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DIFFERENT ATTITUDES TO SIMULATION OF SLOW COOK-OFF EXPERIMENTS

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Abstract:

Heat transfer during the slow cook-off test of PBX was successfully simulated using three computational codes. LS-DYNA and COMSOL Multiphysics are both 3D multipurpose commercial codes based on the finite element method. The simplified 1D simulation was carried out using GNU/Octave and the finite difference method. The codes, their applicability for the modeled problem, advantages and disadvantages are discussed and evaluated. The results were compared to the experimental slow cook-off test of Semtex 1A (czech PETN based putty-plastic explosive) and with the critical temperature according to the Frank-Kamenetskii theory. The best agreement between the simulated and experimental value of the ignition temperature was obtained using GNU/Octave script, but COMSOL Multiphysics seems to be better choice due to its accessibility and advantages in this particular case.

Keywords: cook-off, numerical simulation, COMSOL Multiphysics, GNU/Octave, LS-DYNA

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Introduction

Thermal decomposition of energetic material is strongly exothermic process. If such material is thermally loaded there is a danger of beginning of self-heating process. If heat produced by exothermic reaction is not conducted away to the surroundings, it will accumulate in the material and temperature of the material will rise. Rising of temperature leads to increasing rate of decomposition and self-heating rate subsequently. Indicated decomposition reaction may leads to spontaneous ignition and thermal explosion.
If the decomposition reaction obeys Arrhenius kinetics, the heat transfer can be described (according to Frank-Kamenetskii theory) by the following equation(1)[1]

$$\rho \cdot c\frac{\partial T}{\partial t} = \lambda \cdot \nabla^2 T + Qf(\alpha)\rho \cdot A \cdot exp\left(-\frac{E}{RT}\right) \qquad (1)$$

where ρ is density $[\mathrm{kg \cdot m^{-3}}]$, c is specific heat capacity $[\mathrm{J \cdot kg^{-1} \cdot K^{-1}}]$, T is temperature $[\mathrm{°C}]$, t is time $[\mathrm{s}]$, λ is thermal conductivity coefficient $[\mathrm{W \cdot m^{-1} \cdot K^{-1}}]$, Q is decomposition heat $[\mathrm{J \cdot kg^{-1}}]$, $f(\alpha)$ is reaction model depending on the conversion α (both α and $f(\alpha)$ are dimensionless), A is pre-exponential factor $[\mathrm{s^{-1}}]$, E is activation energy $[\mathrm{J \cdot mol^{-1}}]$and R is universal gas constant $[\mathrm{J \cdot mol^{-1} \cdot K^{-1}}]$. This equation cannot be solved analytically, because of the exponential dependency of the generated heat (the second term on the right side) on temperature. The general reaction model $f(\alpha)$ also makes the solution more difficult. Frank-Kamenetskii solved a simplified form of this equation. For solution some of numerical methods has to be used.
One of the most important experiments focused on this phenomenon is slow cook-off experiment. The slow cook-off tests are standardized in UN Recommendations for transportation of dangerous goods [2], or COS 137601 [3]. This test is used to determine the reaction of an energetic material to a gradually increasing thermal environment and to find the temperature at which reaction occurs. The slow cook-off test has to be carried out for all EIDS (extremely insensitive detonating substance) or for LOVA (Low Vulnerability Ammunition) ammunition. In the case of LOVA, the testing procedure is modified and the whole ammunition objects are tested.

Experiment

Set-up for slow cook-off experiment on Institute of Energetic Materials (IEM) includes tube shaped bomb from mild steel 90 mm long and 21 mm in inner diameter. Bomb is twisted around by kanthal wire and four thermocouples are attached to the bomb surface. Bomb is insulated with industrial insulation and placed in explosive chamber. Beginning temperature is set on the value 50 $[\mathrm{°C}]$below expected ignition temperature. After five hours long period on holding temperature slow heating with heating rate of $3.3\ [\mathrm{°C \cdot hr^{-1}}]$ has been implemented [4].

