

What May Happen After a Thermal Explosion

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ABSTRACT

Thermal explosion may happen when an explosive is in a temperature field, and when its boundary temperature is between the critical and ignition temperatures. Semenov and Frank-Kamenetzky solved the thermal explosion problem analytically in 1D and for a constant boundary temperature [1,2]. Since the 1960s thermal explosion problems have been simulated numerically in 3D and for realistic boundary conditions. In thermal explosion tests it is easier to apply the boundary temperature gradually, and in this way, they become cookoff tests. When thermal explosion happens in a small region of an explosive body, the events that follow, and their overall resultant violence, may be quite diverse, like: 1) a slow decaying pressure wave; 2) a fast non-decaying wave; 3) a strengthening pressure wave that builds up to shock initiation and detonation. The outcome of a thermal explosion depends on: 1) the sensitivity of the explosive; 2) the temperature field throughout the explosive body at the time of thermal explosion; 3) the geometry of the explosive body; and 4) the degree of confinement of the explosive body. To model what may happen after a thermal explosion event, we use our PDSR (= Pressure Dependent Shear Reaction) together with our TDRR (= Temperature Dependent Reaction Rate) reactive flow models. For each computational cell these two models work in sequence. Initially there is a shear reaction handled by PDSR. If as a result, pressure and temperature there go beyond the threshold for reaction out of hot spots, TDRR takes over to compute shock initiation and detonation. We present here computed examples of different outcomes of thermal explosion events.

INTRODUCTION

Thermal explosion is a dangerous safety event when considering the response of explosives to heat. A thermal explosion may happen in an explosive device when it is surrounded by a temperature field that is between what is known as a critical temperature and the explosive ignition temperature. Ignition temperature is the explosive boundary temperature above which a self-sustaining combustion wave propagates into the explosive, given that the combustion products flow away very quickly. Ignition temperature of common explosives is around 500-600K. When the boundary temperature is above the ignition temperature, a steady combustion wave propagates into the explosive, as long as the combustion products are unconfined. Such a combustion wave is usually rather slow, around 1mm/s. When the explosive boundary temperature is below the ignition temperature, a combustion wave is not formed, and heat flows into the explosive at a rate determined by heat transfer. The front temperature of this heat wave may slowly increase because of two reasons: 1) slow bulk reaction with an Arrhenius reaction rate; and 2) slow heat transfer towards the boundary, which decreases as the heat front moves away from the boundary. Because of the highly nonlinear nature of the Arrhenius rate equation, whenever the heat front temperature goes above a certain threshold,

the reaction process accelerates exponentially, and the temperature at the front increases to high values in less than a μs . As a result, the explosive there undergoes a fast bulk reaction, which is known as **thermal explosion**. For decreasing values of the boundary temperature below the ignition temperature, the thermal explosion location in the explosive body moves further away from the boundary. There is therefore a low boundary temperature for which the thermal explosion distance from the boundary is the furthest. For a spherical explosive body this would be the center of the sphere. The boundary temperature for which the thermal explosion location is the furthest from the boundary is known as the critical temperature T_c . When the boundary temperature is below T_c , a thermal explosion event would not happen. The phenomenon of thermal explosion in energetic materials was discovered and analyzed in Russia some 80 years ago by Semenov and Frank-Kamenetzky [1, 2]. As there were no computers at that time, analysis of this highly nonlinear problem was quite difficult. They were able to overcome the difficulties by treating the 1D configurations of the problem with asymptotic approximations. Since the 1960s thermal explosion problems are treated with computer simulations [3], which make it possible to predict the time and location of thermal explosions for explosive bodies of various geometries and boundary conditions.

