A High-Order Relaxation Method for Condensed Explosives Detonation

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Abstract—**The paper gives a high-order precision and high resolution scheme for the governing equations of the detonation in condensed explosives. Based on the relaxation approximation, the nonlinear governing equations of condensed explosives detonation are transformed into linear relaxation systems, in which it can avoid solving Riemann problem and calculating the Jacobian matrix of nonlinear flux, and it is not necessary to split the source term of chemical reaction law. A fifth-order WENOM (Mapped Weighted Essentially Non-Oscillatory) reconstruction in space discretization and a fifth-order IMEX (IMplicit-EXplicit) scheme of linear multistep methods with monotonicity and TVB (Total Variation Boundedness) in time discrtiezation are utilized. The proposed method is applied to numerically simulate the steady structure of a one-dimensional planar detonation wave and the unsteady propagation of a one-dimensional spherically divergent detonation wave in explosives PBX-9502. The test cases demonstrate that the proposed method can obtain very satisfactory numerical results in terms of accuracy and resolution.**

Keywords-relaxation method; detonation wave; condensed explosives; high-order precision scheme; high resolution scheme

I. INTRODUCTION

The design of complex engineering devices that use high explosives to do useful and controlled work requires the capability to numerically simulate detonation with high fidelity [1]. In the past several decades, the Lagrangian method [1] is in the majority because of its nature character to treat with the interface of multimaterial. However, in the recent decade, more attention has been paid to the Eulerian method due to its following advantages: 1) to well preserve conservation of the total energy due to usually using finite volume discretization; 2) to commonly sharpen the discontinuity of detonation wave due to using high resolution scheme; 3) to easily construct high-order precision in temporal and spatial discretization; 4) to conveniently utilize small meshes to improve accuracy due to employing fixed space grids. Representative works show some fruits of Eulerian method [2]-[5]: using second-order Godunov scheme, adopting simple equation of state (usually perfect gas formulation) and chemical reaction model, employing split way to treat with the chemical source term.

The governing equations of the detonation in condensed explosives are nonlinear hyperbolic conservation system with strongly stiff reaction source term of chemical reaction and complex equation of state. It is the strong stiffness of reaction source term and the complexity of equation of state that brings enormous difficulty to numerically compute the detonation by high-order precision and high resolution scheme.

When strongly stiff source term is discretized, insufficient spatial/temporal resolution may cause an incorrect propagation speed of discontinuities. H. C. Yee [6][7] points out that the phenomenon of wrong propagation speed of discontinuities is connected with the smearing of the discontinuities caused by the discretization of the advection term. The smearing introduces a nonequilibrium state into the calculation, thus as soon as a nonequilibrium value is introduced in this manner, the source term turns on and immediately restores equilibrium, while at the same time shifting the discontinuity to a cell boundary. The analysis shows that the degree of wrong propagation speed of discontinuities is highly dependent on the overall amount of numerical dissipation contained by the numerical scheme. So, excellent shock-capturing scheme for detonation wave discontinuity must possess the high resolution, namely low numerical dissipation. At present, most high resolution schemes have utilized Riemann solver [8] based on simple equation of state, such as the perfect gas with gamma law [9]. However, unreacted solid component and gas product component of detonation in condensed explosives usually utilize some complex equation of state [10], such as Jones-Wilkins-Lee (JWL), HOM, BKW, Davis, extremely, SESAME data library, and so on, also, the temperature and pressure of mixing zone in chemical reaction needs to iterative operation when generally considering pressure and temperature as equilibrium state. Apparently, the high resolution scheme based on Riemann solver is difficult to construct numerically flux about the flow equations of detonation in condensed explosives. In order to capture exactly the shock discontinuity, besides the high resolution in spatial discretization, the high resolution in temporal discretization is very necessary. Hundsdorfer et al. [11] show that the unsplitting explicit and implicit scheme is more reliable: the advection term adopts explicit discretization, and the source term adopts implicit discretization.

