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Simulating the explosive shear and friction ignition problem by Thermo-mechanical Coupling technique with Unstructured Polygon Meshs

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Abstract: Non-shock process of shear and friction bring threaten for high explosive safety. In this ignition process, it may be a thermo-mechanical large deformation problem. For simulating explosive safety problem, A cell-centered finite volume scheme is used for discretizing diffusion equations on unstructured arbitrary polygonal meshes of LAD2D, which is a thermo-mechanical coupling technique. Using a composite explosive friction ignition model and developed shear ignition model, We simulate important explosive shear and friction tests, such as ODTX test, the constrained friction test with long pulse duration low pressure, friction sensitivity test of explosive tablet and low velocity shear ignition test, then get the same results with tests. It prove validity of thermo-mechanical coupling technique and program.

Keywords: Shear, Friction, Thermo-Mechanical, Unstructured Mesh.

1 Introduction

High explosives may ignite and burn, when they are subjected to some unexpected insults such as non-shock process of shear or friction[1]. It bring huge threaten for explosive safety. For preventing it, we study the mechanism and process of explosive ignition, and also simulation method. There are two effects including deformation by forces and temperature rise of chemical reaction at the same time, which is found in experiments. In explosive friction problem, many researcher find that the light shock can make explosive ignition in the test[2], in which friction is an important source for hot spots. Glenn[3] make a Intense Pressure and Friction Test(IPFT), which is a repeat test for friction ignition. At early research, the particles of friction surface may quicken the ignition[4]. YanQing Wu found melt materials on the friction surface in test figure[5], thought that it was lubricative and the coefficient of friction became small. In the process of friction, friction work became temperature rise, producing hot spot, at last make explosive ignition. It is some different in explosive shear ignition. If shear stress exist in the explosive by the outside effect such as shock, may produce transverse shear strain, deformation and flow velocity. When shear stress is strong enough, adiabatic shear banding may occur by dissipation of mechanical flow energy into heat, which is mechanism for localization of energy deposition in explosive. A further complexity is that material damage may also influence the ignition process. Bridgman[6] was the first to point out that shear-induced reactions may occur in explosive. Many laboratories[7] found shear-induced reactions and ignition in drop-weight impact test and susan test. Boyle[8] first design an explosive shear test, then basing on split hopkinson pressure bar(SHPB), Kraewinski[9] design an explosive shear test, which can get shear stress, displacement and shock velocity of ignition. It can be a good test for simulation.

For studying and simulating explosive safety problem in this paper, we base on unstructured arbitrary polygonal meshes program LAD2D for large deformation problem, A cell-centered finite volume scheme is used for discretizing diffusion equations in LAD2D[10], and has calculation ability of thermo-mechanical coupling effects. Basing on the explosive friction model[11]and shear model, developed for composite explosive in friction model and explosive reaction rate in shear model from experiment research, simulate typical explosive shear and friction tests.

2 Methods and Simulation Results

A two dimensional lagrangian unstructured mesh Adaptive fluid dynamics (LAD2D) program is used to calculate explosive problem. The management system of unstructured N-polygon meshes, which is suitable for complex geometry and mesh topology changing during fluid computation, finite volume method and closed void slide method made the program good adaptability for large deformation in multi-medium detonation fluid problems. And a cell-centered finite volume scheme is proposed for discretizing diffusion equations on unstructured arbitrary polygonal meshes. It is extent from the conservation scheme [12],which has not found used in unstructured arbitrary polygonal meshes. We use the nonlinear energy type diffusion equations:

$$\begin{aligned} \rho\frac{d\varepsilon}{dt}-\nabla\cdot\left(\kappa\nabla T\right)&=f,\\ T\left(x,r,0\right)&=T^0,\\ \alpha\kappa\nabla T\cdot\vec{n}+\beta T&=g. \end{aligned} \tag{1}$$

Where ρ is the mass density , ε is the mass-specific internal energy, t is time, κ is the heat conduction coefficient, T is the temperature and f is volume specific external energy sources, $\vec{n}$ is the unit outward normal vector. α, β, g is the given value as the function of the space coordinates(x, r). Denote $\vec{F}=-\kappa\nabla T$ as heat flux, $F=-\kappa\nabla T\cdot\vec{n}$ is the normal flux.