The problem of predicting the time and location of a thermal explosion (known as the Frank-Kamenetzky problem) is quite important for explosive safety considerations. Sometimes it is enough to know if a thermal explosion is to be expected, and if so, how to avoid it by some design change. But sometimes it is also important to predict what may happen after a specific thermal explosion. This part is known as **level of violence** of a thermal explosion event. In reality these are two stages of the same process. The first stage (heating stage) includes heat transfer and slow reaction, and pressure rise is minimal. It ends with a very fast pressure rise over a small volume of the explosive. In the second stage a weak pressure wave spreads out of this high-pressure volume, which may subsequently ignite the explosive around it by means of plastic flow localization and shear band formation [4, 5]. Deflagration fronts then spread out of the ignited shear bands, similar to deflagration waves out of hot spots. But reaction out of shear bands (called shear reaction) is much slower and less violent than reaction out of hot spots. This is mainly because the distance between shear bands is an order of magnitude larger than the distance between hot spots. On the other hand, ignition threshold of shear bands is much lower than that of hot spots. Shear bands may ignite from a pressure wave of 0.1-0.2GPa, while hot spots ignite at 1-2GPa.

The second stage of a thermal explosion process may become rather involved, because the shear reaction wave may strengthen to become a detonation wave. Such strengthening may happen in various ways: 1) self-strengthening, when the initial pressurized volume is relatively high; 2) geometric convergence; 3) reflection from a rigid boundary; and 4) interaction of two shear waves. This is why transition from shear reaction to shock initiation and detonation depends strongly on: 1) thermal explosion location; 2) device geometry and 3) its level of confinement.

From the view point of computer simulations, the two stages of thermal explosion are **two entirely separate problems**, to be handled with different computational tools. The first stage (heat transfer + slow reaction) is slow, and its computer simulation may ignore pressure variations and use ms time steps. The second stage may be a fast hydrodynamic process, with

ns time steps and high-pressure waves. This is why the two stages should be treated with different types of codes, the first stage with a heat transfer code augmented by an Arrhenius reaction rate, and the second stage with a hydrocode. What needs to be transferred from one code to the other are the temperature field, the reaction parameter field, and the thermal explosion location.

In what follows we show results from computed examples of the second stage of thermal explosion events.

COMPUTED EXAMPLES

The hydrocode we're using includes two of our previously developed reactive flow models that work consecutively for each computational cell. The first is a shear reaction model that we call PDSR (= Pressure Dependent Shear Reaction). We calibrated PDSR for an LX07 like explosive from our Steven test data. The second is our shock initiation and detonation (or surface burn) model which we call TDRR (= Temperature Dependent Reaction Rate) [6], that we calibrated in the past for the same explosive from pop plot data.

The explosive body in our computed examples is a cylinder of 180mm diameter and 380mm length. We compute only one half of this cylinder, $z > 0$, as it has a symmetry plane at $z = 0$. Around the explosive we have an aluminum envelop 10mm thick. We assume axial symmetry, and the computational mesh is 1 cell per mm in both directions. To start stage 2 of the thermal explosion event we: 1) put an initial temperature T_0 over all the explosive cells. T_0 represents an average of the boundary temperature and the somewhat increased temperature near the thermal explosion location just before the thermal explosion. In the examples that follow we use $T_0 = 350\text{K}$, and the initial temperature of the explosive at the beginning of the second stage has been specified accordingly; 2) choose the thermal explosion location cell. In the examples that follow there are two such locations; 3) let part of the explosive around the cell center detonate out of the cell center with a programmed burn scheme, and we control the mass of the explosive that undergoes thermal explosion by changing the radius of the detonating sphere; and 4) run our combined PDSR-TDRR reactive flow model.