Recently, developing a relaxation method is an effective strategy to numerically solve hyperbolic conservation system [12]-[15]. The main idea of the relaxation method is to transform the nonlinear hyperbolic conservation system into linear hyperbolic relaxation equations by means of relaxation approximation. When the relaxation rate tends to zero and

the subcharacteristic condition is satisfied, the solution of the relaxation equations converges to the solution of the original hyperbolic conservation system. In comparison with upwind schemes such as the Godunov scheme, relaxation method does not require the Riemann Solver and the computation of its Jacobians. These features make the relaxation method particularly suitable for those systems where the Riemann problem is difficult to solve or when it is not possible to perform analytical expression for Jacobians. The relaxation method is gradually applied to gasdynamics [16], shallow water motion [17], multimatierial and multicomponent flow [18], magnetohydrodynamic [19].

In this paper, the relaxation method is applied to numerically simulate the typical detonation problem about the condensed explosives. After the nonlinear governing equations of the condensed explosives are transformed into linear relaxation equations, an improved fifth-order WENOM [20] is utilized to spatially discretize and a fifth-order IMEX scheme of linear multistep methods with general monotonicity and boundedness properties is utilized to temporally discretize [11]. The numerical examples about one-dimensional detonation wave in explosives PBX-9502 demonstrate that our method has high accuracy and high resolution properties.

The paper is organized as follows. In Section II, we give the governing equations of detonation in condensed explosives. In Section III, we establish the relaxation equations for the governing equations of detonation. In Section IV, the numerical scheme for the relaxation equations is gives. In Section V several numerical tests are shown. Some conclusions are presented in Section VI.

II. GOVERNING EQUATIONS OF DETONATION IN CONDENSED EXPLOSIVES

The one-dimensional flow equations of detonation in condensed explosives under Eulerian frame are the following:

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial r} = s(u) \qquad (1)$$

where,

$$u = \begin{bmatrix} \rho r^N \\ \rho v r^N \\ \rho E r^N \\ \rho \lambda r^N \end{bmatrix}, \quad f(u) = \begin{bmatrix} \rho v r^N \\ (\rho v^2 + p) r^N \\ (\rho E + p) v r^N \\ \rho v \lambda r^N \end{bmatrix},$$

$$s(u) = \begin{bmatrix} 0 \\ N r^{N-1} p \\ 0 \\ \rho r^N R(\rho, p, \lambda) \end{bmatrix},$$

where ρ is density, v is velocity, E is total energy, λ is chemical reaction process, p is pressure, N is geometry factor ($N = 0$ for plane, $N = 1$ for cylinder, and $N = 2$ for sphere), and R is chemical reaction rate where three-term Lee-Tarver reaction law is adopted [10]:

$$R = I(\eta_1 - 1 - a)^n (1 - \lambda)^y + G_1 (1 - \lambda)^{y_1} \lambda^{x_1} p^{z_1} + G_2 (1 - \lambda)^{y_2} \lambda^{x_2} p^{z_2}.$$

The unreacted solid component and gas product component of detonation in condensed explosives utilize JWL equation of state. On assumption that the pressure and temperature in the reaction mixing zone is in equilibrium, the state of mixing zone may be expressed as (subscript s denotes solid component and subscript g denotes gas product component):

$$\begin{cases} V = (1 - \lambda) V_s + \lambda V_g \\ e = (1 - \lambda) e_s + \lambda e_g - \lambda q \\ p = A_s \exp(-R_{1s} V_s) + B_s \exp(-R_{2s} V_s) + \dfrac{\omega_s C_{Vs}}{V_s} T \\ p = A_g \exp(-R_{1g} V_g) + B_g \exp(-R_{2g} V_g) + \dfrac{\omega_g C_{Vg}}{V_g} T \\ e_s = \dfrac{A_s}{\rho_0 R_{1s}} \exp(-R_{1s} V_s) + \dfrac{B_s}{\rho_0 R_{2s}} \exp(-R_{2s} V_s) + \dfrac{C_{Vs}}{\rho_0} T \\ e_g = \dfrac{A_g}{\rho_0 R_{1g}} \exp(-R_{1g} V_g) + \dfrac{B_g}{\rho_0 R_{2g}} \exp(-R_{2g} V_g) + \dfrac{C_{Vg}}{\rho_0} T \end{cases}$$

where $V = \rho_0 / \rho$ is the relative volume, e is the internal energy per mass, T is temperature, and q is the specific heat for chemical reaction.

