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Application of the CE/SE Method to a Two-Phase Detonation Model in Porous Media *

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We extend the conservation-element and solution-element method to simulate a two-phase detonation model in porous media. The accuracy of the method is validated by calculating an inert compaction problem. The main characteristics of piston-driven detonation phenomena, including the compaction wave, the onset of combustion, and the transition to detonation, could be predicted successfully.

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Two-phase detonation in porous media is an important process. However, it is very complicated in experiment and numerical simulation since the mechanism is not completely clear. Dynamic compaction is a fundamental phenomenon of two-phase detonation in porous media. Steady compaction waves were observed by Sandusky and Liddiard.^[1] in a piston-driven porous HMX bed. To understand compaction and detonation in porous media better, several two-phase continuum models have been developed^[2-4] The main challenge in the numerical simulation of two-phase detonation models is the method of capturing the strong discontinuity in the field. The most commonly used numerical methods are based on either the MacCormack scheme or Riemann solution. The MacCormack scheme needs strong artificial viscosity to capture shocks and maintain stability, which may reduce the accuracy of the results. The method based on the Riemann solution is complicated in constructing Riemann solvers. To overcome these difficulties, in this Letter we apply the space-time conservation-element and solution-element (CE/SE) method to simulate a two-phase detonation model.

The CE/SE method originally proposed by Chang,^[5] provides a new way to solve the hyperbolic conservation equation. It has many features differing from the existing well-established schemes. The CE/SE method satisfies the local and global flux conservation in space and time and needs simple treatments of boundary conditions. Because of its simplicity and accuracy, the CE/SE method has been successfully applied to many fluid problems. Wu *et al.*^[6] applied the CE/SE method to the gas-phase chemical reaction flow. Wang *et al.*^[7] simulated the critical wedge angle of cellular detonation reflections. Zhang *et al.*^[8] studied the plume dynamics of a pulse detonation engine. Weng *et al.*^[9,10] solved a two-phase flow in interior ballistics and the problem of the pulse detonation engine. The simulation of chemical reac-

tion flow by the CE/SE scheme is mainly gas-phase. In this study, we extend the CE/SE scheme to the simulation of the solid energetic granular detonation problem.

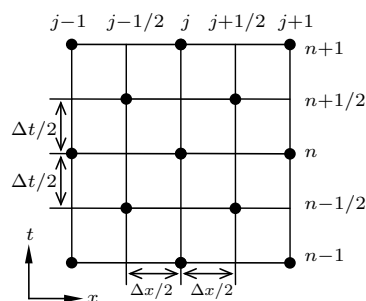


Fig. 1. Staggered space-time mesh of the CE/SE scheme.

The CE/SE method treats time and space as one entity. The concepts of the SE and the CE are introduced. In the SE, variables are continuous. The conservation equation is integrated over the CE. Details are illustrated in Ref. [5]. Figure 1 shows the staggered space-time mesh of the computational region. For the conservation equation $\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$, the CE/SE scheme reads

$$\begin{aligned}
 U_j^n = & \frac{1}{2} \left[U_{j-1/2}^{n-1/2} + \frac{\Delta x}{4} (U_x)_{j-1/2}^{n-1/2} + U_{j+1/2}^{n-1/2} \right. \\
 & \left. - \frac{\Delta x}{4} (U_x)_{j+1/2}^{n-1/2} \right] \\
 & + \frac{1}{2} \frac{\Delta t}{\Delta x} \left[F_{j-1/2}^{n-1/2} + \frac{\Delta t}{4} (F_t)_{j-1/2}^{n-1/2} \right. \\
 & \left. - F_{j+1/2}^{n-1/2} - \frac{\Delta t}{4} (F_t)_{j+1/2}^{n-1/2} \right], \quad (1)
 \end{aligned}$$

where $U_x = \frac{\partial U}{\partial x}$ and $F_t = \frac{\partial F}{\partial t}$ denote spatial and temporal gradients of the variables.