As explained above, the pressure wave spreading out of the thermal explosion is too weak to cause shock initiation, but it may cause shear initiation, which is handled by PDSR. Reaction ignition in PDSR depends on two consecutive criterions: 1) shear localization criterion for starting shear band formation given by:

$$(PD)_L = 0.01\text{GPa} / \mu\text{s} \quad (1)$$

where P =pressure, D =effective plastic strain rate, and L stands for Localization. In the past we calibrated this localization criterion from simulations on the mesoscale [7], and it may be generally stated that around a thermal explosion this location criterion is usually met; and 2) ignition delay (from localization to ignition). Ignition delay (h) depends on the product PD as well, and we calibrated it in the past from Steven test data [7]. Ignition delay is low for high PD and high for low PD . Ignition delay in a cell is determined by the coefficient A_h , calibrated from a preliminary short simulation as explained next. A_h is given by:

$$A_h = 0.635(PD^* - 0.026)^{-0.425} \quad (2)$$

where the coefficients in this equation are in GPa and μs , and where the parameter PD^* depends on the strength of the thermal explosion and is determined as follows: 1) run the simulation without shear reaction for t^* μs , where t^* is the time needed for the pressure wave from the thermal explosion to reach all parts of the explosive; 2) in this preliminary run calculate $PD_{max}(t)$, the maximum value of PD for each time t over the entire computational field; and 3) determine PD^* as the time average of $PD_{max}(t)$. We calibrated the parameters of Eq. (2) from Steven test data obtained in [6]. In the actual run (after the coefficient A_h has been determined) we calculate for each cell the integral:

$$I = \int_{t_L}^t \frac{dt}{h} = \int_{t_L}^t \frac{PD}{A_h} dt \quad (3)$$

where t_L is the shear localization time for that cell. When $I=1$ we have $t-t_L=h$, which means that the ignition delay time for that cell is over, and we start the reaction there.

The average deflagration reaction rate out of shear bands in a cell increases with pressure up to a limit [7]:

$$\begin{aligned} \dot{W} &= R_{sb} P & P \leq P_b \\ \dot{W} &= R_{sb} P_b & P > P_b \end{aligned} \quad (4)$$

where the coefficient R_{sb} decreases with pressure as given in the next equation, which we calibrated from Steven test data [7] as well:

$$R_{sb} = 0.00774(P^* - 0.18)^{-1.039} \quad (5)$$

The coefficients in Eq. (5) are in GPa and μs , and the parameter P^* is determined in the same way as described above for the parameter PD^* .

Whenever pressure and reactant temperature in any explosive cell increase as a result of shear reaction or any other reason, hot spots may form and ignite there, and as a result also deflagration (or surface burn) may propagate out of these hot spots. There are two criterions for this to happen: 1) high enough pressure to enable fast crushing of pores, $P > P_{hs}$ (where the index hs stands for hot spots). We've never calibrated P_{hs} in an orderly fashion, because for shock initiation the pressure needed to meet the other (ignition) criterion is most of the times above P_{hs} . In what follows we use (without checking) $P_{hs}=3\text{GPa}$; and 2) ignition criterion of (self-sustained) deflagration reaction out of hot spots: $T_s > T_{ig}$, where T_s is the reactant temperature. When these two criterions are met in a cell, reaction rate there is changed irreversibly to that of TDRR. In our computed examples we use $T_{ig}=400\text{K}$.

Next, we show results from runs with two locations of the thermal explosion cell: 1) near $r=0$, $z=0$; and 2) near $r=45\text{mm}$, $z=95\text{mm}$. In Fig. 1 the thermal explosion location is at the origin, and the thermal explosion volume extends to $r=1.8\text{mm}$, $z=1.8\text{mm}$. We show the results by maps with lines of equal W (W is the reaction parameter), where $W=0$ to 1 every 0.2.

