A Cell-Centered Lagrangian Method Based on Characteristics Theory For Numerically Simulating Condensed Explosive Detonation

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***Abstract*—The paper proposes a cell-centered Lagrangian method for numerically simulating two-dimensional detonation flows in condensed explosives. The main feature of this method is that the velocity and pressure at the mesh vertex are computed using the characteristics theory in terms of the linearized partial differential equations about the detonation flows, and then the velocity and pressure are used to update the grid coordinates and evaluate the numerical flux across the cell interface. This vertex solver gives the instantaneous evolution solutions for velocity and pressure, which is regarded as a generalization of Riemann solver for one-dimensional Godunov scheme in multidimensional flows.**

Keywords-cell-centered Lagrangian method; characteristics theory; condensed explosive; detonation.

I. INTRODUCTION

The staggered-grid Lagrangian (SGL) method, where the kinematic variables are defined at the vertex of the mesh and the state variables are defined at the center of the mesh cell, is currently the most extensive way to numerically simulating explosive detonation flows [1]. However, SGL method has the following main disadvantages: 1) unable to preserve the conservation of the total energy; 2) always smooth the discontinuity of detonation with artificial viscosity; 3) difficult to adopt high precision for temporal and spatial discretization; 4) easy to produce the spurious motion of the mesh; 5) nonsynchronous time advance between the momentum equation and the mass and internal energy equations.

To eliminate these deficiencies, a highly promising alternative to SGL method is to use cell-centered Lagrangian (CCL) method [2][3], where all physical variables are defined at the center of the mesh cell, and the numerical scheme is constructed by integrating directly the conservation system of detonation flows on each moving cell with finite volume discretization. So, the key technique of CCL method lies in the determination of the velocity at the mesh vertex from the physical variables at the center of mesh cell, especially in multidimensional cases. An important contribution of this paper is to give a new idea to determine the physical variables at the mesh vertex in 2D detonation flows using the characteristics theory of partial differential equation.

The paper is organized as follows. In Section 2, we give the cell-centered finite volume method for detonation flows equations in the Lagrangian formulation. In Section 3, the vertex solver to compute velocity and pressure at vertex of the cell by local evolution Galerkin operator is derived. In Section 4 some numerical tests are shown to demonstrate the excellent performance of this new scheme. Some main conclusions are presented in Section 5.

II. THE GOVERNING EQUATIONS OF DETONATION AND THE FINITE VOLUME SCHEME

The governing equations of detonation flows in Lagrangian formulation are as follows:

$$\frac{d}{dt}\int_{\Omega(t)} d\Omega = \int_{\partial\Omega(t)} \boldsymbol{u}\cdot\boldsymbol{n}dl \tag{1.1}$$

$$\frac{d}{dt}\int_{\Omega(t)} \rho d\Omega = 0 \tag{1.2}$$

$$\frac{d}{dt}\int_{\Omega(t)} \rho\boldsymbol{u} d\Omega = -\int_{\partial\Omega(t)} p\boldsymbol{n}dl \tag{1.3}$$

$$\frac{d}{dt}\int_{\Omega(t)} \rho E d\Omega = -\int_{\partial\Omega(t)} p\boldsymbol{u}\cdot\boldsymbol{n}dl \tag{1.4}$$

$$\frac{d}{dt}\int_{\Omega(t)} \rho\lambda d\Omega = \int_{\Omega(t)} \rho r d\Omega \tag{1.5}$$

where ρ is the density, u and v are component velocities, p is pressure, E is specific total energy, $E = e + (u^2+v^2)/2$, e is specific internal energy, and $\Omega(t)$ is a control volume with the boundary $\partial\Omega(t)$, $\boldsymbol{dl}$ is the differential length of the surface for the control volume, r is the chemical reaction rate of explosives detonation, in which Ignition-Growth model is adopted [4].

