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New numerical algorithms in SUPER CE/SE and their applications in explosion mechanics

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The new numerical algorithms in SUPER/CESE and their applications in explosion mechanics are studied. The researched algorithms and models include an improved CE/SE (space-time Conservation Element and Solution Element) method, a local hybrid particle level set method, three chemical reaction models and a two-fluid model. Problems of shock wave reflection over wedges, explosive welding, cellular structure of gaseous detonations and two-phase detonations in the gas-droplet system are simulated by using the above-mentioned algorithms and models. The numerical results reveal that the adopted algorithms have many advantages such as high numerical accuracy, wide application field and good compatibility. The numerical algorithms presented in this paper may be applied to the numerical research of explosion mechanics.

new algorithm, SUPER CE/SE, numerical simulation, explosion mechanics

The research of explosion mechanics, usually involving many disciplines such as compressible flows, incompressible flows, elastic-plastic flows, chemically reacting flows and two-phase flows, contributes significantly to the field of industry, aeronautics, and military engineering. Numerical simulation of explosion mechanics needs not only accurate numerical schemes and interface capturing methods, but also a perfect combination of the selected numerical algorithms and the physical and chemical models.

The imported commercial software, such as LS-DYNA and AUTODYN, currently plays a dominant role in the application of explosion mechanics in China. Further development based on the imported commercial software is quite difficult, because the kernel modules of the software are always held as commercial secrets. The software of computational explosion mechanics in China has undergone a step-by-step development. The well-established software packages include METH [1] developed by BIAPCM (Beijing Institute of Applied Physics and Computational Mathematics) and MMIC [2] by BIT (Beijing Institute of Technology). The present software packages of computational explosion mechanics mainly adopt well-developed numerical algorithms and models, for example, VOF [3] (Volume of Fluid) method for interface capturing and trajectory method [4] for particle tracing.

This paper has studied the new numerical algorithms in SUPER CE/SE and their applications in explosion mechanics. SUPER CE/SE uses an improved CE/SE (space-time Conservation Element and Solution Element) method [5,6] to discrete governing equations, a local hybrid particle level set method to capture the interface, and a two-fluid model to treat two-phase flows. SUPER CE/SE is also able to adopt common chemical reaction models, such as two-step, de-tailed and Sichel's two-step chemical reaction models. With the above algorithms and models, problems of shock wave reflection over wedges, explosive welding, cellular structure of gaseous detonations and two-phase detonations in gas-droplet system are investigated. Comparisons and dis-

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cussions on the numerical results reveal the applicability of the above algorithms in computational explosion mechanics.

1 Numerical algorithms and models

Computational explosion mechanics refers to many areas of study including computational mechanics, fluid mechanics, solid mechanics, physics and chemistry. In this section, we mainly introduce the basic algorithms in SUPER CE/SE including the improved CE/SE scheme, the local hybrid particle level set method, the common chemical reaction models and the two-fluid model. The models of compressible flow, incompressible flow and elastic-plastic flow can be found in ref. [7,8].

1.1 Improved CE/SE method

The CE/SE method [9] originally proposed by Chang in 1995 is a new numerical framework for solving hyperbolic conservation laws. The CE/SE method substantially differs from the existing well-established CFD methods in that it contains many excellent features such as a unified treatment of space and time, satisfying both local and global flux conservation in space and time and simple treatments for boundary conditions. As a result of its simplicity, generality and accuracy, the CE/SE method has been successfully applied to scientific exploration and engineering. However researchers have found defects in the original CE/SE schemes, such as the complication of mesh structure, the absence of high-order accuracy schemes and the difficulty to extend to three-dimensional situation. To solve these problems, Zhang et al. [10], Zhang et al. [11] and Liu et al. [5,6] have made some progress in this area.