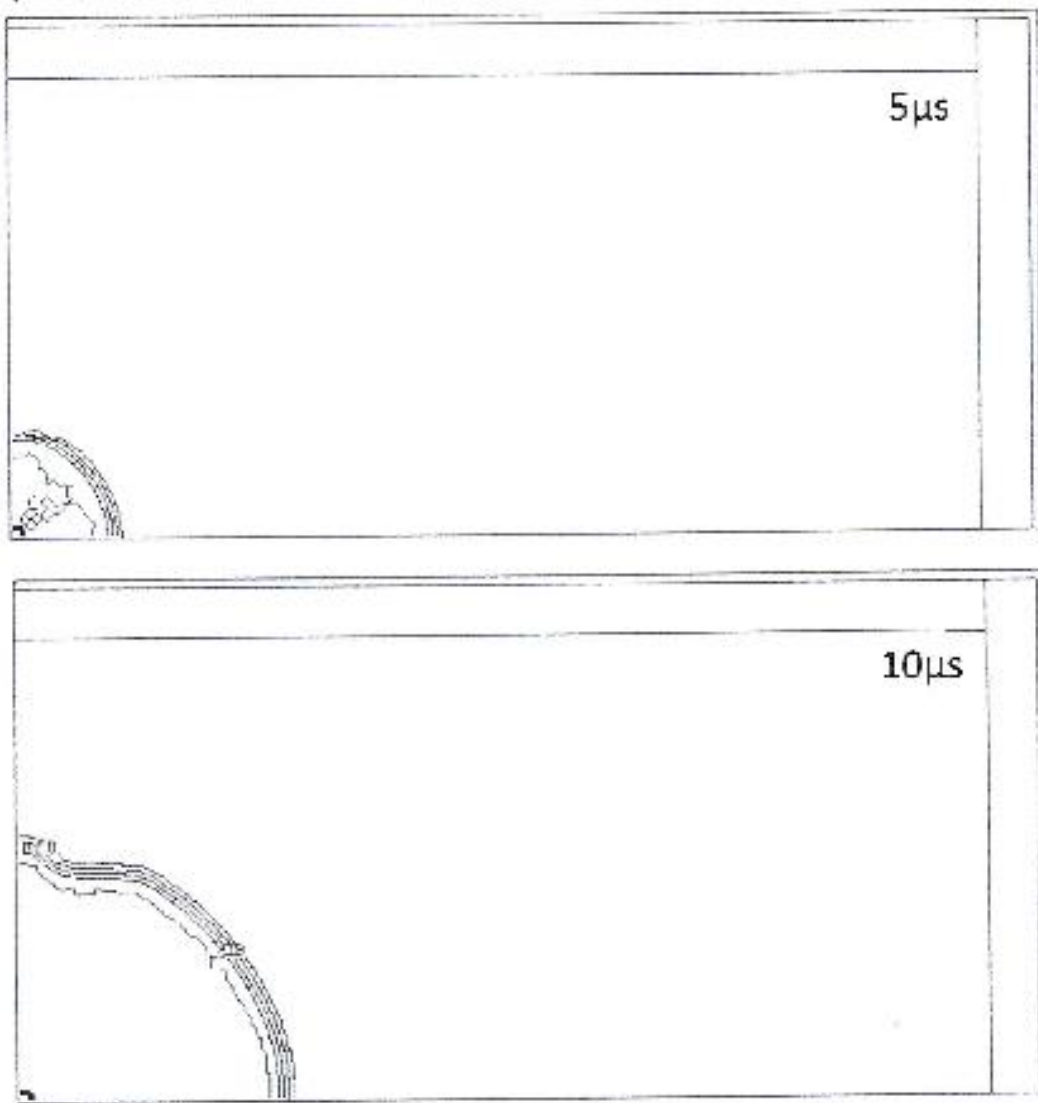


Figure 1: Maps with lines of equal W for thermal explosion at $r=0$, $z=0$ extending to $r=1.8\text{mm}$, $z=1.8\text{mm}$.

We see that for the conditions of Fig. 1 the initial shear reaction quickly turns into a detonation.

In the run shown in Fig. 2, the thermal explosion volume extends in the r direction to only 1.0mm.

