

Effects of Particle Damage during Detonation of Thermobarics on Subsequent Reactions

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1 Physical and Chemical Processes of Detonation, Anaerobic Reaction and Aerobic Reaction of Detonation Products of Thermobaric Weapons

Physical and chemical processes that occur in a non-ideal explosive weapon are very complex. When the initiation train of the weapon triggers a detonation wave in the explosive, it travels down the length of the explosive. Most of thermobarics contain aluminum particles as the source of additional energy. Most of the aluminum particles do not participate in the reaction during the detonation phase. Aluminum particles, of micron sizes, need material diffusion to get oxidized and there is not enough time for the diffusion during the detonation.

The cracking of the aluminum oxide coating has significant implications. If the coating is intact, the ignition of the particles with the surrounding gaseous oxidizers will occur near the melting temperature of the aluminum oxide, near 2050 K. On the other hand, a cracked particle may get ignited close to the melting temperature of aluminum, near 950 K.

As the detonation products expand, their temperature decreases rapidly due to the isentropic nature of the expansion and their composition changes at the same time. However, the temperature is still high enough for a limited duration to heat up some aluminum particles. If the aluminum particles do reach their ignition temperature, they can start chemical reaction with the surrounding gas. At this time, the available oxidizing gases are water vapor, carbon dioxide and carbon monoxide, mostly. The air does not come into play until much later. Any reaction that takes place at this time is therefore called an anaerobic reaction.

The particle size distribution of aluminum plays a critical role during this period. As the particles are accelerated outward and then decelerated at the later stage by the gaseous drag forces, they are heated by the gases at the same time. If the particles sizes are uniformly large, heating of the particles may not be done successfully before the gas temperature drops below or near the ignition temperature of the particles. If the ignition temperature is low, all of the particles may get ignited. If it is high, there may not be enough time to heat and ignite any of the particles. Either most of the particles are ignited or almost no particles get ignited, if a single particle size is used in the simulation.

If particles have a size distribution, smaller particles can get ignited in a relatively short time, thus providing additional heat to the surroundings. This energy contributes to heating of larger particles. The smaller particles burn rapidly and remain closely tied to the local gas, while the larger particles move more readily in the gas and mix with new oxidation sources.

If the charge is cased, the casing has the dual effect of reducing the rate of detonation products expansion and converting energy to case fragment kinetic energy. The reduction of the detonation products expansion rate helps heating up the particles. As detonation products, gases that contain water vapor, carbon dioxide, carbon monoxide, nitrogen, etc. and aluminum particles, expand, the weapon casing is accelerated and stretched and finally broken into fragments. The fragments are further accelerated by the detonation products.

Much energy of the reaction is imparted to the kinetic energy of the fragments. Sometimes, the final kinetic energy of the fragments may exceed that of the remaining internal and kinetic energy of the detonation products.

As the detonation products (a fireball) expand, the volume occupied by the casing fragments becomes relatively unimportant. The products go through an initial turbulent stage, dictated by Rayleigh-Taylor instabilities, augmented somewhat by the initial small jets through the casing cracks. The turbulence is not yet strong enough to be a significant mixing factor, and one can observe some irregularities on the surface of the expanding fireball. Not much air is being mixed into the fireball to start aerobic reactions at this stage.

The fireball now contains the oxidizers mentioned above and mainly three fuel types: hydrogen that was generated during the water-Al reaction, if any, carbon that was generated during oxygen-deficient explosive detonation and CO₂/CO reaction with Al, if any, and the Al particles as well as some hydrocarbon gases.

In the case of an open-air detonation of such weapons, reaction does not progress much further from the processes described above. For small weapons, especially, the event is short and typically there isn't time to mix and heat the Al particles to initiate the anaerobic reaction. Much of the available energy is not realized. The aerobic reaction, even if the fuels are sufficiently mixed with the air, is also limited by the cold (by then) environment.

If the weapon is detonated inside a structure, additional reactions can take place. An air shock wave, generated during the fireball expansion, is reflected from the walls of the structure. The reflected shock plays two important roles. First, it stops the temperature decrease of the air and the fireball. It can actually increase the temperature in some places, depending on how the shock waves are bouncing back and forth. Second, it creates two new types of flow instabilities; Richtmyer-Meshkov and Kelvin-Helmholtz instabilities.

The shock induced increase in temperature allows the continuation of heating of Al particles, whereas the enhanced turbulent mixing created by the two additional instabilities allows air to participate in the reaction of fuels mentioned above. This part is called the aerobic reaction.

