. Since the assumption does not alter the total energy of the confined flow field, it does not influence the theoretical quasi-static pressure corresponding to the steady-state flow field [17], [18]. Based on this assumption, e_{ab} in the initial state equals E_{ab}, and $e_{\text{det}} = E_{\text{det}}$ which represents the detonation energy per unit mass of the explosive. The energy conservation equation of the flow field under this assumption can be expressed as:

$$\frac{p_0}{\gamma - 1}\left(1 - \frac{m/V}{\rho_{\text{TNT}}}\right) + (E_{\text{det}} + E_{\text{ab}})\frac{m}{V} = \frac{p_{\text{qs}}}{\gamma - 1}\cdot\frac{V_{\text{Air}}}{V} + \left[p_{\text{qs}} - A\left(1 - \frac{\omega}{R_1\theta}\right)\exp(-R_1\theta) - B\left(1 - \frac{\omega}{R_2\theta}\right)\exp(-R_2\theta)\right]\cdot\frac{m/V}{\omega\rho}. \quad (32)$$

In eqn (32), p_0 is the initial ambient pressure, p_{qs} is the quasi-static pressure from the thermodynamic model or the UFC standard, and V_{air} is the volume occupied by air. Since there is no mass exchange between the detonation products and the air, ρ can be expressed as

$$\rho = \frac{m}{V - V_{\text{Air}}} = \frac{m/V}{1 - V_{\text{Air}}/V}. \quad (33)$$

Assuming that after the afterburning reaction, the air and detonation products possess identical densities, which is consistent with the quasi-static flow characteristic of the numerical model result. Under this condition, the following equation can be formulated:

$$\frac{\rho_{\text{Air}}\left(1 - \frac{m/V}{\rho_{\text{explosive}}}\right)}{V_{\text{Air}}/V} = \frac{m/V}{1 - V_{\text{Air}}/V}. \quad (34)$$

By solving eqns (31)–(34), the value of E_{ab} under a specified p_{qs} can be determined.

4.2 Validation of the proposed solution

The proposed method was validated based on numerical simulation. The numerical model is a 1/8 symmetric model constructed based on LS-Dyna with the ALE (arbitrary Lagrange–Euler) algorithm in which a spherical TNT explosive was detonated at the centre of a 1 m × 1 m × 1 m confined space, as shown in Fig. 4. The *m/V* ratio was set as 0.01, 0.05, 0.1, 0.5, 1, 5, and 10 kg/m^3 in different cases, respectively. The equations of state EOS for air and the explosive were eqn (29) and (31), respectively, with material parameters detailed in Table 1. The average pressure at the wall's normal reflection point during the 20–25 ms after the explosion was taken as the quasi-static pressure. The initial internal energy of TNT was set as $E_{\text{det}} + E_{\text{ab}}$, and E_{ab} was determined based on eqns (31)–(34). The mesh size employed is 0.30 cm, which is sufficient for model result convergence in all cases.

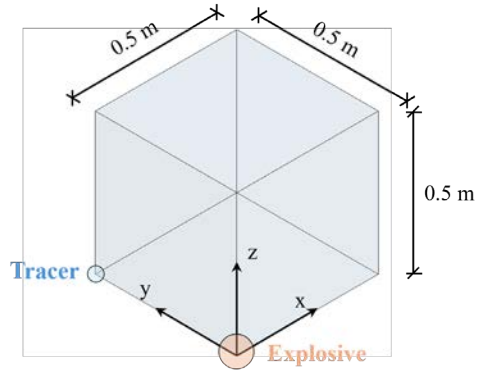


Figure 4: Quasi-static pressure from TNT confined explosion experiments and the corresponding UFC curve.

Table 1: Material parameters of the air and TNT for numerical simulation.

Material	Parameter	Value	Parameter	Value
Air	ρ_{Air}	1.2929 kg/m^3	γ	1.4
	p_0	0.101 MPa		
TNT	ρ_{TNT}	1630 kg/m^3	A	371.25 GPa
	B	3.231 GPa	R_1	4.15
	R_2	0.95	ω	0.30
	E_{det}	4294.5 KJ/kg		

Table 2 compares the accuracy of the proposed method and the simplified method proposed by Hernandez et al. [21] and the method proposed by Zhou et al. [15]. Hernandez provided an empirical method for calculating E_{ab}, while Zhou's method was proposed based on the ideal gas equation. As shown in Table 2, the proposed method achieves an absolute relative error within 3% in all cases. The relative error of Hernandez's method measured in this study does not fully align with the results reported in Hernandez et al. [21]. This discrepancy arises primarily because Hernandez's method cannot account for the influence of equation-of-state (EOS) parameter selection on the results, and the EOS parameters used

Table 2: Accuracy comparison of quasi-static pressure derived from different methods.

m/V	Relative error of the proposed method	Relative error of Hernandez's method	Relative error of Hernandez et al.'s method from [21]	Relative error of Zhou's method
0.01	+0.01%	−6.22%	/	+34.89%
0.05	−1.18%	+0.76%	+1.41%	+16.38%
0.1	−1.24%	+4.63%	+7.65%	+11.20%
0.5	+0.15%	+8.82%	−3.42%	+4.15%
1	+1.03%	+13.42%	+5.23%	+0.71%
5	+2.84%	+35.93%	+5.03%	−6.46%
10	+2.59%	/	/	−8.50%

for simulating air and the explosive in the two studies differ. Although the methods from Hernandez or Zhou achieve lower relative errors in some cases, they fail to maintain satisfactory accuracy across the entire *m/V* range investigated, demonstrating that the proposed method exhibits broader applicability compared to the two existing methods.

5 CONCLUSIONS

This study first conducted a comparative analysis to investigate the necessity of considering reaction equilibrium in the quasi-static pressure thermodynamic model for TNT confined explosion. Then, a simplified calculation method was proposed to determine mole numbers of product compositions, temperature, and pressure in the quasi-static stage. Finally, a practical solution was proposed for determining additional afterburning energy in numerical models for accurate quasi-static pressure simulation. Here are the main conclusions:

1. The thermodynamic model considering reaction equilibrium is a more rational choice for calculating physical quantities related to components and temperature. The introduction of reaction equilibrium in the thermodynamic model shifts the *m/V* for carbon generation from 0.371 kg/m^3 to 3.850 kg/m^3 and reduces the peak temperature from 3578 K to 3060 K. The discrepancies in product components and temperature results become increasingly significant when $m/V > 0.1$ kg/m^3.
2. The proposed simplified calculation method shows good consistency with the thermodynamic model results considering reaction equilibrium. Within the range of $0.01 \text{ kg/m}^3 \leq m/V \leq 10 \text{ kg/m}^3$, the simplified method yields relative errors of less than 15% in the mole number of each component when the mole number exceeds 0.7 mol. The relative errors for temperature and pressure remain below 3% and 4%, respectively.
3. The proposed practical solution for calculating the afterburning energy in numerical models achieves an absolute relative error of quasi-static pressure within 3% and shows a broader applicability range than the two existing methods in the range of $0.01 \text{ kg/m}^3 \leq m/V \leq 10 \text{ kg/m}^3$.

Research in future should conduct additional experiments to measure parameters like quasi-static temperature and heat of detonation in confined explosions across varying *m/V*, which will help validate the applicability scope of the thermodynamic model based on the complete reaction assumption from multiple perspectives.

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