For condensed explosives, there are several huge numbers in the chemical reaction rate. For example, for high explosives PBX-9502, $I = 4.0 \times 10^6$, $G_1 = 1100.0$, $G_2 = 30.0$, so the source term for the chemical reaction rate is regarded as strongly stiff.

III. ESTABLISH OF RELAXATION EQUATIONS

By means of relaxation approximation, the governing equations about condensed explosives may be replaced by the following relaxation system:

$$\begin{cases} \dfrac{\partial u}{\partial t} + \dfrac{\partial w}{\partial r} = s(u) \\ \dfrac{\partial w}{\partial t} + A^2 \dfrac{\partial u}{\partial r} = \dfrac{f(u) - w}{\varepsilon} \end{cases} \qquad (2)$$

where w is a middle variable, $A = diag[a_1, a_2, a_3, a_4]$ is a positive diagonal matrix, $0 < \varepsilon \le 1$ is relaxation rate.

The linear characteristic of relaxation system (2) is utilized to construct simple and effective high resolution scheme. Papers [12]-[13] point out that the solutions of (2) approach the solutions of the original problem (1): $w \to f(u)$, when $\varepsilon \to 0$, and provided the following subcharacteristic condition holds:

$$-a_k \le \frac{\partial f(u)}{\partial u} \le a_k \ (k = 1, 2, 3, 4) \ \text{for all } u .$$

The role of relaxation rate in numerical scheme may be analyzed [14] as follows.

Because w can converge to $f(u)$, there is a Chapman-Enskog expansion:

$$w = f(u) + \varepsilon f_1(u) + \varepsilon^2 f_2(u) + \cdots \qquad (3)$$

Substituting (3) into (2) and collecting terms, a first-order approximation of system (2) can be obtained:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial r} = \boldsymbol{s}(\boldsymbol{u}) + \varepsilon \frac{\partial}{\partial r}\left[\left(\frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial \boldsymbol{u}}\right)\boldsymbol{s}(\boldsymbol{u})\right]$$
$$+ \varepsilon \frac{\partial}{\partial r}\left\{\left[\boldsymbol{A}^2 - \left(\frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial \boldsymbol{u}}\right)^2\right]\frac{\partial \boldsymbol{u}}{\partial r}\right\} \tag{4}$$

Thus, system (4) is dissipative if the subcharacteristic condition holds. It can be thought that introducing relaxation rate is equivalent to introducing numerical dissipation.

In practice, the elements of diagonal matrix in system (2) may be chosen as: $\boldsymbol{A} = max\left(\left|\partial \boldsymbol{f}(\boldsymbol{u})/\partial \boldsymbol{u}\right|\right)$ in the whole flowfield zone. Thus, $\boldsymbol{A}$ is a constant matrix, and the bigger $\boldsymbol{A}$ implies the bigger numerical dissipation.

IV. SOLUTION OF RELAXATION EQUATIONS

Diagonalize the system (2) and holds:

$$\begin{cases} \dfrac{\partial(\boldsymbol{w} - \boldsymbol{A}\boldsymbol{u})}{\partial t} - \boldsymbol{A}\dfrac{\partial(\boldsymbol{w} - \boldsymbol{A}\boldsymbol{u})}{\partial r} = \dfrac{\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{w}}{\varepsilon} - \boldsymbol{A}\boldsymbol{s}(\boldsymbol{u}) \\[2mm] \dfrac{\partial(\boldsymbol{w} + \boldsymbol{A}\boldsymbol{u})}{\partial t} + \boldsymbol{A}\dfrac{\partial(\boldsymbol{w} + \boldsymbol{A}\boldsymbol{u})}{\partial r} = \dfrac{\boldsymbol{f}(\boldsymbol{u}) - \boldsymbol{w}}{\varepsilon} + \boldsymbol{A}\boldsymbol{s}(\boldsymbol{u}) \end{cases} \tag{5}$$