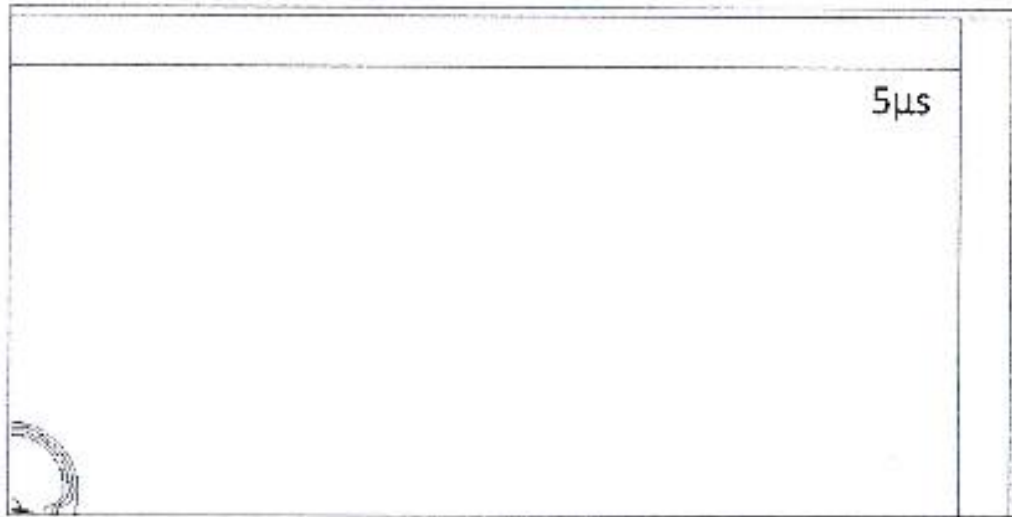


Figure 2: Map with lines of equal W for thermal explosion at $r=0$, $z=0$ extending to $r=1.0\text{mm}$, $z=1.8\text{mm}$.

We see from Fig. 2 that although the thermal explosion volume in this run is much smaller than in the previous run, the shear reaction still turns into a detonation.

In the run of Fig. 3 we diminished the thermal explosion volume in the r direction even further, to 0.9mm .



Figure 3: Map with lines of equal W for thermal explosion at $r=0$, $z=0$, extending to $r=0.9\text{mm}$, $z=1.8\text{mm}$.

We see from Fig. 3 that in this case the thermal explosion volume is too small for it to turn into a detonation. We get a shear reaction that expands very slowly and is much less violent.

In the run of Fig. 4 the thermal explosion center is in the middle of a cell at $r=50.5\text{mm}$ and $z=79.5\text{mm}$, and the volume of the thermal explosion event is that of the entire cell. Because of the axial symmetry the thermal explosion volume is actually a torus with a radial thickness of 1mm and axial thickness of 1mm .

