Numerical Simulation for the Thermal Response of the PBX-2 Explosive with Confinement on Fire*

Zhang Xiao-Li[1], Hong Tao[1] , Dong He-Fei[1] , Lou Jian-Feng[1], Li Jian-ling[2]
[1]Institute of Applied Physics and Computational Mathematics(IAPCM)
Beijing, China

[2]Northwestern Polytechnical University,xi'an,Shanxi province, China

1 Instruction

The weapon and ammunition can usually be heated by the unexpected thermal source.The thermal source can be self-produced, as in the center of a well-insulated, large volume of energetic material, or it can arise from an external event such as a fire. As a rule, the process is called "cookoff ". The heating can be rapid or very slow, or anything in between. The energetic material can be homogeneous, or it may have been damaged, either through thermal expansion and chemical processes or mechanically.

The cookoff refers to any situation in which bulk explosive is heated either directly to ignition (sometimes referred to as fast cookoff) or to a temperature at which relatively slow exothermic reactions eventually generate heat faster than it is removed by dissipative transport processes, leading to self-heating to ignition (slow cookoff). These events split naturally into two quite distinct stages, with different timescales and dominant physics and chemistry. During the preignition (heating) stage, which may last from seconds to days, external heating of the explosive leads to relatively slow processes such as phase changes, slow mechanical and chemical damage, and largely solid-state chemical decomposition. At some point, ignition occurs, by which we mean a transition to faster, and generally much more exothermic, gas-phase chemistry. If the explosive is confined, high pressurization rates will result, with accompanying high-strain-rate deformation of both the explosive and the confinement, and the possibility of compaction and shock wave formation that may lead to a transition from deflagration to a higher order event such as detonation. The post-ignition event may be over in milliseconds or even in microseconds, and is complicated considerably by the thermally damaged state of some or all of the explosive charge[1]. So the process of the cookoff of the weapon is very complicated and the research for the thermal stability of the weapon such as the missle is very important.

The research method of explosive cookoff includes mainly the cookoff experiment and numerical simulation. In 1987, American designed the fast cookoff test , in which the fuel was aviation kerosene and the explosive was subjected to external fire. The cookoff violence was judged by witness plate , fragments size and temperature of the bomb[2]. In 1991, Nakost et al. made cookoff test s in the enveloped and unenveloped pool fire. The surface temperature and heat flux were measured. They

---

* **Correspondence to: xiaoli_zhang79@yahoo.com,hongtao@iapcm.ac.cn**

indicated that the cookoff test in unenveloped scene approached to the reality condition[3]. In 1999 , Sumrall carried out the large scale fast cookoff test on insensitive explosive(TE-T7005) , in which the flame temperature was measured[4].The results showed that only burning reaction occurred. Heretofore, only USA has made such large scale fast cookoff experiments. In 2005,Ren Yan simulated fast cookoff experiment for JB9014 explosive , in which propellant was used as fuel and the flame temperature can reach more than 2000K[5,6].

In the paper, the numerical simulation of the thermal response of the bombs with PBX-2 explosive on fire were carried out by means of FLUENT program, in which the charge size are φ25mm×50mm andφ50mm×100mm. The PBX-2 is comprised about 87% by weight of HMX crystals, about 7% by weight of TATB crystals, about 4.2% by weight of polymeric binder and 1.8% by weight of antioxidant stabilizer. The calculating condition of fire was proofreaded by the experiment. The time to ignition,the location of the ignition and the ignition temperature are obtained. The law of the explosive was analysed. The results of the simulation show good agreement with that of the expeiments.

2 Confirming parameters for model

According to the test results[7,8], the explosive parameters, thermal capacity, thermal conductivity,the activation energy and frequency factor are confirmed by repetitious calculation, as well as the mass flow rate(kg/s) of the combustion gases in simulations.

3 Numerical simulation

Figure 1. shows the schematic geometry of cookoff model. The flame of fuel was considered. The diameter of model domain is 2000 mm and the length is 1500 mm. The domain includes the bomb,oil pool and air.The high temperature combustion gases were ejected into the calculating domain from the mass flow inlet.And the cookoff bomb was heated by the combustion gases.

