Gas Explosions with Limited Boundary Conditions and Their Effects on DDT

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Abstract

Gas explosions using a mixture of ethane and oxygen were investigated to determine what conditions affected the deflagration to detonation transition (DDT). Investigations were done using single 100L bags that were fully filled with the gas mixture orientated horizontally with the ground as well as double 100L bags that were each only filled to 80L orientated vertically with the ground. For each type both near field and far field pressure data was collected to see the pressure variation as a function of distance. The resulting pressures demonstrated exponential decay as predicted for a gas explosion. The peak pressures at one meter (3 feet) away were on average 22.5 PSI for the double 80L bag tests and 15.7 PSI for the single 100L bag tests. At 12 meters (30 feet) the peak pressures decayed to under 1 PSI. The peak pressures varied by 43 percent due to the change in volume from 100L to 160L (double 80L), showing a non-linear relationship between the peak pressures and volume of ethane-oxygen mixture. Each bag was also viewed using the Vision Research Phantom Veo-710S high-speed imaging to find the blast wave velocities within each bag during the explosion. The double 80L bags resulted in full detonation and consistent simultaneous initiation; they exhibited a maximum shock front velocity of 2275 m/s. The single 100L bags demonstrated several failures to detonate resulting in deflagration; the bags that did detonate had shock front velocities 2469 m/s, showing an 8 percent increase in shock front velocity. The shock front velocity showed dependence on the gas dynamic expansion and the chemical energy by the ethane-oxygen mixture. The DDT rate depends on physical and chemical parameters of the reaction (boundary conditions).
1. Introduction to Gas Explosions

1.1. Gas Explosions

A gas explosion is the process where the combustion of a gas cloud, a fuel-oxidizer mixture, causes a rapid increase in pressure and temperature. Gas explosions can be confined, occurring inside of pipes, processing equipment, or perhaps buildings, or unconfined, occurring in open air. The pressure generated from the combustion wave depends upon the velocity of flame propagation and how pressure is able to expand away from the gas cloud (this, in turn, is governed by confinement). When a gas cloud is ignited, the flame can propagate through the flammable portions of the cloud in two different ways: (i) deflagration and (ii) detonation. A deflagration propagates at subsonic speeds relative to the unconsumed gas; standard flame speeds are in the order of 1 – 1000 m s\(^{-1}\). Pressure generated from the explosion may reach several bars, depending upon flame speed. A detonation wave is supersonic and the combustion wave and shock wave are coupled. In a fuel-oxidizer mixture cloud, a detonation wave will propagate with a velocity of 1500 – 2000 m s\(^{-1}\).

1.1.1. Deflagration Theory versus Detonation Theory

The combustion rate of deflagration is controlled by the supply of oxygen to the explosion front. The explosion front travels at subsonic speeds within the unconsumed gas. The propagation mechanism for deflagration is a heat transfer effect – therefore combustion reactions are significantly dependent upon heat and mass diffusion in the region of energy release (Wang et al. 2011). For strong deflagrations, the combustion wave is preceded by a shockwave that is formed from the expansion of combustion products left behind. This combustion wave consists of a preheat zone and reaction layer (Ruming et al. 2011).

In detonations, combustion is initiated by the pressure and temperatures related to the shock wave. The shock wave travels at supersonic speeds in the unconsumed gas. The propagation mechanism is due to the shock compressive heating of the unreacted gases ahead of the propagation front. Detonations generate higher pressures and velocities in comparison to deflagrations. Detonations can further be divided into two different types: (i) stable detonations and (ii) unstable detonations. Stable detonations occur when the detonation travels through a confined system without significant variation in velocity and pressure characteristics. Unstable detonations occur during the transition of the combustion process from deflagration to detonation, known as deflagration to detonation transition (DDT). This transition occurs in a limited special zone, where the velocity of the combustion wave is not constant and pressure is significantly higher than that in stable detonation (Ruming et al. 2011). A detonation wave is described as a shock wave that is immediately followed by a flame (ZND theory). The shock compression heats the gas and ultimately triggers the combustion.
1.2. Ethane Oxygen Mixture

This paper presents an analysis of the propagation of the shock waves generated by gaseous ethane-oxygen explosive mixtures with the assumption of atmospheric air as the surrounding medium.