It can be found that the system (5) is constant linear hyperbolic law with characteristic lines $dr/dt = \pm A$ and Riemann invariables $\boldsymbol{w} \pm \boldsymbol{A}\boldsymbol{u}$.

A semi-discrete finite difference scheme with uniform space sizes for the system (5) can be approximated into:

$$\begin{cases} \dfrac{d\tilde{\boldsymbol{u}}_i}{dt} = \boldsymbol{A}\dfrac{\tilde{\boldsymbol{u}}_{i+1/2} - \tilde{\boldsymbol{u}}_{i-1/2}}{\Delta r} + \dfrac{1}{\varepsilon}\left[\boldsymbol{f}(\boldsymbol{A}^{-1}\dfrac{\tilde{\boldsymbol{w}}_i - \tilde{\boldsymbol{u}}_i}{2}) - \dfrac{\tilde{\boldsymbol{w}}_i + \tilde{\boldsymbol{u}}_i}{2}\right] \\[3mm] \qquad - \boldsymbol{A}\,\boldsymbol{s}(\boldsymbol{A}^{-1}\dfrac{\tilde{\boldsymbol{w}}_i - \tilde{\boldsymbol{u}}_i}{2}) \\[3mm] \dfrac{d\tilde{\boldsymbol{w}}_i}{dt} = -\boldsymbol{A}\dfrac{\tilde{\boldsymbol{w}}_{i+1/2} - \tilde{\boldsymbol{w}}_{i-1/2}}{\Delta r} + \dfrac{1}{\varepsilon}\left[\boldsymbol{f}(\boldsymbol{A}^{-1}\dfrac{\tilde{\boldsymbol{w}}_i - \tilde{\boldsymbol{u}}_i}{2}) - \dfrac{\tilde{\boldsymbol{w}}_i + \tilde{\boldsymbol{u}}_i}{2}\right] \\[3mm] \qquad + \boldsymbol{A}\,\boldsymbol{s}(\boldsymbol{A}^{-1}\dfrac{\tilde{\boldsymbol{w}}_i - \tilde{\boldsymbol{u}}_i}{2}) \end{cases} \tag{6}$$

where $\tilde{\boldsymbol{u}} = \boldsymbol{w} - \boldsymbol{A}\boldsymbol{u}$, $\tilde{\boldsymbol{w}} = \boldsymbol{w} + \boldsymbol{A}\boldsymbol{u}$.

When the system (6) is spatially discretized, the numerical flux $\tilde{\boldsymbol{u}}_{i\pm1/2}$ and $\tilde{\boldsymbol{w}}_{i\pm1/2}$ may adopt a fifth-order mapped weighted essentially non-oscillatory (WENOM) [20]:

$$\tilde{\boldsymbol{u}}_{i+1/2} = w_1 \tilde{\boldsymbol{u}}_{i+1/2}^{(1)} + w_2 \tilde{\boldsymbol{u}}_{i+1/2}^{(2)} + w_1 \tilde{\boldsymbol{u}}_{i+1/2}^{(2)},$$

$$\tilde{\boldsymbol{u}}_{i+1/2}^{(1)} = \frac{1}{3}\tilde{\boldsymbol{u}}_{i-2} - \frac{7}{6}\tilde{\boldsymbol{u}}_{i-1} + \frac{11}{6}\tilde{\boldsymbol{u}}_i,$$

$$\tilde{\boldsymbol{u}}_{i+1/2}^{(2)} = -\frac{1}{6}\tilde{\boldsymbol{u}}_{i-1} + \frac{5}{6}\tilde{\boldsymbol{u}}_i + \frac{1}{3}\tilde{\boldsymbol{u}}_{i+1},$$