The spatial gradients of the variables can be obtained simultaneously,

$$(U_x)_j^n = \frac{|U_x^+|^\alpha U_x^- + |U_x^-|^\alpha U_x^+}{|U_x^+|^\alpha + |U_x^-|^\alpha}, \quad (2)$$

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where

$$U_x^\pm = \pm \frac{U_{j\pm 1/2}^{n-1/2} - U_j^n + \Delta t (U_t)_{j\pm 1/2}^{n-1/2}/2}{\Delta x/2},$$

with $\alpha = 1-2$. The other gradients, such as F_x , U_t and F_t , can be calculated by the chain rule and conservation equations.

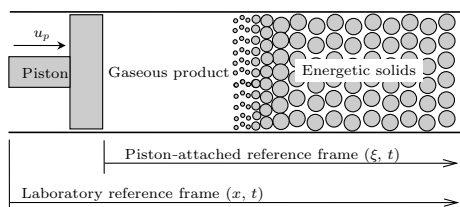


Fig. 2. Schematic of a piston-driven problem.

Figure 2 shows a simple schematic of a piston-driven problem in porous media. The piston moves with a constant velocity in the stationary granular bed. Adiabatic compression of the porous media provides energy to initiate the chemical reaction of solids. Solid mass, momentum, and energy are converted into gas mass, momentum, and energy. The two-phase model equations are given as follows:

$$\frac{\partial(\rho_1\phi_1)}{\partial t} + \frac{\partial(\rho_1\phi_1u_1)}{\partial x} = \Gamma, \quad (3)$$

$$\frac{\partial(\rho_1\phi_1u_1)}{\partial t} + \frac{\partial(\rho_1\phi_1u_1^2 + p_1\phi_1)}{\partial x} = \Gamma u_2 - D, \quad (4)$$

$$\begin{aligned} & \frac{\partial[\rho_1\phi_1(e_1 + u_1^2/2)]}{\partial t} \\ & + \frac{\partial[\rho_1\phi_1u_1(e_1 + u_1^2/2 + p_1/\rho_1)]}{\partial x} \\ & = \Gamma(e_2 + u_2^2/2 + q_{\text{chem}}) - Du_2 - Q, \end{aligned} \quad (5)$$

$$\frac{\partial(\rho_2\phi_2)}{\partial t} + \frac{\partial(\rho_2\phi_2u_2)}{\partial x} = -\Gamma, \quad (6)$$

$$\frac{\partial(\rho_2\phi_2u_2)}{\partial t} + \frac{\partial(\rho_2\phi_2u_2^2 + p_2\phi_2)}{\partial x} = -\Gamma u_2 + D, \quad (7)$$

$$\begin{aligned} & \frac{\partial[\rho_2\phi_2(e_2 + u_2^2/2)]}{\partial t} \\ & + \frac{\partial[\rho_2\phi_2u_2(e_2 + u_2^2/2 + p_2/\rho_2)]}{\partial x} \\ & = -\Gamma(e_2 + u_2^2/2) + Du_2 + Q, \end{aligned} \quad (8)$$

$$\begin{aligned} & \frac{\partial\phi_2}{\partial t} + u_2 \frac{\partial\phi_2}{\partial x} \\ & = \frac{\phi_1\phi_2}{\mu_c} \left[(p_2 - p_1) - (p_{2o} - p_{1o}) \right. \\ & \quad \left. \cdot \frac{\phi_2^2}{\phi_{2o}^2} \frac{(2 - \phi_{2o})^2 \ln(1 - \phi_2)}{(2 - \phi_2)^2 \ln(1 - \phi_{2o})} \right] - \frac{\Gamma}{\rho_2}, \end{aligned} \quad (9)$$

$$\frac{\partial n}{\partial t} + \frac{\partial(u_2 n)}{\partial x} = 0, \quad (10)$$

$$\frac{4}{3}\pi r^3 n = \phi_2, \quad (11)$$

$$\begin{aligned} & \frac{\partial I}{\partial t} + u_2 \frac{\partial I}{\partial x} \\ & = k_I(1 - I) \exp \left[-\frac{T_I}{T_1\phi_1 + T_2\phi_2} \right] \\ & \quad \cdot \left[\frac{p_1\phi_1 + p_2\phi_2 - p_{1o}\phi_{1o} - p_{2o}\phi_{2o}}{p_{1o}\phi_{1o} + p_{2o}\phi_{2o}} \right]^2. \end{aligned} \quad (12)$$