The stoichiometric ratio of ethane-oxygen for combustion was used for this research and represented in the ideal volumetric equation below:

\[ C_2H_6 + 3.5O_2 \rightarrow 2.0CO_2 + 2.5TC \]  
(eq. 1)

Where \( O_2 \), \( CO_2 \) and TC are symbols used to identify the numbers representing the relative volumes of oxygen consumed, carbon dioxide produced, and contraction, respectively, upon the combustion of one volume of ethane.

1.3. Formation of Blast Waves

A blast wave can be defined as a shockwave that decay immediately after the peak is reached. In gaseous explosive mixtures, small perturbations of gas produce signals, in the form of sound waves that propagate away from the source at the speed of sound. When energy is deposited more rapidly within the gas, compressive heating further increases the sound speed in the local gas and energy is transmitted at the local speed (which may now be greater than in the unperturbed air). If dissipation of energy within the compressive wave does not reduce the sound speed of the front of the wave to that of the unperturbed air, then energy accumulates at the front, and a shock wave generated (Needham 2010). Figure 1. Represents the typical overpressure versus time profile for a blast wave at a certain distance from its source (Needham 2010).

![Figure 1. Typical blast wave profile at certain distance from its source](image-url)
The blast wave profile in Fig. 1 depicts an abrupt pressure discontinuity that is followed by positive and negative pressure phases. The negative pressure phase is formed when no more energy can reach the shock front from the source region. These inertial effects produce an overexpansion and, consequently, a rarefaction at the explosion center (Kinney et al. 1985). As the blast wave travels outwards, the peak ($P_s$ in Figure 1) decreased and the positive duration of the blast wave ($t_d$) increases. Ultimately, the blast wave decays to a low overpressure, and the signal takes on some of the characteristics of a sound wave. The peak positive and negative values of overpressure and time duration approach the same value, while material velocity approaches zero (Needham 2010).

The shock front of a blast wave is a significant determining factor in its behavior – depending on explosive charge geometry, various expanding shock wave shapes may be anticipated (e.g. planar, spherical, cylindrical, etc.). The pressure at the shock front minus the ambient pressure is an important descriptor of the shock front. This parameter can be measured directly with instrumentation such as piezoelectric sensors placed at specific ranges in distance. When studying the effects of blast waves on structures, two additional pressures perform a significant role: (i) dynamic pressure and (ii) reflected pressure. However, this paper is concerned only with studying the propagation of the shockwaves, and not the resulting damage.

1.4. Preliminary Predictions

Preliminary calculations were performed for the estimated of blast parameters from gaseous explosive mixtures. These calculations were conducted following the procedure outline in Berg (1984) for the blast prediction of gas cloud explosions. This model is defined as the Multi-Energy Method, and it does indeed overcome some deficiencies of simplified TNT equivalence methods. Using the TNT equivalence method, the blast effects from gas cloud explosions are correlated to those from equivalent explosive charges of TNT – this is a means of quantifying the intensity of the gas explosions. However, blast wave characteristics from TNT and similar high explosives are significantly different from those from a gaseous explosion. High explosives typically produce higher peak overpressures and shorter durations for similar energy content in terms of heat of reaction.

The Multi-Energy Method is based upon numerical simulations of a blast wave from a centrally ignited spherical cloud with constant velocity flames. With this method, the scaled distances are calculated directly from the energy content of the gaseous mixture. MATLAB code was used to compute the estimated overpressure and positive phase duration based upon the volumetric energy of the gas. Figure 2. show the predicted blast overpressure and the positive phase duration for an ethane-oxygen mixture and 1 kg of TNT.
Figure 2. (Left) Blast overpressure against distance for an Ethane-Oxygen mixture and 1 kg of TNT, (Right) Positive phase duration against distance for an Ethane-Oxygen mixture.