$$\tilde{\boldsymbol{u}}_{i+1/2}^{(3)} = \frac{1}{3}\tilde{\boldsymbol{u}}_i + \frac{5}{6}\tilde{\boldsymbol{u}}_{i+1} - \frac{1}{6}\tilde{\boldsymbol{u}}_{i+2},$$

$$w_k = \alpha_k^* / (\sum_{l=1}^{3}\alpha_l^*),$$

$$\alpha_k^* = g_k(w_k^{(JS)}),$$

$$g_k(w) = \frac{w(\bar{w}_k + \bar{w}_k^2 - 3\bar{w}_k w + w^2)}{\bar{w}_k^2 + w(1 - 2\bar{w}_k)},$$

$$w_k^{(JS)} = \alpha_k / (\sum_{l=1}^{3}\alpha_l),$$

$$\alpha_k = \frac{\bar{w}_k}{(\delta + \beta_k)^2},$$

$$\bar{w}_1 = \frac{1}{10}, \ \bar{w}_2 = \frac{3}{5}, \ \bar{w}_3 = \frac{3}{10},$$

$$\beta_1 = \frac{13}{12}(\tilde{\boldsymbol{u}}_{i-2} - 2\tilde{\boldsymbol{u}}_{i-1} + \tilde{\boldsymbol{u}}_i)^2 + \frac{1}{4}(\tilde{\boldsymbol{u}}_{i-2} - 4\tilde{\boldsymbol{u}}_{i-1} + 3\tilde{\boldsymbol{u}}_i)^2,$$

$$\beta_2 = \frac{13}{12}(\tilde{\boldsymbol{u}}_{i-1} - 2\tilde{\boldsymbol{u}}_i + \tilde{\boldsymbol{u}}_{i+1})^2 + \frac{1}{4}(\tilde{\boldsymbol{u}}_{i-1} - \tilde{\boldsymbol{u}}_{i+1})^2,$$

$$\beta_3 = \frac{13}{12}(\tilde{\boldsymbol{u}}_i - 2\tilde{\boldsymbol{u}}_{i+1} + \tilde{\boldsymbol{u}}_{i+2})^2 + \frac{1}{4}(3\tilde{\boldsymbol{u}}_i - 4\tilde{\boldsymbol{u}}_{i+1} + \tilde{\boldsymbol{u}}_{i+2})^2.$$

When the system (6) is temporally discretized, the following ordinary differential equations can be obtained first:

$$\frac{d\boldsymbol{q}}{dt} = \mathcal{F}(\boldsymbol{q}) + \mathcal{S}(\boldsymbol{q}) \tag{7}$$

where $\boldsymbol{q} = [\tilde{\boldsymbol{u}}, \tilde{\boldsymbol{w}}]^T$, $\mathcal{F}(\boldsymbol{q})$ denotes the discretization of the advection term in system (6), $\mathcal{S}(\boldsymbol{q})$ denotes the discretization of the source term in system (6).

Then, a fifth-order IMEX scheme of linear multistep methods with general monotonicity and TVB [11] is adopted to solve the ordinary differential equation (7):

$$\begin{aligned} \boldsymbol{q}_n = {} & \frac{13553}{4096}\boldsymbol{q}_{n-1} - \frac{38121}{8192}\boldsymbol{q}_{n-2} + \frac{7315}{2048}\boldsymbol{q}_{n-3} \\ & - \frac{6161}{4096}\boldsymbol{q}_{n-4} + \frac{2264}{8192}\boldsymbol{q}_{n-5} \\ & + \frac{10306951}{5898240}\Delta t \mathcal{F}_{n-1} - \frac{13656497}{2949120}\Delta t \mathcal{F}_{n-2} \\ & + \frac{1249949}{245760}\Delta t \mathcal{F}_{n-3} - \frac{7937687}{2949120}\Delta t \mathcal{F}_{n-4} \\ & - \frac{3387361}{5898240}\Delta t \mathcal{F}_{n-5} \\ & + \frac{4007}{8192}\Delta t \mathcal{S}_n - \frac{4118249}{5898240}\Delta t \mathcal{S}_{n-1} \\ & + \frac{768703}{2949120}\Delta t \mathcal{S}_{n-2} + \frac{47849}{245760}\Delta t \mathcal{S}_{n-3} \\ & - \frac{725087}{2949120}\Delta t \mathcal{S}_{n-4} + \frac{502321}{5898240}\Delta t \mathcal{S}_{n-5} \end{aligned} \tag{8}$$