A model example

There is a model based on experimental slow cook-off set-up prepared for each of three computational ways. Minor differences depend on capabilities of computational codes. Plastic bonded explosive Semtex 1A was selected as sample for simulation. Physical and kinetic parameters of this explosive was measured on our department and summarized in Table (1) [5]. Physical parameters of steel for COMSOL Multiphysics and LS-DYNA simulations was taken over from the literature [6]. Initial condition is system temperature equal to 85℃ .The convection boundary condition (heat transfer coefficient $100\ W{\cdot}m^{-2}{\cdot}K$) was used, with the surrounding temperature corresponding to the experiment.

Table 1: Kinetic and physical parameters of steel and Semtex 1A

Value	Steel	Semtex 1A
ρ[kg.m^{-3}]	7840	1493.6
λ[W.m-1.K^{-1}]	49.8	0.1531
cp[J.kg-1.K^{-1}]	465	1480.9
E[J.mol^{-1}]	-	2.002.105
A[s^{-1}]	-	1.091.1020
Q[J.kg-1.K^{-1}]	-	4.024.106

LS-DYNA

LS-DYNA is finite element method based multipurpose code for analysis of both static and dynamic cases of heat transfer and construction deformation in 3D geometry [7].
The heat transfer during the slow cook-off test was simulated using the LS-DYNA3D finite element code, the used FE model is in the figure 1. Only one eighth of the geometry was modeled due to symmetry. The model contains 335565 elements of the SOLID164 type.
The process was modeled as the transient heat conduction with the heat source eq.(1). The LS-DYNA code is intended for the simulation of the fast dynamic processes primary. It is also possible to simulate the heat transfer using this code, but there are some limitations. The LS-DYNA code is not able to calculate the kinetics of the chemical reactions. The heat released by the decomposing explosive can be dependent only on the temperature, not on e.g. fraction reacted. Therefore the only one applicable kinetic model is the zero order reaction ($f(\alpha) = 1$ in eq. (1)).

COMSOL Multiphysics

COMSOL Multiphysics is commercial multipurpose software using finite element method for analysing, simulating and solving dynamic and static physical and engineering problems [8]. COMSOL Multiphysics also contains modules for many different cases.
Heat Transfer module was used for simulation of heat transfer. Model of only one eighth of tube bomb in 3D geometry was prepared for simulation due to symmetry (figure 2). Time step

has been modified as follows. According to former simulation time to ignition has been estimated as cca.
52400 s and time steps were reduced during the simulation. Diffusion module was used for calculation of chemical reaction. Due to this module, COMSOL Multiphysics is capable to simulate chemical reaction of first and second order.

COMSOL Multiphysics' post-processor is capable to prepare simple figures. Figure 3 shows temperature time dependency for first order reaction. Moreover, figures of physical field can by can also be created by this postprocesr. Figure 3 obr:Comsol is temperature field in the ignition time.

GNU/Octave
GNU Octave is a high-level interpreted language, primarily intended for numerical computations. It provides capabilities for the numerical solution of linear and nonlinear problems, and for performing other numerical experiments [9]. Finite difference method based script has been written in Octave for solving of temperature field. One dimensional model of explosive tube without steel cover was prepared for this simulation and time step reduction was implemented [10].

Calculation according to Frank-Kamenetskii
Calculation according to Frank-Kamenetskii theory is a simplified solution of equation (1). Used simplifications are: heat transfer to the surroundings is not taken into account, zero order reaction is expected and everything is modeled in 1D geometry. Frank-Kamenetskii theory ascribes all heat resistance to heat conductivity of the sample [1]. Moreover Frank-Kamenetskii theory assumed inhomogeneity of the temperature field in the sample.
Frank-Kamenetskii theory defines critical temperature beyond which no stable state is possible and heat explosion occurs. Critical temperature according to Frank-Kamenetskii theory is defined as:

$$\frac{E}{T_{crit}} = R \cdot \log \frac{r^2 \rho Q A E}{T_{crit}^2 \lambda \delta R} \qquad (2)$$

meaning of the symbols follows:

- T_{crit} is critical temperature **[°C]**
- r is specific dimension, diameter in case of cylinder or sphere, thickness in case of slab **[m]**
- δ is dimensionless shape factor (0.88 for slab, 2.00 for cylinder, 3.22 for sphere)

Results

Outputs from all simulations are time-temperature dependencies and ignition temperature. These parameters along with the experimental results are in table 2.

