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Packing Configurations of PBX-9501 Cylinders to Reduce the Probability of a DDT

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Abstract: The detonation of hundreds of explosive devices from either a transportation or storage accident is an extremely dangerous event. This paper focuses on identifying ways of packing/storing arrays of explosive cylinders that will reduce the probability of a Deflagration to Detonation Transition (DDT). The Uintah Computational Framework was utilized to predict the conditions necessary for a large scale DDT to occur. The results showed that the arrangement of the explosive cylinders and the number of devices packed in a "box" greatly effects the probability of a detonation.

Keywords: DDT, Deflagration, Detonation, Impact to Detonation, Inertial Confinement

1 Introduction

In August of 2005, a tractor-trailer carrying 16,000 kg of seismic boosters overturned, caught fire and detonated in Spanish Fork Canyon, Utah. The damage was catastrophic, creating a crater 10 m deep by 24 m wide with burning debris found up to 400 m away. It was apparent by the size of the crater that the explosion transitioned from a deflagration into a fully developed detonation. Though these accidents are rare the damage caused by the detonation of thousands of kilograms of explosives can be extremely detrimental. The focus of this research is to mitigate the risk of detonation of solid Class 1.1 explosives in either a transportation or storage accident.

The results from this paper showed that the way the explosives are packed is important in mitigating this risk. To the best of the authors' knowledge the probability of DDT as a function of packaging arrangement has not been studied. Here we describe spatial layouts of the devices which were computationally tested to determine which would reduce the probability of a denotation. Two hypotheses were tested in these computational experiments:

1. How does the number of explosive cylinders in a "box" contribute to the propensity for a detonation?
2. Does changing the arrangement of the "boxes" filled with explosives alter the propensity for a detonation?

To analyze these hypotheses four variables were examined: (1) the spacing between the boxes, (2) the arrangement of the boxes, (3) the number of cylinders in each box, and (4) the arrangement of cylinders in the box. The Uintah computation tool was used to simulate these different configurations. Once simulated the configurations were visually examined to determine if a detonation occurred. Section 2 discusses the computational framework used to model the DDT scenario and previously identified DDT initiation mechanisms in an array of cylinders. Section 4.1 discusses how changing the number of cylinders in a box effects the deflagration to transition to a detonation. Section 4.2 examines different packing configurations to reduce the probability of a detonation.

2.1 Current Packing and Storage Protocol

In the 2005 transportation accident, 8,400 seismic boosters were being transported ac- cording to the existing U.S. government regulations. Each booster was filled with Pentolite, an equal part mixture of PETN and TNT, which is commonly used for underground oil and gas exploration. Two sizes of cylindrical boosters were on board and were enclosed in open-ended plastic tubes. There were 5,000 large boosters each containing 2.5 *kg* of explosive. Each one was 0.737 m long and they were packaged 10 to a box. The smaller boosters weighed 1.13 kg each and were 0.33 m in length and were packaged 20 to a box. All of the seismic boosters were packaged in fiberboard 4G boxes in accordance to the Code of Federal Regulations (CFR) Title 49 §173.62 instruction 132. The CFR states that boosters must only be packaged with materials of the same classification, meaning no detonators can be transported in the same load. They must also be packaged in boxes made of steel, aluminum, wood, plywood, reconstituted wood, fiberboard or solid plastics. The mass of the explosives in a box or their spatial arrangement is not defined in

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*Supporting information for this article is available on the WWW under http://www.pep.wiley-vch.de or from the author.((**Please delete if not appropriate**))* the regulations and is at the discretion of the manufacturer [1]. The only limitation on the quantity of explosives transported is the maximum weight limit set by each state. For Utah, where the 2005 accident occurred, regulation 23 CFR §658.17 defines a maximum of 36,000 kg, well above the weight in the accident.