On Lagrangian hydrodynamics, a control volume moves along with the fluid particle with the trajectory equations:

$$\frac{dx}{dt} = u\,,\ \frac{dy}{dt} = v \tag{2}$$

For a given control volume Ω with the mass $m_\Omega = \int_\Omega \rho d\Omega$ and area $A_\Omega = \int_\Omega d\Omega$, the average value of any physical variable f is $\overline{f}_\Omega = \frac{1}{m_\Omega}\int_\Omega \rho f d\Omega$. Thus, for 2D flows, (1.2) becomes an algebraic equation $\overline{\rho}_\Omega A_\Omega = m_\Omega = \text{const}$, and Eqs. (1.1) and (1.3)-(1.5) can be written as the following semi-discrete expression:

$$\frac{d\,\overline{\boldsymbol{q}}_\Omega}{dt} = -\frac{1}{m_\Omega}\int_{\partial\Omega} \boldsymbol{H}\cdot\boldsymbol{n}dl + \overline{\boldsymbol{r}}_\Omega \tag{3}$$

where $\overline{\boldsymbol{q}}_\Omega = \left(-\overline{\tau}_\Omega, \overline{u}_\Omega, \overline{v}_\Omega, \overline{E}_\Omega, \overline{\lambda}_\Omega\right)^T$, $\boldsymbol{H} = \left(u, p, 0, pu, 0\right)^T\boldsymbol{i} + \left(v, 0, p, pv, 0\right)^T\boldsymbol{j}$, $\overline{\boldsymbol{r}} = \left(0,0,0,0,\overline{r}_\Omega\right)^T$, $\overline{\tau}_\Omega = 1/\overline{\rho}_\Omega$.

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For any non-overlapping structured quadrilateral mesh with sides denoted by I_k (k=1,2,3,4), the semi-discrete finite volume discretization of Eq.(3) can be written as:

$$\frac{d\,\overline{\boldsymbol{q}}_\Omega}{dt} = -\frac{1}{m_c}\sum_{k=1}^{4}\int_{I_k} \boldsymbol{H}\cdot\boldsymbol{n}\,dl + \overline{\boldsymbol{r}}_\Omega \tag{4}$$

Due to the fact that a semi-discrete model describes the instantaneous behavior of the dynamical system at its initial time, the full discretization of Eq.(4) can be turned into the following form by means of the trapezia rule to evaluate the numerical integration of the interface flux in structured grids:

$$\begin{aligned}\overline{\boldsymbol{q}}_\Omega^{(n+1)} = \overline{\boldsymbol{q}}_\Omega^{(n)} - \frac{\Delta t}{2m_\Omega}\left\{\sum_{i=1}^{4}\left[\boldsymbol{H}_i\left(\boldsymbol{E}_0\,\overline{\boldsymbol{q}}_\Omega^{(n)}\right) + \boldsymbol{H}_{i+1}\left(\boldsymbol{E}_0\,\overline{\boldsymbol{q}}_\Omega^{(n)}\right)\right]\cdot\boldsymbol{n}_{i,i+1}\Delta l_{i,i+1}\right\} \\ + \boldsymbol{r}\left(\overline{\boldsymbol{q}}_\Omega^{(n+1)}\right)\end{aligned} \tag{5}$$

where $\boldsymbol{E}_0$ is the vertex solver to compute the instantaneous solutions at the mesh vertex at time $t_n^+ = t_n + 0$, namely there is $\boldsymbol{q}(t_n^+) = \boldsymbol{E}_0\boldsymbol{q}(t_n)$, and subscript i is the numbering of the vertices counterclockwise for a quadrilateral grid.

From Eq.(2) and Eq.(5), the velocity and pressure of a vertex of a mesh cell must be obtained. Here, the velocity and pressure of a vertex are solved by the characteristics theory of partial differential equation.

III. VERTEX SOLVER $\boldsymbol{E}_0$ BY CHARACTERISTICS THOERY

To obtain the analytical expressions of the vertex solver $\boldsymbol{E}_0$ by means of the characteristics theory of hyperbolic partial differential equations, the quasilinear and heterogeneous detonation equations (6.1) can be transformed into a locally linearized and homogeneous system (6.2) in terms of the primitive variables:

$$\frac{d\,\boldsymbol{w}}{dt} + \boldsymbol{A}(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial x} + \boldsymbol{B}(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial y} = \boldsymbol{r}_w\,,\quad \boldsymbol{w}_0 = \boldsymbol{w}(t_n) \tag{6.1}$$