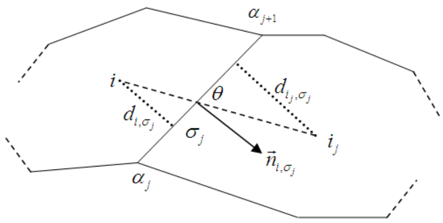


Figure 1: The stencil of the diffusion scheme on polygonal meshes

In figure 1, the vertex unknowns has been expressed by the neighboring cell-centered unknowns. The Diamond finite volume diffusion scheme on unstructured arbitrary polygonal meshes :

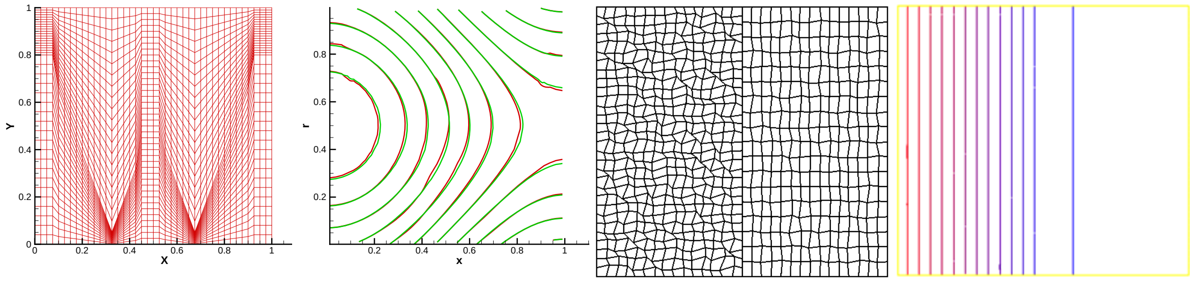
$$m_i\frac{\varepsilon_i^{n+1}-\varepsilon_i^n}{\Delta t}+\sum_{j=1}^{l_i}F_{\sigma_j}^{n+1}L_{\sigma_j}=A_i f_i^{n+1} \tag{2}$$

Where m_i is the mass of the cell i , Δt is the time step, l_i is the total number of the edges for cell i, $F_{\sigma_j}^{n+1}$ is the discretized normal flux on edge σ_j. The diamond diffusion scheme will reduce to the so-called nine-point scheme on quadrilateral mesh. The discretized normal flux can be write like this:

$$F_{\sigma_j}^{n+1}=\begin{cases}-\kappa_{\sigma_j}^{n+1}\left[\dfrac{T_{i_j}^{n+1}-T_i^{n+1}}{d_{i_j,\sigma_j}+d_{i,\sigma_j}}-D_{\sigma_j}\left(\dfrac{T_{\alpha_{j+1}}^{n+1}-T_{\alpha_j}^{n+1}}{L_{\sigma_j}}\right)\right], & \sigma_j-\text{internal edge}\\ -\kappa_i^{n+1}\dfrac{g_{\sigma_j}-\beta_{\sigma_j}T_i^{n+1}}{\alpha_{\sigma_j}\kappa_i^{n+1}+\beta_{\sigma_j}d_{i,\sigma_j}}, & \sigma_j-\text{boundary edge}\end{cases} \tag{3}$$

$$\kappa_{\sigma_j}^{n+1}=\frac{d_{i_j,\sigma_j}+d_{i,\sigma_j}}{\dfrac{d_{i_j,\sigma_j}}{\kappa_{i_j}^{n+1}}+\dfrac{d_{i,\sigma_j}}{\kappa_i^{n+1}}},\ D_{\sigma_j}=\frac{(\boldsymbol{R}_{i_j}-\boldsymbol{R}_i)}{\left|\boldsymbol{R}_{i_j}-\boldsymbol{R}_i\right|}\cdot\frac{(\boldsymbol{R}_{\alpha_{j+1}}-\boldsymbol{R}_{\alpha_j})}{L_{\sigma_j}}\frac{\left|\boldsymbol{R}_{i_j}-\boldsymbol{R}_i\right|}{d_{i_j,\sigma_j}+d_{i,\sigma_j}},$$