The regulations for storing high explosives are defined by the United States Bureau of Alcohol, Tobacco and Firearms (ATF), Title 27 of CFR §555. It describes the ventilation system requirements, permits, required markings, and what material each component of the storage facility can be constructed from. It also states the required spatial separation from surrounding buildings, roadways, and highways. According to Title 27 CFR §555.213 the maximum quantity of high explosives allowed in a building is 136,000 kg. Similar to the transportation regulations, detonators cannot be in the same building as class 1.1 explosives. There are no regulations on how the explosives are packed or stored inside the building. Boxes can be stacked side by side and on top of one another.

2 Computational Methods

The Uintah Computational Framework [2,3], developed at the University of Utah was utilized to predict a DDT in large arrays of explosive cylinders in a variety of spatial arrangements. The framework utilizes the fluid-structure interaction algorithms of the Material Point Method (MPM) [4,5,6,7], a low and high-speed compressible CFD algorithm (ICE) [8], and a fluid-structure interaction algorithm (MPMICE) [6,9,10]. ICE is a finite volume method and uses an adaptive hexahedral mesh. MPM was used to evaluate the evolution of the solid material by using Lagrangian points (particles) and an Eulerian mesh to evolve the governing equations. The particle's state vector is interpolated back to the cell-center where the exchange of mass, momentum, and energy occurs. This allows multi-phase materials to use the same Eulerian mesh. The governing equations and the algorithms to solve them can be found in [6,8,10,11,12]. Embedded within the MPMICE component is a validated DDT model to represent the reaction of solid explosive → gaseous products at multiple initial temperatures and pressures [13,14,15,16]. The DDT model utilizes a modified Ward, Son, and Brewster (WSB) burn model [14,16,17] to evaluate the mass conversion rate, the ViscoSCRAM constitutive model [18] to model the damage in the solid, and the JWL++ simple reactive flow model [19] to describe detonation. The commonly used JWL equation of state [19,20] was used for the solid explosive and the product gases. Detonation occurs in Uintah's DDT model when the localized pressure is greater than the pressure threshold, 5.3 GPa [13,14]. Further details on the model can be found in [13,14,15,16,21]. The Uintah framework has a long history of high performance computing and has shown good strong and weak scaling characteristics up to 512K cores on DOE's Mira [22,23,24]. Uintah's strong scalability enabled us to run large 2D and full 3D simulations at high grid resolutions (2 mm). The reaction model has been validated at many resolutions including 2 mm [15,25]. Using this advanced computational tool it was possible to predict if a thermally ignited array of explosives would undergo a DDT event.

2.1 Common Simulation Setup

This research focused on the smaller of the two cylinders involved in the 2005 accident, 0.054 m in diameter and 0.33 m in length. Due to the abundance of experimental data and Uintah's validated DDT model, solid PBX-9501 (95% 1,3,5,7-octahydro-1,3,5,7-tetranitro- 1,3,5,7-tetrazocine (HMX) and 5% of a plastic binder) was the explosive examined. For simplicity the fiberboard material was not modeled, instead 10 mm air gaps separated the "boxes." These simulations consisted of only two materials, the solid reactant modeled by MPM particles and the product gas modeled by ICE. The explosives and surrounding gas were initially at ambient pressure and temperature, and the explosives were ignited by hot product gas at 2500 K in the *x*− corner of the domain. All explosive devices were one to two cells away from the computational boundaries to reduce boundary effects. The 2D simulations were performed using symmetric/reflective boundary conditions for the *x*−, *y*−, *z*−, and a wall on the *z*+ face. All other boundaries conditions were set to a zero gradient for the primitive variables (temperature, velocity, density and pressure) and the edge of the computational domain was positioned far from the area of interest to minimize, nonphysical boundary condition effects. The 3D simulations were the same with the addition of the *z*− and *z*+ boundaries being set to a zero gradient for the primitive variables.

There are two ways to package cylinders in a box, tight packing where the cylinders are in a hexagonal configuration or loose packing where the cylinders are in a square configuration. For this study both configurations were examined and preliminary simulations showed that the loose packing distribution is less likely to transition to a detonation. Therefore we only presented the simulations consisting of explosives loosely packed in a "box."