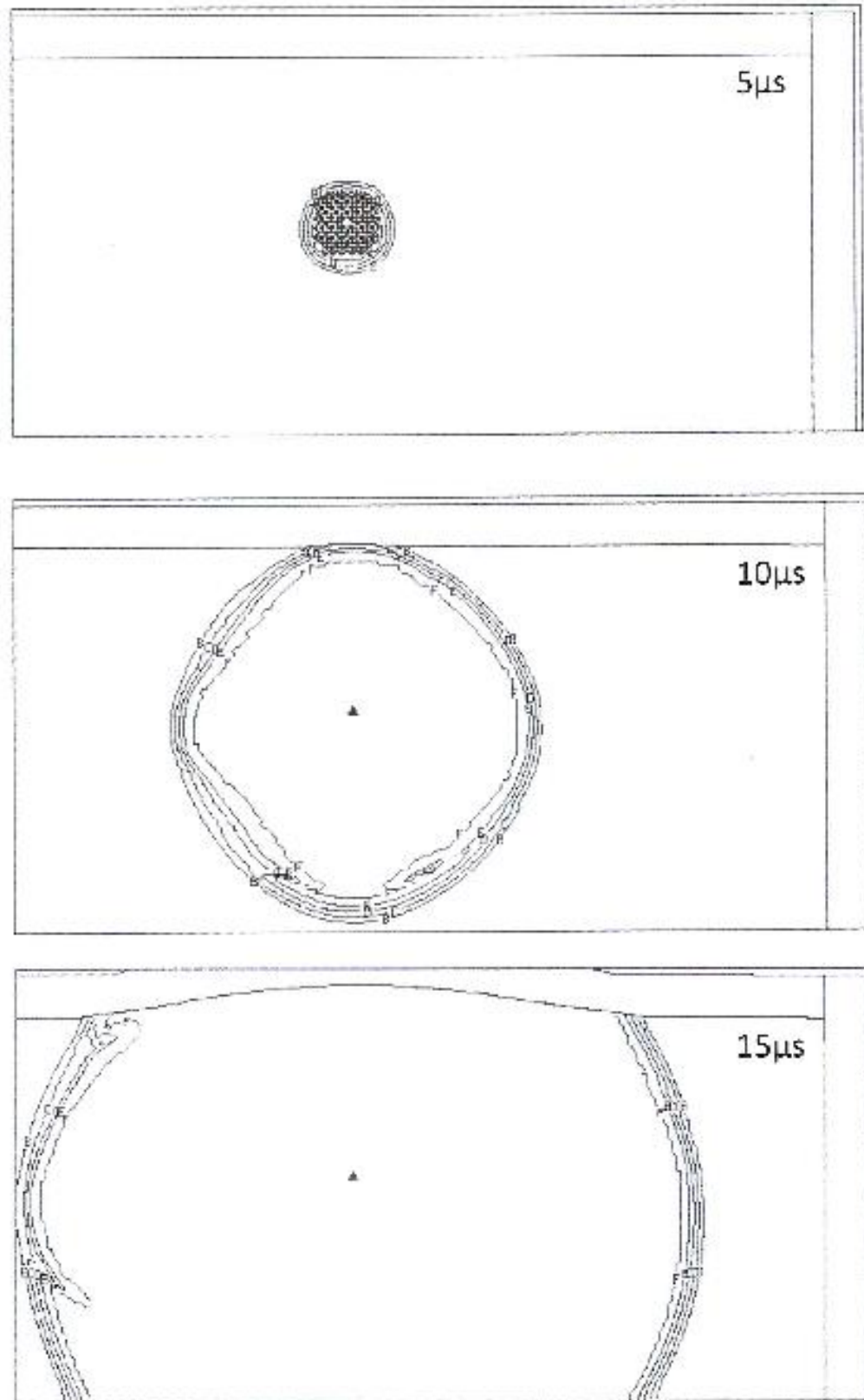


Figure 4. Maps with lines of equal W for thermal explosion at $r=50$ to 51mm , $z=79$ to 80mm .

We see from Fig. 4 that three cells around the thermal explosion cell undergo shear reaction, which then develops quickly into a detonation.

From the above examples we learn mainly that whether a detonation wave develops or not, depends on the details of the thermal explosion event. This includes the shape and volume of the small part of the explosive that undergoes bulk reaction as a result of the fast and localized heating that triggers the thermal explosion.

SUMMARY

We use our combined PDSR-TDRR reactive flow model to predict what may happen after a thermal explosion event. We do not evaluate the first stage of the thermal explosion event, the stage of heat transfer and slow reaction. Instead, we define the thermal explosion event in terms of the following parameters: 1) location of the center of a small volume of explosive that undergoes bulk reaction as a result of fast heating; and 2) extent of this volume around the above center.

To start the second stage of the thermal explosion event we detonate the above small volume of explosive with a programmed burn scheme from its center. We then use our combined PDSR-TDRR reactive flow model to predict the resulting reactive flow. From the example that we ran we conclude the following: 1) the outcome of a thermal explosion event (whether it is a mild shear reaction or a violent detonation) depends mainly on the size of the volume of explosive that undergoes bulk reaction at the end of stage 1; 2) the geometry and location of the above volume is of some importance, but to lesser extent; and 3) the influence of distant confinement seems to be less important than is usually believed. To better understand what determines the size of the explosive volume that undergoes bulk reaction as a result of fast heating, we need to concentrate in the future on simulating in detail the end part of stage 1.

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