In these equations, the subscripts 1 and 2 denote the variables of the gas and solid, respectively. The subscript o represents the initial state. The variables are as follows: ρ the density, u the velocity; p the pressure, e the specific internal energy, ϕ ($\phi_1 + \phi_2 = 1$) the volume fraction, n the number of particles per unit volume, and r the radius of the spherical solid particles. The variable I ($0 < I < 1$) is an ignition parameter introduced by Gonthier and Powers^[11] to model the induction period occurring prior to the onset of combustion in piston-driven detonation experiments. In the source terms of the equations, $\Gamma = \frac{3}{r}\rho_2\phi_2ap_1^m H(I - I_{ig})$ is the interphase mass transfer, H is the Heaviside function, $D = \beta \frac{\phi_1\phi_2}{r}(u_1 - u_2)$ is the interphase drag force, $Q = h \frac{\phi_1\phi_2}{r^{1/3}}(T_1 - T_2)$ is the interphase convection heat transfer, q_{chem} is granular chemical energy, T is the temperature, I_{ig} , k_I and T_I are the constant parameters associated with ignition. The equations of state for the simulation are $e_1 = c_{v1}T_1$, $p_1 = \rho_1 R_1 T_1 (1 + b\rho_1)$, $e_2 = c_{v2}T_2 + \frac{\rho_{20}\sigma}{\gamma_2\rho_2}$, $p_2 = (\gamma_2 - 1)c_{v2}\rho_2 T_2 - \frac{\rho_{20}\sigma}{\gamma_2}$.

To deal with the moving boundary of the piston, Eqs. (3)–(12) in the laboratory reference frame (x, t) are transformed into a piston-attached reference frame (ξ, t) . The transformation is given by $\xi = x - \int u_p dt$ and $v_i = u_i - u_p$ ($i = 1, 2$), where u_p is the piston velocity. In this study, we assume the piston moved in a constant velocity of 100 m/s.

To verify the accuracy of our method, we first simulate an inert compaction problem. We presume that the chemical reaction would not occur in the granular solids. The interactions of gas and solid are only coupled with the inter-phase drag and inter-phase heat transfer. The computational domain is $0 < \xi < 0.5$ m with 501 meshes. The initial conditions and the model parameters used for the simulation are given as $\rho_{1o} = 10$ kg/m³, $\rho_{2o} = 1900$ kg/m³, $T_o = 300$ K, $\phi_{2o} = 0.73$, $r_o = 1.0 \times 10^{-4}$ m, $c_{v1} = 2400$ J/(kg·K), $R_1 = 850$ J/(kg·K), $b = 1.1 \times 10^{-3}$ m³/kg, $c_{v2} = 1500$ J/(kg·K), $\gamma_2 = 5$, $\sigma = 8.98 \times 10^6$ m²/s², $\beta = 1 \times 10^4$ kg/(m²·s), $h = 1 \times 10^7$ J/(K·s·m^{8/3}), $\mu_c = 1000$ kg/(m·s), $q_{\text{chem}} = 0$.

Figure 3 shows the numerical results of the velocity (relative to the laboratory reference frame), volume fraction and pressure of the granular solids. Here ξ is

the position to the piston. A compaction wave quickly developed and propagated away with a steady speed of 411 m/s. The solid volume fraction and pressure for the steady wave are 0.964 and 64.5 MPa. These values of the compaction wave speed D , the solid volume fraction ϕ_2 and the pressure p_2 agree well with the pre-

vious reports,^[1,11,12] which are given in Table 1. We simulate the case on a finer grid of 1000 meshes for further validation. The calculated compaction wave trace is shown in Fig. 4. The result is independent of the grid number.