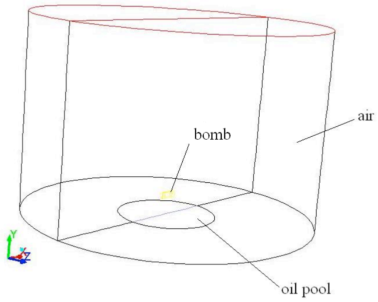


Figure 1. Schematic geometry of cookoff model

The model domain was symmetric cylinder. The half model of the domain was set up to decrease the computing time. The schematic geometry of the cookoff bomb and the keypoints distribution which were focused were shown in Figure 2.Five keypoint were selected to measure the temperature change of the cookoff bomb in numerical simulation. Number 1 is ignition position. Number 2 lies in the side of the cylindrical surface, Number 3 and Number 4 lie in the top of cylinder surface. Number 5 is the center position.The calculation grid of model is shown in Figure 3.

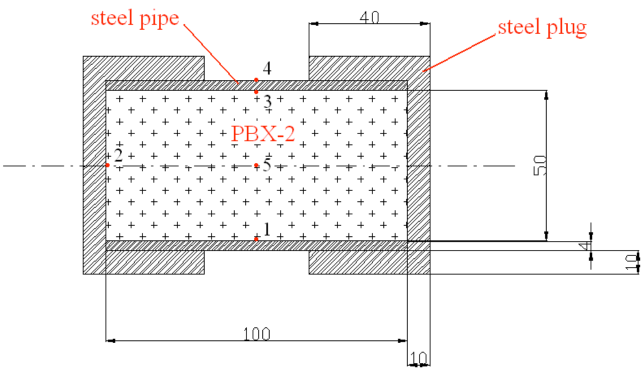


Figure 2. The schematic geometry of the keypoint distribution in simulation

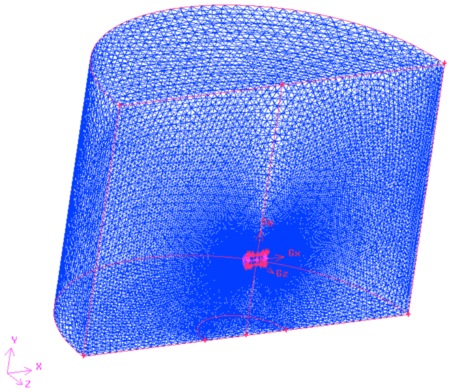


Figure 3. The calculation grid of model

The assumptions were as follows :

☐ Consider explosive as the solid and no phase change occurs.
☐ No gap exists between explosive and steel pipe.
☐ Thermal decomposition reaction of explosive obeys Arrhenius equation.
☐ All physical chemistry parameters of explosive are constant.

The calculating model equation as follows:

$$\rho c \frac{dT}{dt} = \lambda \nabla^2 T + S \tag{1}$$

It is the thermal conductive equation with source term. where $\rho$is the density,c is specific heat at constant pressure, λ is the thermal conductivity;S is the heat source term of the explosive decomposing reaction.

The self decomposing can be described by Arrhenius equation as follows[9] :

$$S = \rho Q Z \left(1 - \alpha\right)^n \exp(-E / RT) \tag{2}$$

where S is the heating source term of decomposition reaction ; $\rho$is the TNT density (kg·m^{-3}) ; Q is the reaction heat (J·kg^{-1}) ; Z is the frequency factor (s^{-1}) ; E is the activation energy (J·mol^{-1}) ; α is the reaction fraction; n is the reaction order,here the zero order reaction is adopt, namely n=0. R is the gaseous constant (J·mol^{-1}·K^{-1}) . Eq. (2) can be implemented a subroutine in C language and imported to the hydrodynamic code[10].