A third-order Runge-Kutta method [21] is used for starting procedure of this IMEX scheme.

Finally, the relaxation scheme with temporal-spatial fifth-order precision about the detonation flows in condensed explosives turns into the expression (8). It is worthy to indicate that the discretization procedure does not solve Riemann problem.

V. NUMERICAL EXAMPLE

In this section, the steady structure of one-dimensional planar detonation wave and the unsteady propagation of a

one-dimensional spherically divergent detonation wave in condensed explosives PBX-9502 are calculated. The JWL parameters and chemical reaction rate of PBX-9502 can be found in [22]. The values for Von Neumann spike are (cm-g-μs unit): $p_N = 0.375$, $V_N = 0.675$ and $u_N = 0.253$ respectively; and the corresponding values for Chapman-Jouguet state are: $p_{CJ} = 0.285$, $V_{CJ} = 0.753$, $u_{CJ} = 0.192$ and $D = 0.7665$.
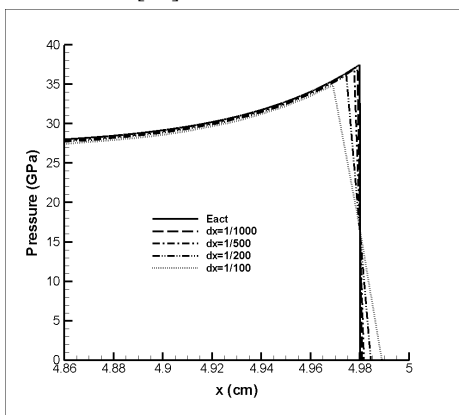
Several values of relaxation rate are tested, and here the results for relaxation rate $\varepsilon = 10^{-7}$ are shown.

A. Steady structure of 1D planar detonation wave

When the detonation arrives at the steady state, the distribution of physical variables in chemical reaction zone can be exactly obtained by means of the Rankine-Hugoniot relations of detonation wave.

The calculating length of explosives takes 5.0cm, and the explosives is initiated by the Chapman-Jouguet condition at its left hand side. The distributions of pressure, relative volume, velocity and mass fraction in chemical reaction zone are obtained, and comparisons are made with the exact solutions. Figure 1(a-d) gives the results where the mesh sizes are $\Delta x = 1/100$, $1/200$, $1/500$, $1/1000$ cm respectively. At the same time, the relation of the Chapman-Jouguet velocity and Von Neumann pressure to the mesh sizes is given in Figure 2(a-b). From Figure 1, the shock front of detonation wave is well resolved, and the spurious oscillation does not appear in the vicinity of the shock discontinuity. From Figures 1 and 2, when the mesh size is less than $1/500$ cm (about 50 meshes in the reaction zone), the calculating solutions agree well with the exact solutions.