The overpressure and duration values shown in Figure 2 were used to set up a data collection system that recorded the voltage-time signal generated by the sensors. This procedure is outlined in the experimental testing section of this paper.

2. Experimental Procedure

2.1 Test Setup

Figure 3. EPRI Bang and Clean Experimental Test Setup
All testing was performed at the Explosives Research Laboratory in Idaho Springs, CO. Two test series were conducted to measure the near-field blast overpressure at a 1m standoff distance from the blast. Test series one included four tests of 100L stoichiometric single bag mixtures of ethane and oxygen. Test series two included six tests of 80L (each) stoichiometric double bag mixtures of ethane and oxygen.

The bags and pressure sensors were mounted 1.5m above the ground. A gas filling system was used for precise flow metering of the ethane and oxygen into bags. Teledyne Electric Bridge-Wire Detonators using only the electric spark were used, they had a 4000 volt pulse, with 1500 amps peak current into low resistance load at 8 Joules. For initiation the Teledyne FS 17 firing set was use. Another series of tests was conducted with for Far-Field pressure measurements ranging from distances of 1 meter to 12 meters. The same eight gauges were used and both single 100L and double 80L bag were tested.

2.2 Instrumentation

The blast overpressure and impulse were recorded using five piezoelectric pressure gauges PCB models 137A23. These free-field ICP pressure probes are specifically designed for measuring field blast and shock tunnel pressure time profiles using a stable quartz piezoelectric element in an Invar housing. The five sensors were dynamically calibrated by PCB using a hydraulic pulse technique with +/- 1 percent uncertainty.

Figure 3. Bag Setup, double bags were orientated vertically (out of plane) and initiation occurred above the bags
The gauge diaphragm is insulated using common vinyl electrical tape to minimize possible signals generated by flash temperatures due to the passing of the shock front. Additionally, the bodies of the gauges were isolated from the ground by placing vinyl electrical tape in the contact surface with the steel stand (Figure 5.).

The pressure sensors are connected by coaxial cable to a PCB sensor signal conditioner model 482C05. The outputs are also connected to the channels of two Tektronix DPO72004C Oscilloscopes where the signal provided by each gauge was recorded. Triggering was implemented from the firing system and a signal differentiator that provided a 2-volt output to the high-speed camera and the oscilloscopes. A high-speed camera, Phantom Veo, recorded a close view of the exploding bag for understanding the flame propagation across the ethane-oxygen mixture.

Figure 4. Free-field Blast Pencil Probe

Figure 5. Blast Pencil Setup
3. Results

3.1 Peak Pressure 100L Gas vs. TNT

Eight gauges were used for the near-field and far-field tests and data was obtained by using a variety of standoff gauge distances as mentioned earlier. For the near field tests, five pressure gauges were arranged in a semi-circle all one meter from the center of the bag, refer to Figure 3. and three were in a concentric semi-circle 2m from the center of the bag. For the far field tests, the gauges were arranged at varying distances from 1m to 12m away from the center of the bag. 12 meters was the max distance obtainable due to the size of the test range. The oscilloscope data was recorded for all 8 gauges. Each set of shot data was then put into a MATLAB program to determine peak pressure readings for each gauge and duration of the positive phase of each detonation. The data for each shot that did not detonate was removed and plotted separately to show the pressure differences between a bag that transitions to detonation and one that only deflagrates. The following plot, Figure 6, shows a comparison between the far field data for the Single 100L shots and a numerical calculation for the pressure decay at the same distances of 100 grams of TNT.