In figure 2, We do some test on some different meshs, get the right result. Now the program LAD2D can be used for the conduction calculation in the fluid mechanics process.



a. Continuous coefficient diffusion problem b. Discontinuous coefficient diffusion problem

Figure **2**: The numerical test on different polygonal meshes

2.1 Explosive Fiction Ignition Simulation

We have a composite explosive friction ignition model. Melting temperature of explosive is lower than igniting temperature, which is observed in test[5]. So it is needed to do the melting simulation, in the energy equation:

$$\rho \frac{dE}{dt} - \nabla \cdot \left(\kappa \nabla T\right) = f,$$
$$E = \varepsilon + \Delta E \tag{4}$$

E is internal energy include melting energy, changing with the β, which is the fraction of melting material.

$$\Delta E = \beta L \qquad \begin{array}{l} \beta = 0 \ \ if T < T_{solidus} \\ \beta = 1 \ \ if T > T_{liquidus} \\ \beta = \dfrac{T - T_{solidus}}{T_{solidus} - T_{liquidus}} 1 \ \ if T_{solidus} < T < T_{liquidus} \end{array} \tag{5}$$

T is temperature, L is latent heat. And the Friction force is reduce with temperature rising, so we assume that friction coefficient is linear changed with temperature of friction face.

We also develop the model for composite explosive, which some parameters of model is lacking. The reaction heat Q is calculated as mass fraction f of single compound explosives(one composite explosive may contain more than one single compound explosive):

$$Q_{\text{composite explosive}} = Q_{\text{explosive1}} * f_{\text{explosive1}} + Q_{\text{explosive2}} * f_{\text{explosive2}} + \ldots \tag{6}$$

Consider just one single compound explosives melting, whose melting temperature is lowest. So melting temperature, latent heat L and friction coefficient use this single compound explosive's parameters. We give parameters of some composite explosive in table 1.

$$L_{\text{composite explosive}} = L_{\text{explosive1}} * f_{\text{explosive1}}$$
$$\mu_{m\text{composite explosive}} = \mu_{m \text{ explosive1}} \tag{7}$$

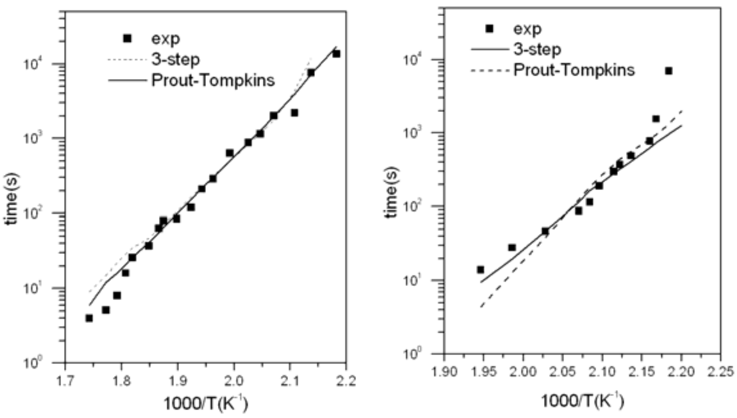
Table 1 The parameters of composite explosives

	r **(kg/m³)**	***C*** **(J/kg•K)**	***k*** **(J/s•m•K)**	***Q*** **(J/kg)**	***E*** **(J/mol)**	***Z*** **(s⁻¹)**	***L*** **(J/kg)**	***T*m** **(K)**	***k*m** **(J/s•m•K)**
JOB-9003	**1850**	**1020**	**0.302**	**0.2442**	**2.00e6**	**1.43e5**	**4.78e12**	**1.82e5**	**541.5**
GO-	**1700**	**966.93**	**0.20**	**0.2164**	**1.84e6**	**1.428e5**	**4.45e13**	**1.84e5**	**541.5**