The improved CE/SE method used in SUPER CE/SE constructs SEs and CEs shown in Figure 1 on rectangular meshes and is extended to second-order accuracy. This construction of SE and CE on rectangular meshes has many

advantages such as simple mesh structure, clear physics concept, easy to extend to three-dimensional cases and convenient high-accuracy Taylor expansions. The physical variables Q, E and F at every mesh point $(t, x, y) \in SE(j, k, n)$ are approximated by their second-order Taylor expansions Q^* , E^* and F^* as

$$M^{*}(\delta x, \delta y, \delta t)_{P'}$$

= $M_{P'} + (M_{x})_{P'} \delta x + (M_{y})_{P'} \delta y + (M_{t})_{P'} \delta t$
+ $\frac{1}{2} (M_{xx})_{P'} (\delta x)^{2} + \frac{1}{2} (M_{yy})_{P'} (\delta y)^{2} + \frac{1}{2} (M_{tt})_{P'} (\delta t)^{2}$
+ $(M_{xy})_{P'} \delta x \delta y^{2} + (M_{yt})_{P'} \delta y \delta t + (M_{xt})_{P'} \delta x \delta t,$ (1)

where $M=Q, E, F, \delta x = x - x_{P'}, \delta y = y - y_{P'}, \delta t = t - t_{P'}$. A second-order accuracy CE/SE scheme can be constructed by eq. (1).

1.2 Local hybrid particle level set method

How to accurately trace the interface of materials is a challenge confronted in the Eulerian method for multi-material simulations. The Level Set method [12], originally proposed by Osher and Sethian in 1988, is an effective Eulerian algorithm for interface capturing. The level set method essentially refers to a level set function whose zero isoline exactly determines the material interface is introduced to describe the development of the material interface. The level set method can deal with very complicated topologic changes of interfaces, because it is not necessary to reconstruct interface fronts just like some "wave front tracing" methods.

Adalsteinsson [13] proposed a fast local algorithm for the level set method which confines the solving region to a narrow band surrounding the interface. This algorithm has the time complexity of O(Nw), where N is the number of grid points and w is the width of the narrow band. Applying the idea of fast local algorithm, Peng [14] proposed a fast level set method based on PDE (Partial Difference Equa-



Figure 1 Mesh construction of the improved CE/SE method. (a) Solution element SE(P'); (b) conservation element CE(P').

tions), which has merits such as easy to be implemented and time complexity of O(N).

Enright [15] introduced non-mass Lagrangian particles to the level set method to solve the problem of mass losing. Based on this idea, he proposed a hybrid particle Level Set method in 2002.

1.3 Common chemical reaction models

The two-step reaction model simplifies a complicated chemical reaction into an induction reaction and an exothermic reaction. The rates of *a* (progress parameter for induction reaction) and β (progress parameter for exothermic reaction), ω_{α} and ω_{β} , are given as below [16]:

$$\begin{cases} \omega_{\alpha} = -k_{\alpha}\rho \exp\left(-\frac{E_{\alpha}}{RT}\right), \\ \omega_{\beta} = \begin{cases} 0 \quad (\alpha > 0), \\ \omega_{\beta}^{+} + \omega_{\beta}^{-} = -k_{\beta}p^{2} \left[\beta^{2} \exp\left(-\frac{E_{\beta}}{RT}\right) -(1-\beta)^{2} \exp\left(-\frac{E_{\beta} + Q}{RT}\right)\right] \\ (\alpha \le 0), \end{cases}$$
(2)

where ρ is the mass density, *p* the pressure, *T* the temperature, *R* the gas constant, *Q* the heat release parameter, k_{α} and k_{β} the constants of reaction rates, and E_{α} and E_{β} the activation energies. The two-step reaction model does not need large computing resource because it only takes the heat release parameter *Q* into account. However, the two-step reaction model can describe the essential characteristics of detonations.

The detailed chemical reaction model is extensively used to describe the transformation of reactants into products at the molecular level through a large number of elementary steps. Concentrations of reactants, intermediates and products can be computed by integrating the sets of differential equations describing the rates of formation and destruction of each species. In the current study, an eight-species (H₂, O₂, H, O, HO, HO₂, H₂O, H₂O₂), twenty-reaction model for a hydrogen-oxygen detonation is used [17].

Sichel et al. [18] proposed a new two-step reaction model by considering multi-component densities. Sichel's two-step reaction model supposes that all mass percentage, Y_i , change linearly with the progress parameter of exothermic reaction β .

$$Y_{i} = (Y_{Ri} - Y_{Pi})\beta + Y_{Pi},$$
(3)

where Y_{Ri} and Y_{Pi} are the mass fractions of the *i*th species in the initial reactant and balanced product, respectively. Sichel's two-step reaction model can obtain more accurate gasdynamics parameters than the two-step reaction model, though the numerical mass distributions are approximated.