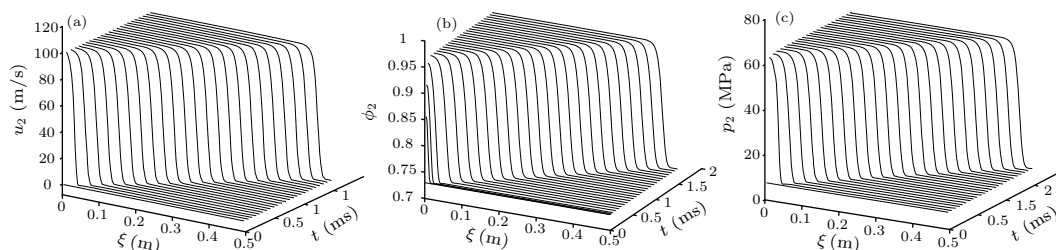


Fig. 3. Numerical results of the compaction wave in granular solids: (a) velocity, (b) volume fraction, and (c) pressure.

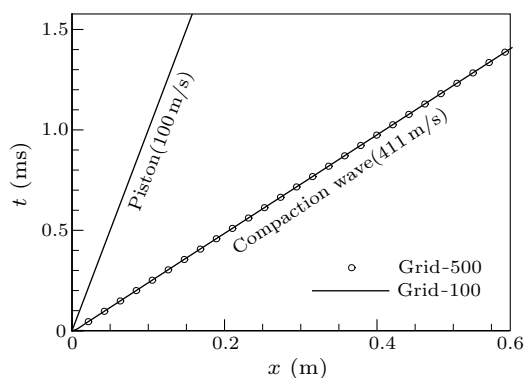


Fig. 4. Calculated compaction trace.

We numerically simulate the detonation process based on the inert compaction problem. Here the granular solids begin to combust when the ignition variable I exceeds a certain threshold. Equation (12) is an evolution equation for the ignition variable. It models the ignition variable as an increasing function of pressure and temperature of the gas and solid.^[11] The computational domain is $0 < \xi < 0.5$ m with 501 meshes. The initial conditions and the model parameters used for the simulation are given as $\rho_{1o} = 10 \text{ kg/m}^3$, $\rho_{2o} = 1710 \text{ kg/m}^3$, $T_o = 300 \text{ K}$,

$\phi_{2o} = 0.7$, $r_o = 1.0 \times 10^{-4} \text{ m}$, $c_{v1} = 2400 \text{ J/(kg}\cdot\text{K)}$, $R_1 = 850 \text{ J/(kg}\cdot\text{K)}$, $b = 1.1 \times 10^{-3} \text{ m}^3/\text{kg}$, $c_{v2} = 1500 \text{ J/(kg}\cdot\text{K)}$, $\gamma_2 = 5$, $\sigma = 8.98 \times 10^6 \text{ m}^2/\text{s}^2$, $\beta = 1 \times 10^4 \text{ kg/(m}^2\cdot\text{s)}$, $h = 1 \times 10^7 \text{ J/(K}\cdot\text{s}\cdot\text{m}^{8/3})$, $\mu_c = 100 \text{ kg/(m}\cdot\text{s)}$, $q_{\text{chem}} = 5.84 \times 10^6$, $a = 2.9 \times 10^{-9} \text{ m/(Pa}\cdot\text{s)}$, $m = 1$, $I_{ig} = 0.5$, $k_I = 1.0 \times 10^6 \text{ s}^{-1}$, and $T_I = 2690 \text{ K}$.

Table 1. Comparison of the present results with the data in references.

Values	Sandusky ^[1]	Gonthier ^[11]	Yang ^[12]	Present
D (m/s)	432	418	402	411
ϕ_2	0.952	0.96	0.958	0.964
P_2 (MPa)	62.1	67.1	66.3	64.5

Figure 5 shows the velocity (relative to the laboratory reference frame), density and pressure of the gaseous product. A compaction wave quickly forms due to the moving piston. The velocity and density increase to 100 m/s and 67 kg/m³, respectively. The pressure increases to 20 MPa from the initial value of 2.57 MPa. As time goes on, the ignition is predicted to occur at the piston surface. The velocity, temperature and pressure increase rapidly. The detonation forms subsequently and strengthens in the propagation process. Lastly, the accelerating detonation grows into a steady detonation with a speed of 6160 m/s.