Figure 3(a-b) shows the change of pressure and velocity at several typical times on the course of unsteady propagation of the detonation, in which the discretized mesh is $\Delta x = 1/500$ cm and the corresponding time are: t=0.06, 0.12, 0.24, 0.48, 0.96, 1.44, 1.92, 2.40, 2.88, 3.36, 3.84, 4.32, 4.80, 5.28μs. From the results, the pressure grows much quickly, and reaches the steady state about 3.84μs after initiating CJ conditions. The change agrees well with the experimental results [10].
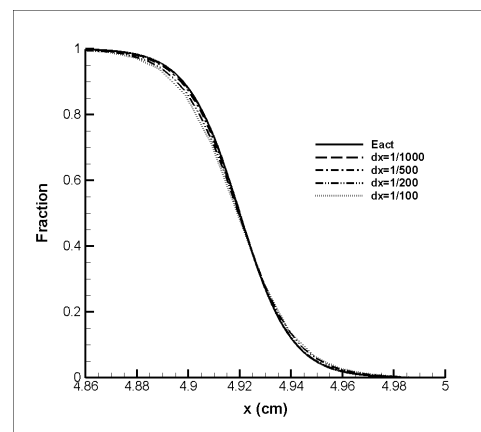

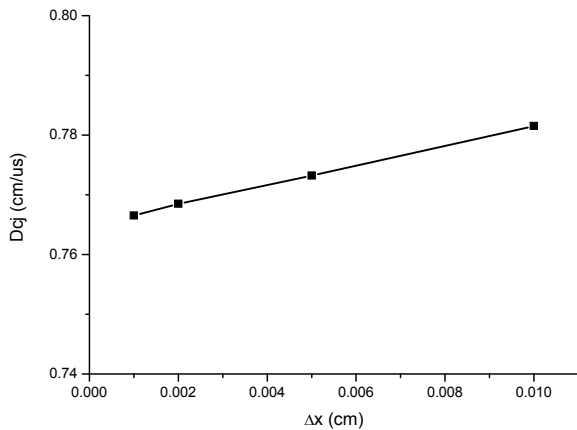(b) Velocity profile under different mesh sizes
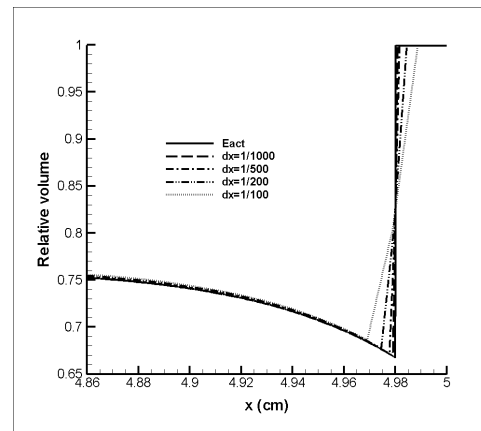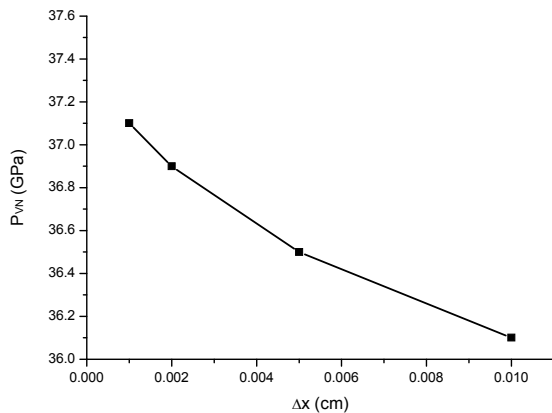

(c) Relative volume profile under different mesh sizes

(d) Fraction profile under different mesh sizes

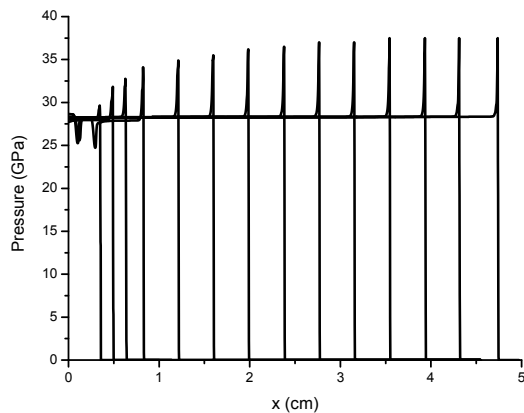Figure 1.   Distributions of physical variables in chemical reaction zone of PBX9502