1.4 Two-fluid model

In this paper, we assume the gas-droplet system has the following characteristics: the flow is unsteady; the initial temperature of the gas and the droplets is the same; the radii of droplets are uniform; droplets are homogenously distributed initially; the phase of droplets is considered a continuous medium; the shape of droplets always remains spherical even in the process of separation, and evaporation; the temperature distribution in every droplet is uniform; the total volume of droplets can be ignored compared with the volume of gas; the interactions between droplets are ignored; when the fuel reaches the gaseous state, chemical reactions occur and accomplish immediately; the chemical energy is absorbed only by gas, which is considered ideal.

With these assumptions, the governing equations for gas phase can be expressed as

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \frac{\partial \boldsymbol{E}}{\partial x} + \frac{\partial \boldsymbol{F}}{\partial y} = \boldsymbol{S},\tag{4}$$

where

$$Q = (\rho, \rho u, \rho v, E),$$

$$E = (\rho u, \rho u^{2} + p, \rho u v, (E+p)u),$$

$$F = (\rho v, \rho u v, \rho v^{2} + p, (E+p)v),$$

$$S = (I_{p}, -F_{x} + u_{p}I_{p}, -F_{y} + v_{p}I_{p}, -(u_{p}F_{x} + v_{p}F_{y}) + ((u_{p}^{2} + u_{p}^{2})/2 + q_{r})I_{p}).$$

The governing equations for droplet phase can be expressed as

$$\frac{\partial \boldsymbol{Q}_{p}}{\partial t} + \frac{\partial \boldsymbol{E}_{p}}{\partial x} + \frac{\partial \boldsymbol{F}_{p}}{\partial y} = \boldsymbol{S}_{p}, \qquad (5)$$

where

$$\begin{aligned} \boldsymbol{Q}_{p} &= (\rho_{p}, \rho_{p}u_{p}, \rho_{p}v_{p}, N), \\ \boldsymbol{E}_{p} &= (\rho_{p}u_{p}, \rho_{p}u_{p}^{2}, \rho_{p}u_{p}v_{p}, Nu_{p}), \\ \boldsymbol{F}_{p} &= (\rho_{p}v_{p}, \rho_{p}u_{p}v_{p}, \rho_{p}v_{p}^{2}, Nv_{p}), \\ \boldsymbol{S}_{p} &= -(I_{p}, -F_{x} + u_{p}I_{p}, -F_{y} + v_{p}I_{p}, 0). \end{aligned}$$

Eqs. (4) and (5) describe the conservation (including density, momentums and total energy) of gas phase and droplet phase, respectively. ρ and ρ_p are the mass densities of gas phase and droplet phase, respectively; u, v, u_p and v_p the velocity components of gas phase and droplet phase, respectively; p the pressure, $E=p/(\gamma-1)+\rho(u^2+u^2)/2$ the total energy density, N the droplet numbers per unit volume, q_r the energy density of fuel, I_p the density variation by the phase change, F_x and F_y the forces components acting on droplets. The parameters of I_p , F_x and F_y can be found in ref. [19]. Mass, momentums and energy transfers are implemented by source items in governing equations.

2 Applications

2.1 Compressible flow

Numerical simulation of compressible flow needs a

high-accuracy numerical scheme that can capture shock waves accurately. The improved CE/SE method can capture strong discontinuity surface accurately [6]. In order to show the advantages of the improved CE/SE method in compressible flow, shock wave reflections are simulated and discussed.

When a shock wave encounters a wedge, the incident shock wave is reflected by the wedge surface, whereas the induced nonstationary flow behind it is deflected by the wedge corner, and that process is called shock wave reflection. Both experiments and theories show four types of shock wave reflections including regular reflection, single-Mach reflection, complex-Mach reflection and double-Mach reflection [20].