![Single Bag - 100L](image)

**Figure 6.** The pressure decay in PSI of single 100L bags vs. 100 grams of TNT
The single 100L bags have a very similar pressure profile as 100 grams of TNT. This demonstrates that the gas explosion does indeed reach pressures similar to that of high explosives as well as exhibit similar overpressure decay. In the next plot, Figure 7, the far field profiles for 100L shots that detonate are compared to the shots that deflagrated. The shots that deflagrated had significantly lower pressures by an order of $10^1$ (note y-axis is logarithmic). When the tests were conducted it was clear when a shot would not transition to a detonation because of these low pressures being seen in the oscilloscopes, less than 1 PSI at 1m away was typical of the shots that deflagrated, whereas 15-12 PSI was typical of a shot that detonated.

![Figure 7. Comparison between single bag 100L shots that detonated vs. deflagrated](image)

To further illustrate the differences seen between shots that detonated and shots that deflagrated the blast profile can be evaluated from the high-speed imaging. Figure 8. shows a spherical blast wave indicative of a detonation. As the wave moves across the bag many features of a typical detonation wave are present. Figure 9. Shows the propagation of a deflagrating gas mixture. During deflagration the blast moves more linear in a path directly out of the tube where the blast is initiated and slowly propagates as compared to the detonation.
3.2 Velocity of Shock Front for Single and Double Bags

To further verify the discrepancies seen between a detonation and a deflagration of the gas mixture, the velocity of detonation was computed using Vision Research Phantom Camera Control 2.8. In this case only one of each type (single vs. double bag) was studied but there is a clear difference between the velocities as seen in figures 10 and 11. The single bag shot that detonated in Figure 10 peaked at velocity of 2469.4 m/s at 176.4 mm from the initiation then slowed down as the blast wave move across the bag. This velocity decay mirrors the pressure decay seen in the far-field analysis. The double 80L bag in Figure 11. showed a much different velocity as it peaked at 1794.3 m/s.

Figure 8. High-speed still images of single 100L bag detonation

Figure 9. High-speed still images of single 100L bag deflagration
Figure 10. Velocity profile of blast wave in a 100L bag

Figure 11. Velocity profile of blast wave in the double 80L bags
3.3 Peak Pressure Double 80L Gas vs. TNT

The Double 80L bag also followed a similar profile to that of the 100L single bag but with a slightly higher magnitude of about 1-5 PSI across the varying distances. This also shows that the double 80L bag has slightly higher pressure than that of the 100 grams of TNT. The other notable difference with the double 80L shots was the higher variation in peak pressures. This can be seen in Figure 13 with a 5 PSI variance between the shots.

![Double Bag - 80L](image)

**Figure 12.** Plot showing double 80L peak pressures vs. 100 grams on TNT
One possible cause that it was observed in some of the high-speed videos that there was sympathetic detonation in the 80L double bags. This appears to be a sympathetic detonation because the bag initiates in the corner nearest to the first bag rather than the middle of the bag where the jet flame enters into the bag. There was a 596.95 μs (micro-seconds) delay between the first bag and the second bag’s initiation. It took 347.06 μs for the shock front to go from the nozzle to the end of the bag and then another 249.89 μs went by before initiation of the second bag.

Figure 13. Plot showing variance in pressure for double 80L shots

Figure 14. The left frame shows full detonation of the right bag then the second frame shows the blast initiating in the top right corner of the left bag
Figure 15 shows the discrepancy between a double 80L shot that had the two bags initiate simultaneously and a shot that had a sympathetic initiation. The velocities obtained for the bags that initiated as intended were consistent with velocities above 1600 m/s. However, for the bag that was initiated sympathetically had values much lower, and the velocity increased as the reaction went along the bag. This indicates that the second bag did not transition from deflagration to detonation as a result of critical diameter being reduced from 25.7 mm (1 inch) at the nozzle to a smaller diameter due to the non-fully inflated bag. Moving from a confined state within the tube leading to the bag and transitioning into a partially confined state within the bag, the jet flame will not be able to sustain a high enough velocity to transition from deflagration to detonation. It can also be noted that the deflagration velocities increased as they traveled along the length of the bags but never transition to detonation as seen in Figure 15. In Figure 15 the different colored lines represent 3 different tests for the double 80L bags. The lines with triangles represent the left bags and the stars represent the right bags. Test 1 (green) shows both bags detonating simultaneously, while Test 2 (black) showed the right bag detonate and the left bag deflagrate, and finally Test 3 (blue) showed the left bag detonate and the right bag had a slower velocity detonation. It can be seen that at about 275 mm into the bags showed a steady detonation velocity across the tests that detonated.