Table 2: Comparison of results

Simulation	Reaction model	Ignition temperature [°C]
COMSOL	(1-α)	139.5
	(1-α)2	139.1
Octave	(1-α)	137.3
	(1-α)2	137.5
LS-DYNA	1	138
Experiment	-	136,9

LS-DYNA

Simulation with reaction model of zero order was carried out on LS-DYNA and time temperature dependency is figured out on figure 4.

COMSOL Multiphysics

Two simulations with two different reaction models were carried out in COMSOL Multiphysics. Ignition temperature for reaction model of second order is 139.5 ℃ and for reaction model of first order is 139.1℃ . Time-temperature dependency for reaction model of first order is figured out on figure 5.

GNU/Octave

Simulation of slow cook-off test has been carried out with script written in GNU/Octave. Results of two simulations are ignition temperatures for reaction model of second order (137.5℃) and for reaction model of first order (137.3℃).

Frank-Kamenetskii theory

Critical temperature obtained according to Frank-Kamenetskii theory is 127℃ . Critical value of shape factor for infinite cylinder 2.0 was substituted into (1) and equation was solved.

Summary

There were simulations of slow cook-off experiments carried out using three different computational codes. LS-DYNA and COMSOL Multiphysics are both 3D multipurpose commercial codes based on the finite element method. The simplified 1D simulation was carried out using GNU/Octave and the finite difference method.

Simulated ignition temperature in comparison with the experimental one was selected as the main comparative criterion. The experimentally obtained ignition temperature was 136.9℃ . But ignition temperatures obtained by each simulation way are quite close to each other and also in very good agreement with experimental result. Therefore it is also necessary to take the advantages and disadvantages of each computational way into account.
The worst and more or less informative result is the critical temperature by Frank-Kamenetskii theory equal to 127℃ . Simulation with the LS-DYNA code provides ignition temperature of 138℃ , but is strongly limited to zero order reaction model. Result of GNU/Octave script for reaction of first order is 137.3℃ and is the immediate to the

experimentally obtained temperature. But there are some disadvantages like difficult modification to 2D geometry, simulation carried out on explosives itself only and the fact that it is not intended for wider use.
Advantages of both LS-DYNA and GNU/Octave are included in COMSOL Multiphysics software. Ignition temperature from this computation is 139.5℃ , but its big advantage is its easy understandable pre-processor, because task can be easily modified due to graphical interface and it is possible to simulate almost any geometry. COMSOL Multiphysics has also very powerful post-processor and physical field, figures animation can be easily created.
As a result, the COMSOL Multiphysics comes out as the best choice mainly due to its modularity and easy usage and it is worth to be more studied. GNU/Octave script is more precise but is highly restricted.