The computing area is 4.0×4.0. There is a supersonic inflow on the left boundary and the other boundaries are rigid. Other computational conditions are given in Table 1. Figure 2 shows the four types of shock wave reflections simulated by SUPER CE/SE. All the four types of shock wave reflections agree well with experiment results [20]. The numerical results indicate that SUPER CE/SE can discriminate the complex flow field in complex-Mach reflection and double-Mach reflection only using 400×400 meshes. This nu-

 Table 1
 Computational conditions of four shock wave reflections

	Mach number	Wedge angle (°)	Computational meshes
(a) Regular reflection	3.84	60	200×200
(b) Single-Mach reflection	1.5	30	200×200
(c) Complex-Mach reflection	5.2	20	400×400
(d) Double-Mach reflection	4.64	40	400×400



Figure 2 Four types of shock wave reflections. (a) Regular reflection (200×200) ; (b) single-Mach reflection (200×200) ; (c) complex-Mach reflection (400×400) ; (d) double-Mach reflection (400×400) .

merical case exhibits a high numerical resolution of SUPER CE/SE.

2.2 Incompressible flow

Incompressible flow is the foundation of elastic-plastic flow, though it may not be applied very broadly to explosion mechanics. The method of artificial compression is used in SUPER CE/SE to couple pressure and velocities. Numerical results show that the improved CE/SE method achieves high accuracy in both steady and unsteady incompressible flows [7].

2.3 Elastic-plastic flow

Elastic-plastic flow is one of the most important research topics in explosion mechanics. Currently, three plastic constitutive models, ideal plastic model, linear hardening model and Johnson-Cook model and two equations of state that Mie-Gruneisen and Jones-Wilkins-Lee (JWL) integrated into SUPER CE/SE. SUPER CE/SE have been used to simulate many problems of elastic-plastic flow such as impact [21], penetration [22], and explosive welding [23]. The full simulation of explosive welding needs to carry out a coupling computation of gas, fluid and solid, which most commercial software can't tackle. We have solved this difficult problem by adopting the local hybrid particle level set method to trace the interface of materials. The explosive welding, also called explosive combination, is a special welding technique in engineering that utilizes the explosive energy to drive two different metal boards welding together at a quite high velocity.

The computational model is shown in Figure 3(a). The target plate is LY12 aluminum with dimensions of 40 mm \times 7 mm. The rigid wall boundary condition in the *x* direction is imposed in the bottom of the target. The flyer plate is steel with a length of 40 mm and thickness of 1 mm. The distance between the target and the flyer plate is initially set to be 4 mm. The explosive is ignited on the left at the initial time. The computational area is 45 mm \times 20 mm. The number of computing meshes is 1350 \times 600. The total computing time is 15 µs.

Figures 3(b) and (c) show the density contours at 9 and 15 μ s, respectively. We can find a wavy interface between the steel plate and the aluminum plate from Figure 3(b). The numerical results also imply that the point of the highest velocity locates at the impact point, which leads to the highest value of the plastic strain, the shear stress and the pressure. The maximum pressure appears at the impact point that varies from 1 to 16 GPa. The extremely high pressure and plastic deformation result in a significant temperature increase which exceeds the melting points of the two metal plates on the impact interface. The two plates are welded together when the temperature of the material interface decreases rapidly.



Figure 3 Density contours at different time periods. (a) 0 µs (computing model); (b) 9 µs; (c) 15 µs.

2.4 Chemically reacting flow

A coupling problem of chemical reaction and mechanics function has to be investigated in explosion mechanics, so chemical reaction models are very important for accurate simulations. SUPER CE/SE has been applied to simulation of gaseous detonations [6]. In this paper, we investigate three chemical reaction models (the two-step reaction model, the detailed chemical reaction model and Sichel's two-step reaction model) in SUPER CE/SE by simulating the cellular structure of gaseous detonations

The computational model is a detonation propagating in a stoichiometric H₂-O₂ gas, and the initial pressure and temperature are 1 atm and 298 K, respectively. The detonation wave is generated by igniting on the left with a high initial pressure and temperature. Computing parameters of stoichiometric H₂-O₂ gas for the three chemical reaction models are given as follows. (1) Two-step reaction model: $Q=1.33\times10^7$ J/kg, $k_a=3.0\times10^8$ m³/kg·s⁻¹, $k_{\beta}=1.875\times10^{-5}$ m⁴/N²·s⁻¹, $E_a=2.261\times10^7$ J/kg, $E_{\beta}=4.6151\times10^6$ J/kg [16]. (2) Detailed chemical reaction model: reference [17]. (3) Sichel's two-step reaction model: $a=1.2\times10^8$, $b=8\times10^3$, c=0[18]; $CP(H_2, O_2, H, O, HO, HO_2, H_2O, H_2O_2)=(1.978\times10^{-2},$ $0.10042, 4.49\times10^{-3}, 3.27\times10^{-2}, 0.14027, 2.3209\times10^{-4},$ $0.70209, 2.2772\times10^{-5}), which are calculated from the de$ tailed chemical reaction model.