$$\frac{d\,\hat{\boldsymbol{w}}}{dt} + \boldsymbol{A}(\boldsymbol{w}_0)\frac{\partial\hat{\boldsymbol{w}}}{\partial x} + \boldsymbol{B}(\boldsymbol{w}_0)\frac{\partial\hat{\boldsymbol{w}}}{\partial y} = 0\,,\quad \hat{\boldsymbol{w}}_0 = \boldsymbol{w}(t_n) \tag{6.2}$$

where $\boldsymbol{w} = \hat{\boldsymbol{w}} = \begin{bmatrix}\rho\\ u\\ v\\ p\\ \lambda\end{bmatrix}$, $\boldsymbol{A}(\boldsymbol{w}) = \begin{bmatrix}0 & \rho & 0 & 0 & 0\\ 0 & 0 & 0 & \frac{1}{\rho} & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & \rho c_\lambda^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\end{bmatrix}$, $\boldsymbol{r}_w = \begin{bmatrix}0\\ 0\\ 0\\ r\frac{\partial p}{\partial\lambda}\\ r\end{bmatrix}$,

$\boldsymbol{B}(\boldsymbol{w})$ is similar to $\boldsymbol{A}(\boldsymbol{w})$, and c_λ is the sonic speed.

We can prove the equality $\boldsymbol{w}(t_n^+) = \hat{\boldsymbol{w}}(t_n^+)$ as follows.

***Proof*:**

From the Taylor expansion, it holds:

$$\begin{aligned}\boldsymbol{w}(t_n+\tau) &= \boldsymbol{w}(t_n) + \frac{d\boldsymbol{w}}{dt}\tau + O(\tau^2)\\ &= \boldsymbol{w}_0 - \boldsymbol{A}(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial x}\tau - \boldsymbol{B}(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial y}\tau + \boldsymbol{r}_w\tau + O(\tau^2)\\ \hat{\boldsymbol{w}}(t_n+\tau) &= \hat{\boldsymbol{w}}(t_n) + \frac{d\hat{\boldsymbol{w}}}{dt}\tau + O(\tau^2)\\ &= \hat{\boldsymbol{w}}_0 - \boldsymbol{A}(\hat{\boldsymbol{w}}_0)\frac{\partial\boldsymbol{v}}{\partial x}\tau - \boldsymbol{B}(\hat{\boldsymbol{w}}_0)\frac{\partial\hat{\boldsymbol{w}}}{\partial y}\tau + O(\tau^2)\end{aligned},$$

There is

$$\begin{aligned}&\boldsymbol{w}(t_n+\tau) - \hat{\boldsymbol{w}}(t_n+\tau)\\ &= \left(\boldsymbol{A}(\boldsymbol{w}_0)\frac{\partial\hat{\boldsymbol{w}}}{\partial x} - \boldsymbol{A}(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial x}\right)\tau + \left(\boldsymbol{B}(\boldsymbol{w}_0)\frac{\partial\hat{\boldsymbol{w}}}{\partial y} - \boldsymbol{B}(\boldsymbol{w})\frac{\partial\boldsymbol{v}}{\partial y}\right)\tau + \boldsymbol{r}_w\tau + O(\tau^2)\end{aligned} \tag{7}$$

A limit operation is carried out for the Eq.(7), and we have:

$$\lim_{\tau\to 0}\left(\boldsymbol{w}(t_n+\tau) - \hat{\boldsymbol{w}}(t_n+\tau)\right) = 0\,,$$

namely, $\boldsymbol{w}(t_n^+) = \hat{\boldsymbol{w}}(t_n^+)$.

End.

Because of $\hat{\boldsymbol{w}}(t_n^+) = \lim_{\tau\to 0}\hat{\boldsymbol{w}}(t_n+\tau)$, the expression of $\hat{\boldsymbol{w}}(t_n^+)$ may be obtained from $\hat{\boldsymbol{w}}(t_n+\tau)$ firstly, and the limit operation can be carried out secondly.