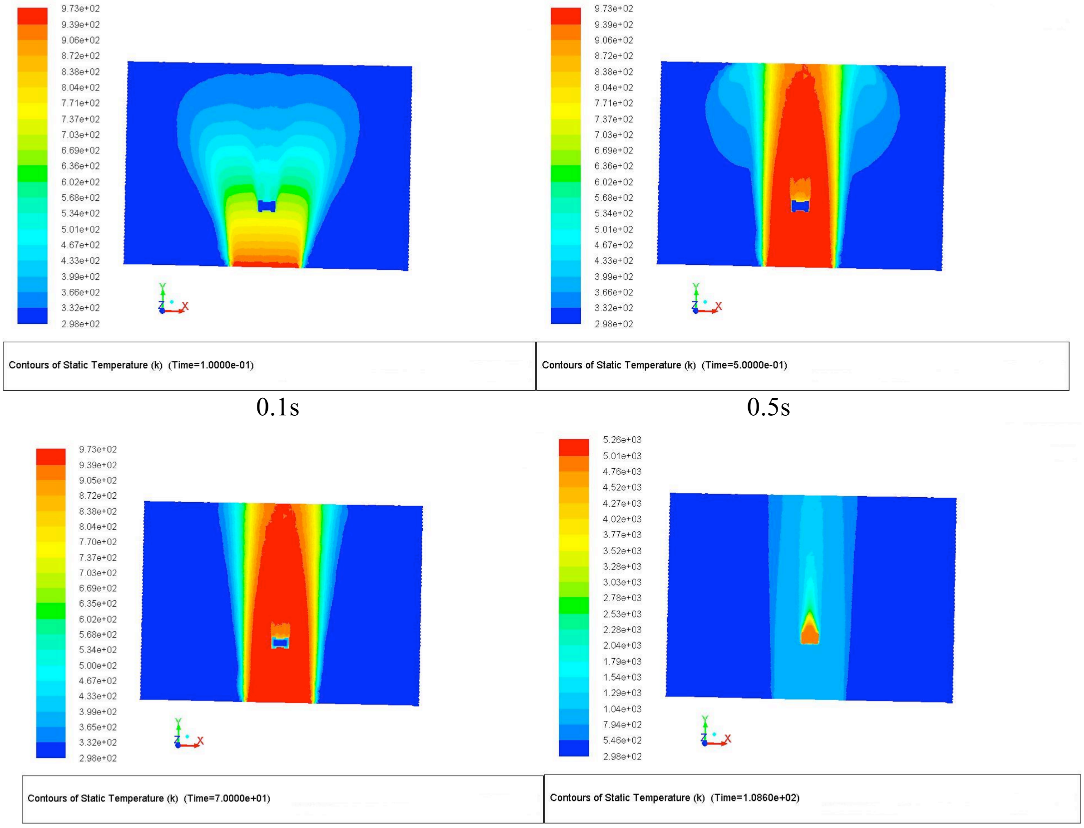
4 Boundary condition

According the experiments condition, the diameter of the oil pool is 500mm.So in numerical simulation, the high temperature (973 K) combustion gases was ejected into the mass flow inlet, the diameter of which is 500mm. The combustion gases were described by high temperature mass flow generated from the kerosene. The combustion gases flow is turbulent flow. The k -εturbulent model was employed[11] . The initial temperature was 278 K. The numerical simulation of explosive cookoff was conducted by computational fluid dynamics(CFD) software , FLUENT. Tab.1 shows the parameter of the materials.

Table 1:The parameters of the materials

materials	Density /kg·m^{-3}	thermal capacity /J·kg^{-1}·K^{-1}	thermal conductivity /w·m^{-1}·K^{-1}	reaction heat /kJ·kg^{-1}
PBX-2	1850	1020	0.302	4780
steel	8030	502.48	16.27	—

5 Calculated results and discussion



0.1s 0.5s

70s 108s

Figure 4. Temperature distribution on domain section at different time

Figure 4. shows the temperature distribution on domain section at different time for fire cookoff of theφ50mm×100mm bomb. At 0.5s , the high temperature zone lied in the underside and all sides of the bomb. But average temperature on top surface was lower . At 70s , the test item was completely engulfed by the flame. Only the flame temperature on the narrow zone above the bomb was a little lower. At 108s ,the bomb burst.

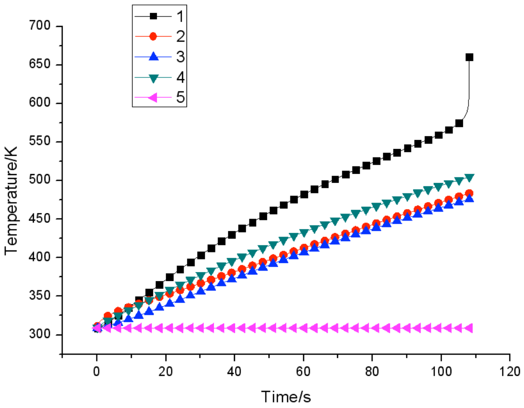


Figure.5. The curve of temperature change of the keypoints

Figure 5 shows the calculated temperature vs. time curves of ignition position and three monitored positions on axis vertical of PBX-2 bomb. It is seen that temperature on the underside explosive rose rapidly, but the upside temperature rose slower than that of the ignition location before reaction.Moreover , there was almost no change in temperature of the explosive inside. The inflexion in the curve is considered as the ignition point. The curve of ignition position reveals that the ignition temperature (550 K) and ignition time (108s) of PBX-2 explosive can be confirmed from the inflexion.Contrast to the measure results, the ignition time of the calculating(108s) is a little shorter than that of the experiment(120s) by Dai Xiao-gan[12]. It could be the fire condition,for example the temperature,the direction etc, would be affected by the circumstance and weather,while the heating condition in numerical simulation is fixed(700□). So the heating rate of the explosive of numerical simulation is faster than that of the expeiment. As a result, the ignition time of the explosive in simulation is earlier.