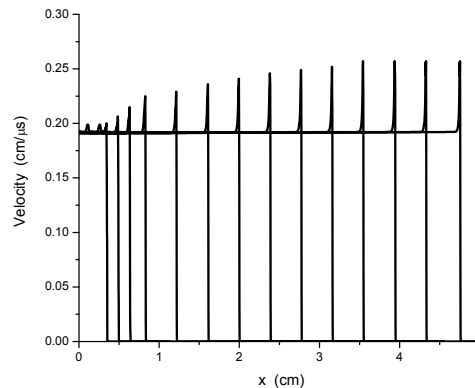(a) Pressure profile under different mesh sizes

(a) Detonation CJ velocity

(b) Detonation CJ pressure

Figure 2.   Relations of the CJ velocity and Von Neumann pressure to the mesh sizes in PBX9502
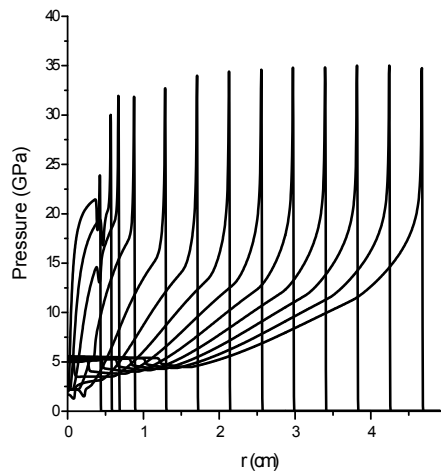

(b) Velocity

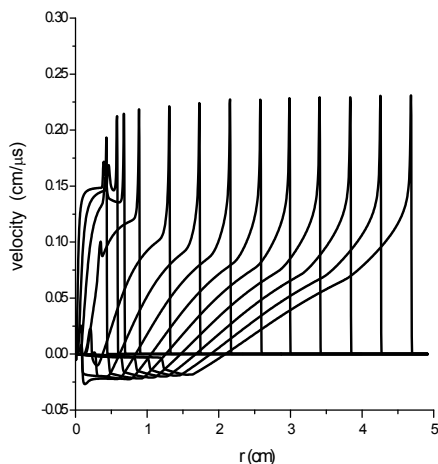Figure 3.   Pressure and velocity of planar detonation wave in PBX9502

B.   Unsteady propagation of 1D spherically divergent detonation wave

When a divergent detonation wave propagates in spherical way, the physical variables behind the shock front will sharply descend. A poor numerical scheme is usually unable to correctly treat with the effect of geometry factor to result in detonation extinguishing [1].

The calculating radius of spherical explosives takes 5.0cm, and the explosives is initiated by the CJ condition at the center. Figure 4(a-b) shows the change of pressure and velocity at several typical times on the course of unsteady propagation of the detonation wave, in which the discretized mesh is $\Delta r = 1/500$ cm and the corresponding time are: t=0.06, 0.12, 0.24, 0.48, 0.96, 1.44, 1.92, 2.40, 2.88, 3.36, 3.84, 4.32, 4.80, 5.28μs. From the results, the pressure and velocity grow along with increasing distance and reach quasi-steady state about 3.84μs after initiation, whose values are lower than the corresponding planar ones.

(a) Pressure

(a) Pressure

(b) Velocity

Figure 4.   Pressure and velocity of spherically divergent detonation wave

VI.   CONCLUSION

This paper presented the relaxation method for numerically simulating the detonation in condensed explosives, and a temporal-spatial fifth-order precision scheme is utilized to discretize the relaxation equations, which does not require solving Riemann problem and calculating the Jacobian matrix of nonlinear flux and splitting the source term of chemical reaction law. The calculating results for the steady structure of a one-dimensional planar detonation wave and unsteady propagation of a one-dimensional spherically divergent detonation wave in PBX-9502 demonstrate the high precision and high resolution of the present method. The present method will be generalized to two-dimensional detonation problems in condensed explosives.

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