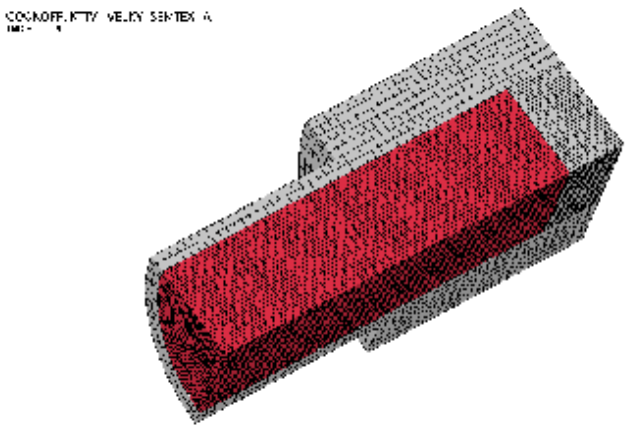

Figure 1: Model of 1/8 of tube bomb created in LS-DYNA

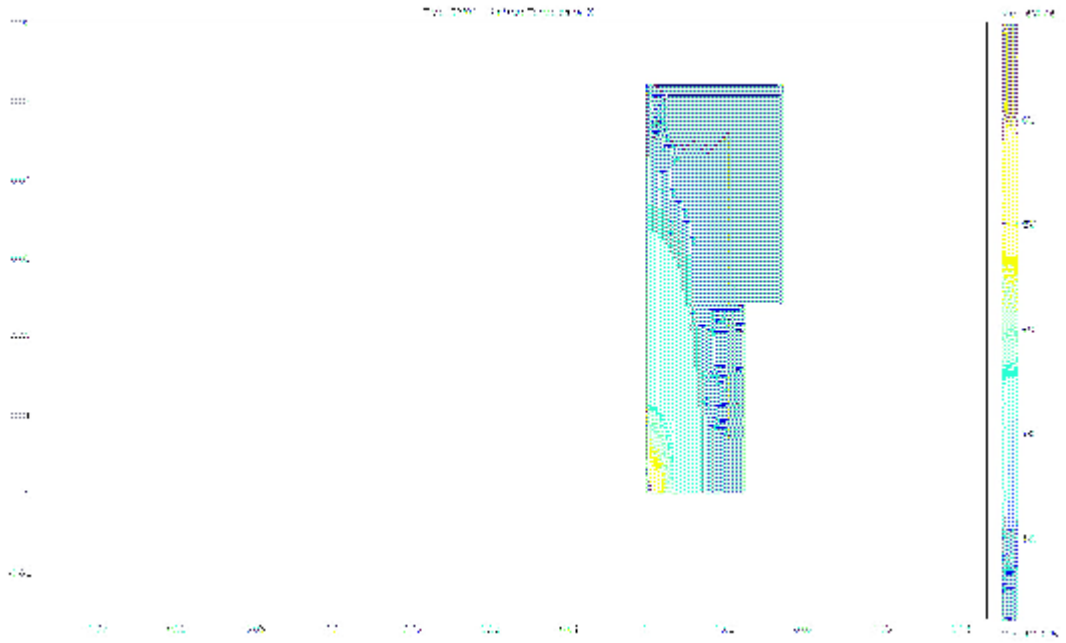

Figure 2: Model of 1/8 of tube bomb created in COMSOL Multiphysics.