924									
JO-9159	**1860**	**1050**	**0.369**	**1.99e6**	**2.21e5**	**5e19**	**1.99e5**	**541.5**	**0.2164**
GH-923	**1650**	**1090**	**0.197**	**1.7364e6**	**1.998e5**	**1.702e17**	**1.2329e5**	**477.1**	**0.305**
JH-9005	**1770**	**1230**	**0.195**	**0.305**	**2.02e6**	**1.97e5**	**2.02e18**	**1.43e5**	**477.1**

The Friction sensitivity test is simulated for four composite explosives(JO-9159, JH-9005, JOB-9003 and GH-923). The test is 1D problem. The test result is RDX(76) > JO-9159(15%) > Tetryl(12) > JH-9005(<=12%) > TNT(4-6%) ~ JOB-9003(5%) > GH-923(<=5%) > TATB(0-4) ~ DATB(0-4), which is given order of the mass percent of reaction explosive. The more percent means shorter ignition time during same test time. So the result of simulation is RDX(0.42ms) < JO-9159(0.44ms) < Tetryl (0.46ms) < JH-9005(0.48ms) < JOB-9003(0.55ms) < GH-923 (0.57ms) < TNT(0.65ms) < TATB(0.77ms) < DATB(0.83ms). The order is same with test. So the friction model is suitable for many different explosive.

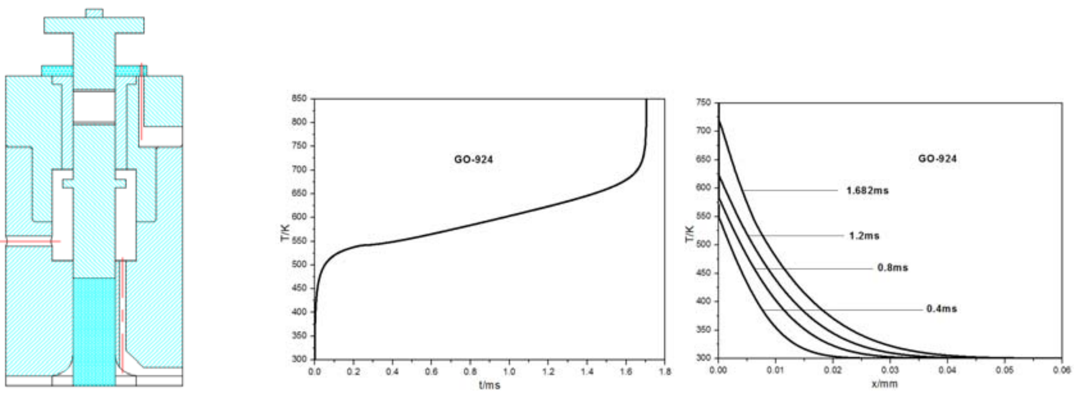
ODTX(One-Dimensional Time-to-Explosion) test[13] is pure heat conduction problem. In test, explosive will ignition under a still temperature in a certain time. This time is recorded. The two reaction model is used, which is 3-step reaction model[14] and single step Prout-Tompkins model[15]. The result of simulation is fit with test time point in figure 3.



TNT RDX

Figure 3: The simulation results of ODTX test

The constrained friction test with long pulse duration low pressure is simulated too. In the test, big mass drop hammer do low pressure long pulse to explosive. Explosive rubs against metal wall. Velocity and stress data of metal stick can be gotten from test. The result is ignition time 1~3ms in the condition of pressure 120MPa, friction velocity 7.7m/s. In figure 4, the result of simulation is ignition time 1.682ms, fit with test.