In simulation,the ignition time of the bomb that the charge size ofφ25mm×50mm is 107s, while in the fire cookoff expeiment[12], the ignition time is 140s, the reason is the same as theφ50mm×100mm bomb.

6 Conclusion

The numerical simulation of the thermal response of the bombs with PBX-2 explosive on fire were carried out by means of FLUENT program, in which the charge size areφ25mm×50mm and φ50mm×100mm. From the simulation result,we get some useful conclusion:

Firstly, the ignition location is on the bottom of the cookoff bomb, where the heating rate is most fastest. Under the condition of the temperature of fire is 700□,the ignition time of the two charge size of the bomb, φ25mm×50mm andφ50mm×100mm, is about 110s, and the ignition temperature is about 280□.

Secondly, the temperature in the center of the bombs almost do not increase.Because the thermal decomposition takes place in the surface of the explosive cylinder, where the temperature has reached the ignition temperture,while the temperature in the center of the explosive remains normal temperature.

Finally, the fire is one kind of fast cookoff condition. The ignition loction of the explosive is on the surface of the explosive cylinder.The thickness of the steel pipe is the same.As a result, the ignition time of the two charge size, φ25mm×50mm andφ50mm×100mm, is almost the same.The charge size can hardly affected the ignition law of the cookoff bomb.

Acknowledgements

This work is supported by the national natural science foundation of China (No. 11302031, No.11372053), Foundation for development of Science and Technology of CAEP (No. 2012A0101004, No.2013B0101014),Robust Munitions Center,CAEP(RMC2014B02)

References

[1] Blaine W. Asay.Cookoff. Non-Shock Initiation of Explosives[C].ShockWave Science and Technology Reference Library.Vol.5.403

[2] Rooijers A J T , Leeuw M W. Literature study of cookoff , PML-1987-22 [R] .Virginia : Naval Surface Weapon1 Center , 1987.

[3] Nakost J T , Kent L A , Sobolik KB. Fast cookoff testing in enclosed facilities with reduced emissions , Sand-91-0470C[R] . Albuquerque , NM: Sandia National Laboratories , 1991.

[4] Sumrall T S. Large scale fast cookoff sensitivity resultsof a melt castable general purpose insensitive high explosive [J] . Propellants , Explosives , Pyrotechnics , 1999 ,24 : 61-64.

[5] Ren Y. Investigation on explosive thermal characterunder high temperature [D] . Beijing : School of Mechtronics Engineering , Beijing Institute of Technology , 2005. (in Chinese)

[6] Wang P,CHEN L, WANG X F.etc. Cookoff Test and Numerical Simulation for Explosive Heated by Fire[J]. Journal of Beijing Institute of Technology,2009,18(2):146-151. (in Chinese)

[7] Dai X G,LV Z J,SHEN C Y,etc.Reaction Rule for Different Size PBX-2 explosives in Fast Cook-off Test[J].Chinese Journal of Explosives and Propellants,2008,31(3):47-49. (in Chinese)

[8] Wang P, Chen L, Lu J Y, etc.Cookoff experiments of the explosive on fire and the numerical simulation[C]. The 4th Academic Conference of Calculating Explosion Mechanics,Qinghai province,August 2008,347-354.

[9] Wang P , Chen L , Wang Y , et al. Numerical simulation of explosive cookoff at different heating rate[C] □Huang Ping , Wang Yajun , Li Shengcai. Theory and Practice of Energetic Materials , VOLVII. Beijing :Science Press ,2007 :701-704.

[10] Fluent Inc. FLUENT User's Guide [M]. New Hampshire : Fluent Inc ,2006.

[11] Wang F J. Analysis of computational fluid dynamics [M] . Beijing : Tsinghua University Press , 2004 :11. (in Chinese)

[12] Dai X G,Lv Z J,Shen C Y,etc. Slow cookoff experiments and the numerical simulation of the two charge sizes of JOB9003 explosive[C].The 8th Academic Conference of Explosion Mechanics of China,Jiang xi province,September 2007, 29-32.