![Double 80L Bag Velocities](image)

**Figure 15.** Plot showing the velocities within the double 80L bags as a function of distance from the initiation point
3.4 Pressure Profile for Near Field Data

The near field data for pencil probes one through five were evaluated to determine the pressure peaks for each shot that detonated as well as the profile for peak pressures around the bag as shown in Figure 16. Only one of the four shots conducted using 100L bags did not detonate. All the double bag 80L shots detonated for the near-field shot series.

![Single 100L Pressure Peaks at 1m](image)

**Figure 16.** Plot of pressure peaks for single 100L bags at pencil gauge positions 1-5

![Positions of pencil gauges 1-5](image)

**Figure 17.** Positions of pencil gauges 1-5 (black rectangle is the initiation point)

From the peak pressure results based off the position of highest pressure for 100L bags is unclear. From shots 2 and 3 it would appear that the highest pressure is obtained at the gauge 4 positions, which is 45 degrees off the axis of initiation. However, shot 3 appears to have its highest pressure at the end of the bag along its longitudinal axis. More data is needed to get a clear understanding of how the peak pressure changes depending on orientation from the bag. It is also important to note that the only shots that deflagrated were shots using single 100L bags.
For the double 80L bag tests, the pressure profile has a clearer pattern. Positions 1-5 can be seen in Figure 18 and indicates that the highest-pressure values are obtained at positions one and five. The pressure values decrease as the gauges move radially to position three. This decrease in pressure may be due to the direction of the blast wave propagation moving outward and down, meaning it will reach gauges 1 and 5 before the rest of the gauges.
5. Discussion and Conclusions

A total of 10 tests were conducted for the ethane-oxygen gas mixtures at the Explosive Research Laboratory at Colorado School of Mines in Idaho Springs. These tests were designed to study the DDT characteristics of the gas explosion related to limited boundary conditions such as the critical diameter. Among all the tests the stoichiometric conditions were the same with the only change being related to the volume and resulting pressure of the gas mixture. Results demonstrated that the jet flame coming from the confinement of the hose leading to the bags was reaching velocities causing the deflagration of the gas mixture to transition into a detonation. However, the critical diameter of the nozzle leading into the gas tubes would sometimes decrease to a point where the transition to detonation would not occur. More tests that have instrumentation to record the exact diameter leading into the bag would help further this conclusion. It was also observed that as the shock front velocities within the bags increased the peak pressures also increased as expected.

For confirmation of both the detonation velocities and the peak pressure profiles of the gas explosion, more shot data would be needed. Especially when referring to the 100 Liters single bag shots not enough consistency was obtained to be able to clearly state what causing failures to detonate and what variable were changing the peak pressure profiles. These failures may be attributed to premature rupture of the bag as seen in the high-speed images. The boundary conditions changed resulting in the pressure within the bag to decrease causing the jet flame to not attain velocities high enough to transition into detonation.

The 80 Liter double bag studies were more consistent leading to the idea that shear volume adds to the consistency of detonation but this idea still needs to be validated. Especially when noting that there were several instances that one bag would reach detonation velocities while the other would have much lower velocities. It is also important to study the exact characteristics that make the mistiming of the 80L bag initiation and resulting sympathetic detonation.

In the near-field studies it was shown that the orientation of the bags had an effect on the profile of pressure peaks at 1 meter due to the geometry of the bag. The bags had a width to length ratio of 1 to 3, when orientated horizontally there was a significant effect on the profile of pressure peaks due to the asymmetry. When positioned vertically there was little effect because the bags were now symmetric with respect to the gauges.
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Citations