In summary, there are three distinct types of reactions taking place in a given non-ideal explosive weapon, and they are more or less separated temporally and spatially: detonation, anaerobic reaction and aerobic reaction. For blast weapons, the question of how quickly these last two reactions occur is of fundamental importance as is the total energy released.

2 SHAMRC Code and Numerical Simulations

SHAMRC is a second order, fully conservative, inviscid code with two- or three- dimensional geometries. It handles multi materials in two phase turbulent chemically reacting flows. Turbulence in the viscous flow regime (below the Kolmogorov scale) is ignored. The SHAMRC code incorporates the above physics and chemistry processes into models. It describes the detonation process assuming that none of the aluminum particles react during the detonation. In the absence of any other knowledge of what aluminum particles, one of the most important fuels present in many thermobaric explosives, look like after going through an initial detonation, the code assumes that they keep their original (before formulation) size and their temperature remains as that of the original temperature. Further, non-spherical particles are approximated as being spherical with the same surface-to-volume ratio as the actual particles.

The amount of carbon, water, carbon dioxide, methane, and other burned explosive materials released during the passage of the detonation front are estimated using CHEETAH (with the inert aluminum assumption), and a simple LSZK equation of state is used to describe the gaseous part of the products. The weapon casing, if it is present, is allowed to fragment when the total average strain of the casing exceeds 100%, and the fragment size distribution is estimated and statistically distributed when such information is given (from an arena test or from similar tests, for example). As the aluminum particles fly inside the fireball, they undergo momentum (drag) and energy (heating) exchange processes with the surrounding gases. If the temperature of the aluminum particles reaches 2050 K (melting temperature of the aluminum oxide coating on the surface of the particles), and if there is oxidizer present nearby, the aluminum particles are assumed to ignite, start burning and releasing energy. Their burn rates are variable as specified by laboratory data, and specified by a simple cubic law formula. After the detonation, the model allows the gaseous products to react with aluminum particles and atmospheric oxygen.

Three thermobarics formulations (TBX A, TBX B and TBX C) were selected for detailed study of SHAMRC capability [1]. TBX A contains a large amount of large aluminum particles (more than 30 weight %),

a liquid explosive and no binder in the explosive matrix. TBX B contains a small amount of a bit smaller aluminum particles and an adequate amount of binder. TBX C contains a large amount of small aluminum particles in a large amount of binder.

The test bed in which these formulations were tested consisted of a two-room, vented, reinforced concrete, non-responding structure with each room measuring 12 ft x 15 ft x 8ft. The rooms were labeled as the source (blast) room and the adjacent room with the charge being placed in the source room. Each room had an exterior doorway covered with responding wooden doors and an external open window. The nominal eight-pound charges were encased in 12 pound steel cases. The interior walls of the source room and portions of the secondary room were protected from fragment damage with a layer of steel. The experimental setup focused on measuring the air blast pressures in the source room and the adjacent room. Pressure gauges were placed in the walls and the ceilings of both rooms and dynamic pressure was measured between the two rooms.

Figure 1 shows the comparison between the experimental data and the code simulations for the three thermobarics at the same gauge location. For TBX A, the comparison is relatively poor. The first major shock (at around 7 ms as measured) is slower and weaker for the numerical simulations compared against the measured. This implies that a significant amount of energy at or immediately following the detonation (in a few milliseconds) is not properly accounted for. The second major shock (at around 18 ms as measured) prediction is still further behind the measured, indicating that some afterburning (both anaerobic and aerobic) also may not be fully accounted for. The third peak is completely lost in the simulation.