Figure 4(a) shows the cellular pattern by experiment, and Figures 4(b)–(d) shows the numerical cellular patterns using the two-step reaction model, the detailed chemical reaction model and Sichel's two-step reaction model, respectively. All the three chemical reaction models can simulate the cellular structure of gaseous detonations, though the ap-

pearances of the cellular pattern differ. In order to research the accuracy of the three chemical reaction models, we list cell parameters of the three numerical cellular patterns to compare with the experimental pattern in Table 2. This comparison shows that all the three numerical cellular patterns agree well with the experiment results.

2.5 Two-phase flow

SUPER CE/SE is also able to simulate gas-particle twophase flows. Many chemical reaction systems in explosion mechanics, for example, the gas-droplet combustion and explosion system, can be converted into gas-particle two-phase flows for numerical simulation. The two-fluid model is introduced in SUPER CE/SE to treat the particle phase. In this paper, O_2 - C_6H_{14} (fuel droplet) two-phase planar detonations are simulated at different equivalence ratios. In the numerical simulation of a two-phase detonation, the complex interactions should be considered between the two phases, such as mass transfer, momentums transfer and chemical reactions.

Figure 5 shows the detonation velocities of C_6H_{14} fuel (droplet diameter is 50 µm) at different equivalence ratios by C-J (Chapman-Jouquet) theory, experiments [24] and numerical simulations, respectively. We can find that the numerical results can predict the correct profile and are much closer to the experiment than those by C-J theory. Comparing the results of two-phase detonation with the gaseous detonation, we realize that the simulation and the experiment in two-phase detonations are more inconsistent than in gaseous detonations. Obviously, there are more errors in two-phase experiments than in gaseous experiments. For example, the



Figure 4 Cellular patterns by experimental and numerical simulations (220×200 meshes). (a) Experiment; (b) two-step reaction model; (c) detailed chemical reaction model; (d) Sichel's two-step reaction model.

Table 2 Cell parameters of experimental and numerical cellular patterns

	Cell width/cell length (d/l)	Exit angle α (°)	Entrance angle $\beta(^{\circ})$	Angle of transverse wave trace $\omega(^{\circ})$
Experiment	0.5-0.6	5-10	32-40	≈ 30
Two-step reaction model	0.59	9.2	33.0	30.5
New two-step reaction model	0.60	11.2	31.5	29.0
Detailed chemical reaction model	0.51	9.5	38.2	28.5

detonation velocities may be 300 m/s different in different experiments under the same experimental conditions as in reference [24]. Furthermore, some substantial errors might occur in experiments. For example, the experimental results in Figure 5 produce an unexpected error that the detonation velocity is lower at ϕ =0.6 than ϕ =0.5. The experimental conditions such as droplet size, droplet distribution are usually very difficult to be well-proportioned. These unclear experimental conditions also lead to difficulties in numerical validation.

3 Conclusions

In this paper, we have presented the new algorithms in SUPER CE/SE and their applications in explosion mechanics. The main researched algorithms and models include the improved CE/SE method, the local hybrid particle level set method, three chemical reaction models (including the two-step reaction model, the detailed chemical reaction model and Sichel's two-step reaction model) and the two-



Figure 5 Detonation velocities of C_6H_{14} fuel at different equivalence ratios.

fluid model. Problems of shock wave reflection over wedges, explosive welding, cellular structure of gaseous detonations and two-phase detonations in gas-droplet system are simulated and discussed. The discussions of the numerical results show that: (1) The improved CE/SE method has many advantages, such as clear in physical concept, accurate to capture a shock wave, convenient to implement boundary conditions and easy to be extended to three-dimensional situations; (2) the interface capturing method and the various kinds of chemical and physical models can be integrated with the improved CE/SE method perfectly; (3) SUPER CE/SE can compute multi-material simultaneously and achieves high computational accuracy, wide application range and good compatibility. SUPER CESE can be widely applied to research of explosion mechanics and aeronautic and military engineering.

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