For convenience, Eq.(6.2) can be transformed into the following quasi-diagonalized system by means of left multiplication of the eigen-matrix:

$$\frac{d\,\boldsymbol{v}}{dt} + \boldsymbol{\Lambda}_A\frac{\partial\boldsymbol{v}}{\partial x} + \boldsymbol{\Lambda}_B\frac{\partial\boldsymbol{v}}{\partial y} = \boldsymbol{s} \tag{8}$$

where $\boldsymbol{v}$ is the eigenvector, $\boldsymbol{v} = \boldsymbol{R}^{-1}\hat{\boldsymbol{w}}$, $\boldsymbol{R}$ is the right eigen-matrix of a matrix pencil $\boldsymbol{C} = \cos\theta\boldsymbol{A}(\boldsymbol{w}_0) + \sin\theta\boldsymbol{B}(\boldsymbol{w}_0)$ ($\theta\in[0,2\pi]$) and has the right eigenvectors $\boldsymbol{r}_l$ ($l = 1,2,3,4,5$); and there are $\boldsymbol{\Lambda}_A = diag[\lambda_{A,1},\lambda_{A,2},\lambda_{A,3},\lambda_{A,4},\lambda_{A,5}]$ and $\boldsymbol{\Lambda}_B = diag[\lambda_{B,1},\lambda_{B,2},\lambda_{B,3},\lambda_{B,4},\lambda_{B,5}]$.

Obviously, it can be found from the characteristics theory of two-dimensional first-order hyperbolic partial differential equations that, given the physical state $\boldsymbol{w}_0 = \tilde{\boldsymbol{w}} = (\tilde\rho,\tilde u,\tilde v,\tilde p,\tilde\lambda)$ at initial time-space point $\tilde P = (x,y,t)_{t=t_n}$, the every characteristics variable v_l ($l = 1,2,3,4,5$) at any time-space point $P = (x,y,t)_{t=t_n+\tau}$ would evolve for the time τ along the corresponding bicharacteristics line and then can be written into [5][6]:

$$\begin{aligned}&v_l(P,\theta) = v_l[\tilde P(\theta)]\\ &\quad + \int_{t_n}^{t_n+\tau} s_l[x-\lambda_{A,l}(\theta)(t_n+\tau-\xi),\ y-\lambda_{B,l}(\theta)(t_n+\tau-\xi),\ \xi]d\xi\end{aligned} \tag{9}$$

By left multiplying Eq.(9) through $\hat{\boldsymbol{w}} = \boldsymbol{R}\boldsymbol{v}$ and then integrating with respect to θ from 0 to 2π, it leads to:

$$\hat{\boldsymbol{w}}(P) = \frac{1}{2\pi}\int_0^{2\pi}\left\{\sum_{l=1}^{5}\boldsymbol{r}_l\left[v_l\left(\tilde P(\theta)\right) + s_l(\theta)\right]\right\}d\theta \tag{10}$$

For discretized structured grids, $\tilde P = (x,y,t)_{t=t_n}$ is assumed to be time-space position of any vertex. Obviously, the vertex is shared by four grid cells, and θ_{ka} and θ_{kb} are respectively assumed to be the starting and ending angles of the kth ($k\le 4$) grid cell of the shared vertex, thus Eq.(10) can be rewritten into:

$$\begin{aligned}u(P) = \frac{1}{2}u(\tilde P) + \frac{1}{2\pi}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\left[-\frac{p(\tilde Q)}{\tilde\rho\tilde c_\lambda}\cos\theta + u(\tilde Q)\cos^2\theta + v(\tilde Q)\sin\theta\cos\theta\right]d\theta\\ + \frac{1}{2\pi}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\int_{t_n}^{t_n+\tau} S[\boldsymbol{z}+\tilde c_\lambda(t_n+\tau-\xi)\boldsymbol{n}(\theta),\xi,\theta]\cos\theta\,d\xi\,d\theta\,\frac{1}{2\tilde\rho}\int_{t_n}^{t_n+\tau}\frac{\partial p(z,\xi)}{\partial x}d\xi\end{aligned} \tag{11}$$