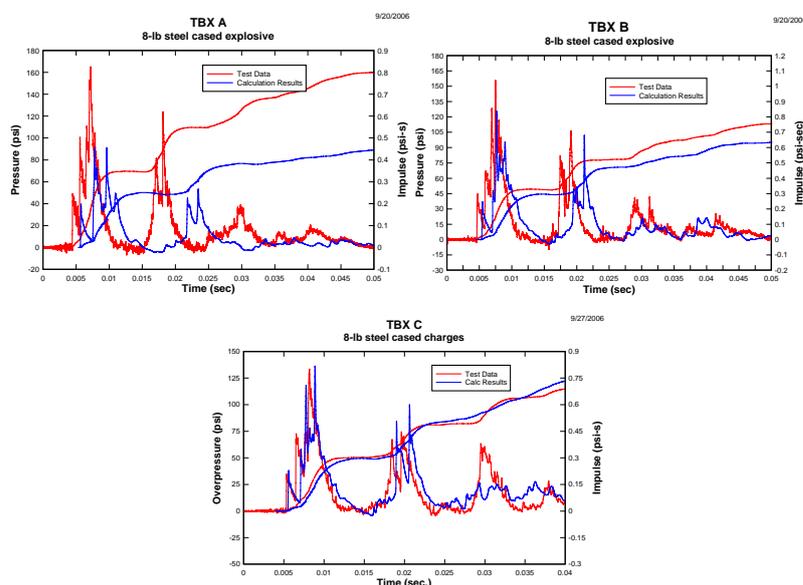


Fig. 1 Comparison between SHAMRC and test results for Thermobarics A, B and C

A most probable source for the errors in the simulation is as follows: “Are the particles damaged during the initial detonation to an extent that a significant part of aluminum oxide coating is removed, exposing aluminum to the detonation product gases?” As the detonation wave travels down the explosive, high pressures of hundreds of kilo-bars disturb the physical morphology of aluminum particles. It has been shown in meso-scale numerical simulations that [2] aluminum flakes break during the detonation. Even for spherical particles, they are largely deformed to an extreme extent [3] that aluminum oxide coatings may crack and expose fresh aluminum to the detonation products. In some explosives with a large amount of binder with smaller aluminum particles, this deformation may be limited, whereas other explosives with a small amount of binder with large aluminum particles are envisioned to cause more deformation. During the shock/detonation interaction, meso-scale simulations further show that mass-averaged particle temperature reaches 25-30% of the post-shock/detonation flow temperature [3]. Local hot spots at the particle surfaces become much hotter. Experiments show that the reaction of the expanding 10-50 μm aluminum particle cloud occurs 10-40 μs behind

the detonation front [4], while the reaction of the 10 μm aluminum particles in more confined detonation products takes place within microseconds [5]. These data clearly indicate that the oxide layers are compromised by the detonation wave and fragmentation of the aluminum particles would also not be excluded. Aluminum reaction mechanism is another uncertainty. Experimental results have also provided clear evidence of dependence of aluminum reaction on chemical kinetics and pressure.

Deformation and cracking of the oxide layer could lower the effective ignition temperature of the particles or some portion of the particle mass. Most of other possibilities for the source of the error can be discounted in the light of other observations. TBX A does not contain any binder and large aluminum particles may suffer some mechanical damage during detonation.

The comparison for TBX B that contains a smaller amount of medium size aluminum particles in a medium amount of binder is better. The first major pressure peak is somewhat slow, indicating that the first part of the anaerobic reaction may not be fully accounted for. The comparison for TBX C that contains a larger amount of very small aluminum particles in a large amount of binder is much better. This may be because of the fact that smaller aluminum particles are well protected inside a large amount of soft binder materials such that the least amount of particle morphology change is expected during the detonation. Therefore, the "intact particles during detonation" assumption may hold best for TBX C.

3 Particle Damage during Detonation Assumption

One way to observe the damage done to aluminum particles during detonation is to subject small samples of thermobarics in an inert gas chamber, detonate them and collect particle samples for examination. However, it would be difficult to quantify the extent. Another tool would be the meso-scale modeling as shown in Ref 2. However, the detailed description of aluminum oxide coating (about 3 nanometers thin) on the particles of tens of micrometers is still beyond the reach of current state of numerical simulations.

In this paper, a parametric study was performed in order to see if the assumption of particle damage during detonation can explain experimental data. First, two types of experiments were performed using TBX A: the thermobarics that contain liquid explosives, no binder, and a large amount of large aluminum particles. In one experiment, an almost bare charge of TBX A was detonated in between two vertical walls. In the other, TBX A was encased in a heavy steel casing and then detonated in a room with two doors and a window. The two experiments represent a wide spectrum of physical conditions imposed on the thermobarics. Careful pressure measurements at many different gauge locations were obtained.

Second, numerical simulations are in progress to determine if the "particle damage during detonation" assumption can explain the results of both experiments. An additional variable, the amount of exposed aluminum, will be introduced in SHAMRC. Results of this comparison will be presented in the final paper. . Further, the simulations will show the effects of target configurations on the efficiency of the thermobarics. The reaction efficiency is enhanced by the presence of walls through enhanced mixing from three different types of instabilities as well as from enhanced chemistry from elevated temperature and pressure.

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