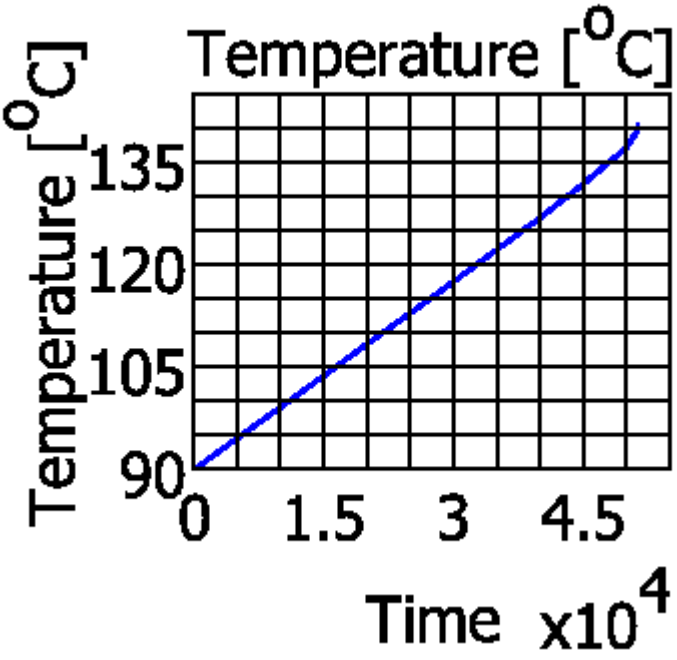

Figure 3: Time temperature dependency from COMSOL Multiphysics calculation

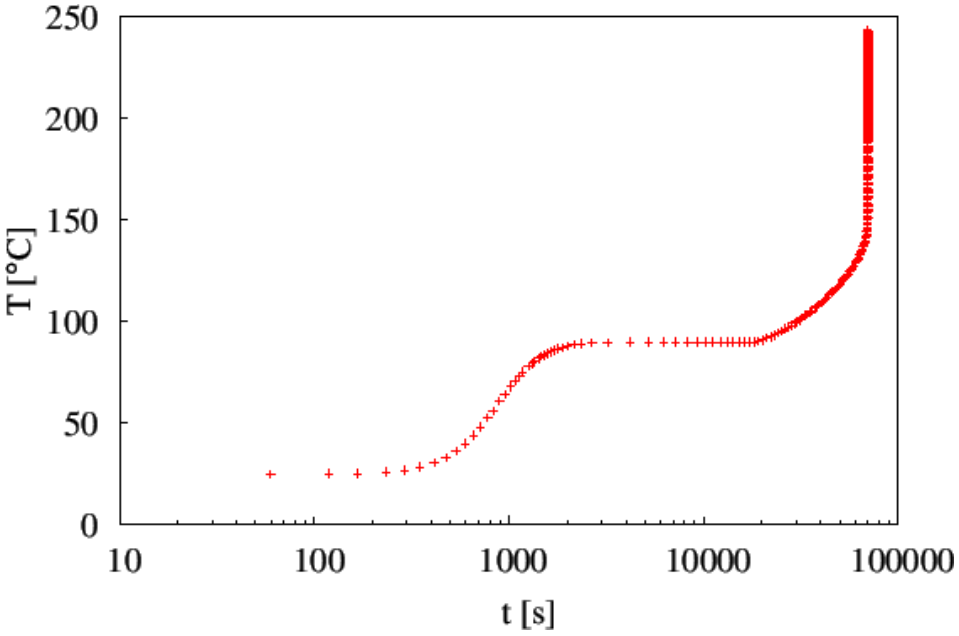

Figure 4: Time temperature from LS-DYNA calculation

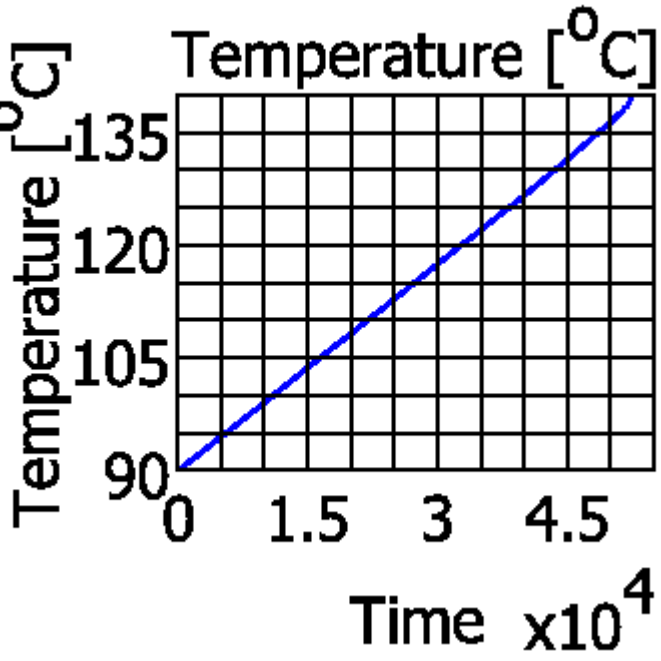

Figure 5: Time temperature dependency from COMSOL Multiphysics calculation

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