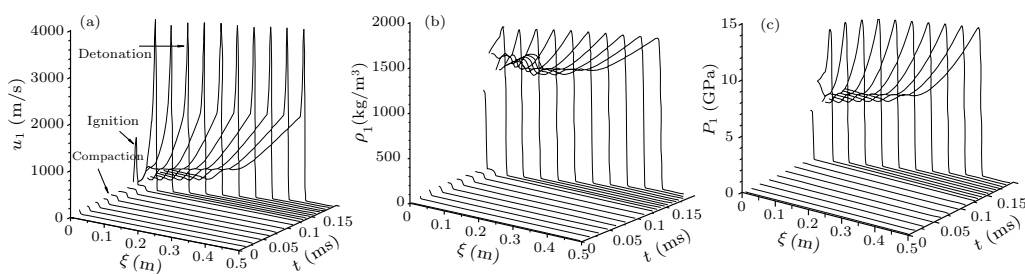


Fig. 5. Numerical results of the gaseous product: (a) velocity, (b) density, and (c) pressure.

Figure 6 shows the gas velocity profile at $t=0.2$ ms. The velocity increases rapidly in the reaction zone due to the detonation. The detonation is a rarefaction wave which reduces the velocity at the end of the reaction zone ($\phi_2 = 0$) to that of the piston. In front of the piston, a compaction zone is produced and the gas velocity is equal to the piston velocity. An interaction zone is predicted between the compaction zone and the rarefaction zone.

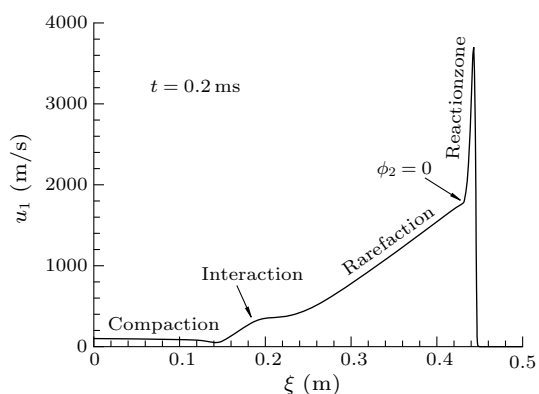


Fig. 6. The gas velocity profile at $t = 0.2$ ms.

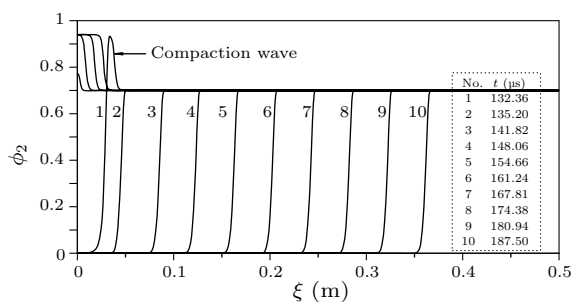


Fig. 7. Evolution of the solid volume fraction.

Figure 7 shows the evolution of the solid volume fraction. At the beginning of the piston movement, the granular solids are compacted from a volume fraction of 0.7 to 0.94. The inert compaction wave propagates away from the piston with a speed of 295 m/s. After about 128 μ s, the combustion is predicted to occur. The solid volume fraction continuously decreases. The granular near the piston surface is completely consumed at about 132 μ s. After about 135 μ s the detonation overtakes the compaction wave and propagates steadily.

Table 2 is the comparison of the numerical results

with the experiment and numerical simulation, which are cited from Ref. [11] directly. The values of the compaction wave speed D_c (relative to the laboratory reference frame), the solid volume fraction behind the lead compaction wave ϕ_2 and the detonation wave speed D_d agree very well with each other.

Table 2. Comparison of the results with Ref. [11].

Values	Experiment ^[11]	Simulation ^[11]	Present
D_c (m/s)	400	401.98	395
ϕ_2	0.90	0.94	0.94
D_d (m/s)	6200	6169.4	6160

In conclusion, the CE/SE method is applied to simulate a two-phase detonation model in porous media. The accuracy of the method is validated by comparing with other researches. An inert compaction problem is calculated first, the development and the structure of the compaction wave are validated by the data of the published experiment and simulations. A two-phase detonation process is numerically simulated by introducing a chemical reaction parameter. The numerical results have indicated the main characteristic of the detonation phenomenon, including the compaction wave, the rarefaction wave, the onset of combustion, and the transition to detonation, induced by low-velocity impact.

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