$$v(P)=\frac{1}{2}v(\tilde{P})+\frac{1}{2\pi}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\left[-\frac{p(\tilde{Q})}{\tilde{\rho}\tilde{c}_{\lambda}}\sin\theta+u(\tilde{Q})\cos\theta\sin\theta+v(\tilde{Q})\sin^{2}\theta\right]d\theta$$
$$+\frac{1}{2\pi}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\int_{t_n}^{t_n+\tau}S[z+\tilde{c}(t_n+\tau-\xi)\boldsymbol{n}(\theta),\xi,\theta]\sin\theta d\xi d\theta-\frac{1}{2\tilde{\rho}}\int_{t_n}^{t_n+\tau}\frac{\partial p(z,\xi)}{\partial y}d\xi \quad (12)$$

$$p(P)=\frac{1}{2\pi}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\left[p(\tilde{Q})-\tilde{\rho}\tilde{c}_{\lambda}u(\tilde{Q})\cos\theta-\tilde{\rho}\tilde{c}_{\lambda}v(\tilde{Q})\sin\theta\right]d\theta$$
$$-\frac{1}{2\pi}\tilde{\rho}\tilde{c}_{\lambda}\sum_{k=1}^{4}\int_{\theta_{ka}}^{\theta_{kb}}\int_{t_n}^{t_n+\tau}S[z+\tilde{c}(t_n+\tau-\xi)\boldsymbol{n}(\theta),\xi,\theta]d\xi d\theta \quad (13)$$

Equtions.(11)-(13) are the exact evolution solutions of the locally linearized and homogeneous system (6.2). The instantaneous evolution solutions of Eqs.(11)-(13) at time $t_n^{+}=t_n+0$ can be obtained by means of the limit operations in terms of $\tau\to 0$, and then the analytical expressions of the vertex solver $\boldsymbol{E}_0$ are as follows:

$$u(t_n^{+})=\frac{1}{\pi}\sum_{k=1}^{4}\left[-\frac{\tilde{p}_k}{\tilde{\rho}\tilde{c}_{\lambda}}(\sin\theta_{kb}-\sin\theta_{ka})\right.$$
$$\left.+\tilde{u}_k\left(\frac{\theta_{kb}-\theta_{ka}}{2}+\frac{\sin 2\theta_{kb}-\sin 2\theta_{ka}}{4}\right)-\tilde{v}_k\frac{\cos 2\theta_{kb}-\cos 2\theta_{ka}}{4}\right] \quad (14)$$

$$v(t_n^{+})=\frac{1}{\pi}\sum_{k=1}^{4}\left[\frac{\tilde{p}_k}{\tilde{\rho}\tilde{c}_{\lambda}}(\cos\theta_{kb}-\cos\theta_{ka})\right.$$
$$\left.-\tilde{u}_k\frac{\cos 2\theta_{kb}-\cos 2\theta_{ka}}{4}+\tilde{v}_k\left(\frac{\theta_{kb}-\theta_{ka}}{2}-\frac{\sin 2\theta_{kb}-\sin 2\theta_{ka}}{4}\right)\right] \quad (15)$$

$$p(t_n^{+})=\frac{1}{2\pi}\sum_{k=1}^{4}\left[\tilde{p}_k(\theta_{kb}-\theta_{ka})-\tilde{\rho}\tilde{c}_{\lambda}\tilde{u}_k(\sin\theta_{kb}-\sin\theta_{ka})+\tilde{\rho}\tilde{c}_{\lambda}\tilde{v}_k(\cos\theta_{kb}-\cos\theta_{ka})\right] \quad (16)$$

IV. NUMERICAL EXAMPLES

The steady structure of 1D planar detonation wave, unsteady propagation of 1D spherically divergent detonation wave and 2D rectangular diffraction of planar detonation wave in high explosive PBX9502 [1] are investigated. Here, only the results of 1D planar detonation wave are given. The calculating length of explosive takes 5.0cm, and the explosive is initiated by the Chapman-Jougeut condition [1] at its left hand side. The distributions of pressure and velocity in chemical reaction zone are obtained, and comparisons are made with the exact solutions. Figure 1 gives the results where the mesh sizes are $\Delta x=1/100$, $1/200$, $1/500$, $1/1000$ cm respectively. 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. Meanwhile, 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. It means that this method has good resolution and convergence. Figure 2 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 faster and the steady state reaches about 3.84μs after initiating by Chapman-Jougeut conditions, and the propagation velocity is about 0.7670 cm/μs after the steady state. The change course is almost identical with the experimental results [7].