(a) test (b) temperature curve of friction interface (c) temperature distributing

Figure **4**: The constrained friction test arrangement with long pulse duration low pressure and result of simulation

A friction sensitivity test of explosive tablet is like friction sensitivity test, but used a steel plate on which 250~380mm quartz sand stuck, in figure 5. The result test is explosive ignition with displacement 102 mm and velocity 2.7m/s, so longest ignition time must smaller than 37ms. The result is JOB-9003:36.5ms, GH-923:21.4ms. The result is fit test too. All these results have proved the validity of conduction calculation.

(a)friction test (b) steel plate with quartz interface (c) Temperature curve of friction

Figure **5**: the friction sensitivity test of explosive tablet and the result of simulation

2.2 Shear Ignition Simulation

Consider the numerical simulation of shear test[16], just consider the shear work transfer into heat, a simple formula of shear temperature rise is used:

$$T_{shear} = T_0 + \frac{\eta_{eff} \cdot \int_0^t \sigma(t)\dot{\varepsilon}(t)\mathrm{d}t}{\rho C} \tag{8}$$

η_{eff} is energy transform coefficient, $\sigma(t)$ is shear stress, $\dot{\varepsilon}(t)$ is shear strain rate. C is specific heat

The heat form reaction is consider using the reaction rate formula:

$$\frac{1}{w}\frac{dw}{dt} = Z\exp(-E/RT)$$

$$\frac{dF}{dt} = I(1-F)^{2/9}\eta^4 + G(1-F)^{2/9}F^{2/3}p^z \tag{9}$$

Which is combine with Arrhenius rate and ignition and growth rate. Damaged Johnson Cook constitutive model is used for calculating shear stress and damage of explosive.

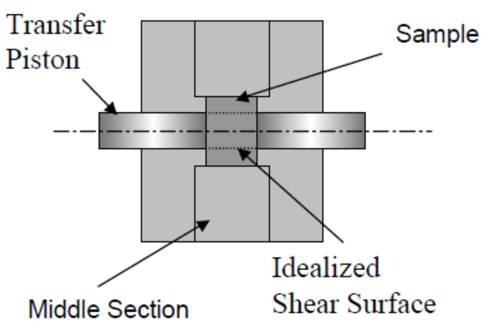
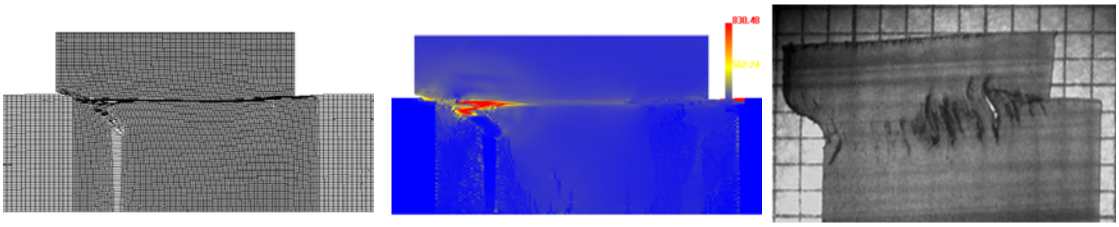


Figure **6**: The low velocity shear ignition test



(a) (b) (c)

Figure **7**: The simulation results of meshs(a), temperature (b)and results of test(c)

In figure 6, a low velocity shear ignition test[9] is simulated. In figure 7(b), there is high temperature in the explosive which is caused by shearing. And in shear position, some chemical reaction happen in the test. The result is agreement with the test qualitatively in figure 7(c), which prove validity of thermo-mechanical coupling technique and program LAD2D.

3 Conclusion and Future Work

Many explosive friction and shear test is simulation with developed friction and shear model using LAD2D. The results are fit with tests, which means the thermo-mechanical coupling technique of LAD2D can used to simulating the explosive heat conduction problem. The changed model for composite explosive is reasonable and easy implementing. This work make contribution for quantified work. The temperature rise formula just considering shear work, has to be developed for detailed effect, for comparing the test displacement in the future.

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