These numerical examples demonstrate the excellent performance of the presented cell-centered Lagrangian method.

V. CONCLUSIONS

This paper proposes a cell-centered Lagrangian method for 2D detonation flows in condensed explosives. Its main feature is that the vertex solver is based on the characteristics theory in terms of the linearized partial differential equations of the detonation flows, which is essentially a multidimensional Riemann solver taking "multidimensional effect" into account in a natural way. From the calculated course, the CCL method is able to preserve the conservation of the total energy by solving the total energy equation, to preserve the good resolution of the discontinuity of detonation without artificial viscosity, to eliminate the unphysical motion of mesh, and keep the synchronous time advance between the momentum equation and the mass and internal energy equations. Our future most important works will be on the generalization of high-order precision and high resolution, and the extension to arbitrary Lagrangian-Eulerian method.

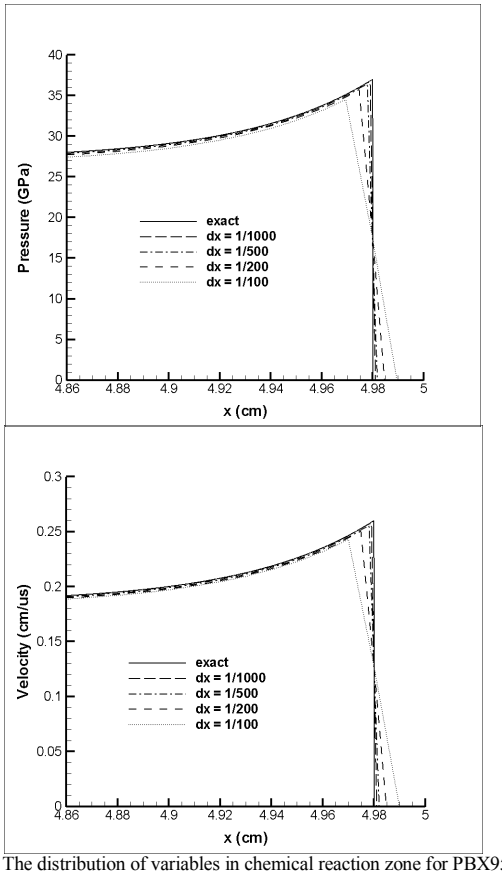

Fig.1 The distribution of variables in chemical reaction zone for PBX9502

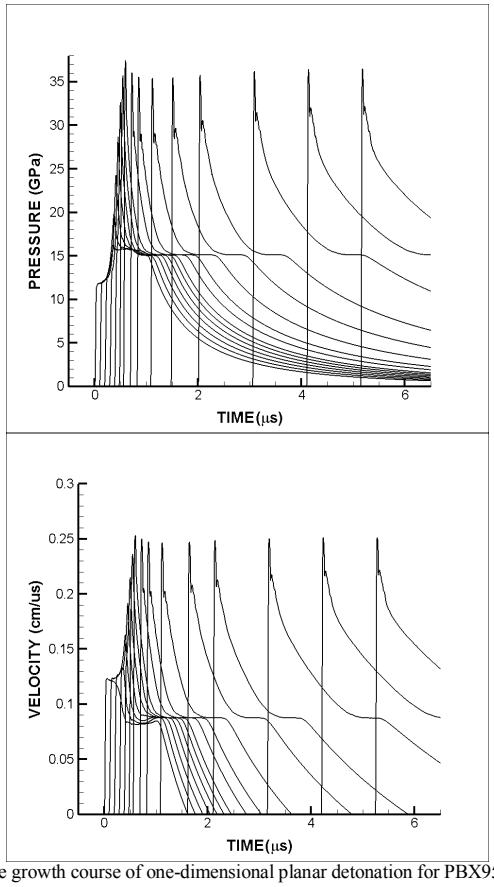

Fig.2 The growth course of one-dimensional planar detonation for PBX9502

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