A large 3D simulation was run with 1280 PBX-9501 cylinders packaged 20 to a "box" and stacked one on top of the other, as shown in Figure 1. The simulation consisted of 64 "boxes," 4 in each direction, correlating to 1/8th of the original tractor trailer in the 2005 accident. The domain for this simulation was 12 m^3 resulting in 350 million cells containing 980 million PBX-9501 particles. This was run on 64 thousand cores on DOE's Mira costing over 24 million core processing units. Under these conditions our results showed that the array transitioned to a denotation at 0.66 msec. From this simulation there was strong evidence that the packing arrangement used in most storage facilities and during transportation will transition to a DDT. This result provided motivation to study new ways of packing/storing explosive cylinders

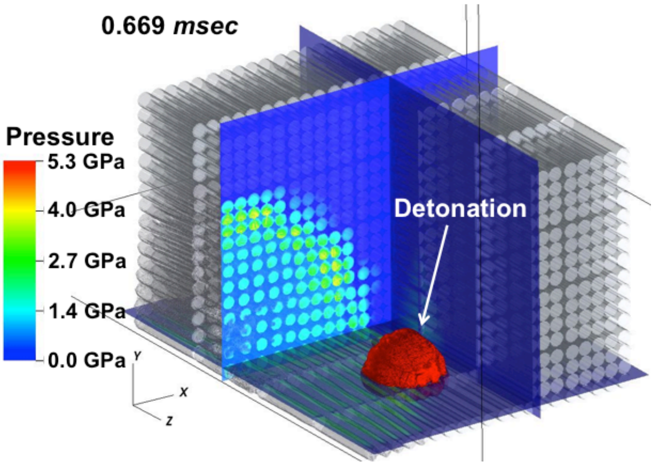

Figure 1. Contour plots of the pressure and shadow of the explosive cylinders in the 3D simulation.

to prevent a detonation. The level of computational resources required to preform a parametric study of this type is exceedingly expensive on current computational platforms. We therefore investigated using low-cost, fast running, 2D simulations for our study. We ran a series of 2D simulations and compared the position and time of the detonation against the large 3D results. Analysis of the state of the cylinders at the point of detonation showed that a similar physical mechanism caused the detonation in each simulation [25]. The global maximum pressure in the domain as a function of time was also compared and good qualitative agreement was observed. The good level of agreement in the main variables of interest justified our use of low cost 2D simulations for the parametric study.

3 DDT Initiation Mechanisms

Previous work on identifying the previously unknown physical mechanisms involved in initiating a DDT in an array of explosive cylinders was presented in [25]. Two dominant mechanisms were identified, inertial confinement and Impact to Detonation Transition (IDT). Inertial confinement only occurs when the explosive cylinders are packaged closely together. As the deflagration progresses outward the inertial mass of the surrounding explosives slows the movement of the deforming deflagrating cylinders, causing them to compact into one another. In the compaction zone a high-density barrier forms, trapping the product gases and increasing the local pressure behind the barrier. As the pressure increases the burn rate accelerates, until a detonation is reached [25]. The second mechanism, IDT, was observed when the explosive cylinders were packaged further apart, allowing for the gases and explosive fragments to accelerate to velocities of ≥500 m/s before impacting nearby deflagrating cylinders. Due to the deflagration, these nearby explosives are typically at an elevated pressure (≈3 GPa). Once impact occurs the deflagration quickly transitions to detonation. The observations suggested that the mechanical insult generates stress waves in the explosive, that reflect, and produce the pressures required for a detonation. A full discussion of these physical mechanisms can be found at [25].

4 Results and Discussion

This study examined two strategies to reduce the probability of a DDT in packed PBX- 9501 cylinders. The first was to change the number of explosives in a “box” and the overall volume or the global Packing Volume Fraction (PVF). The global PVF is the total PBX-9501 volume divided by the total volume that the “boxes” occupy (not the computational domain volume). The second was to change the way in which the “boxes” are organized while keeping the size of the boxes constant. This is referred to as the packing configuration. Figure 2 illustrates the four different packing configurations presented.

4.1 Critial Packing Volume

This section examines hypothesis one; how the number of explosive cylinders in a “box” contributes to the propensity for a detonation. In these simulations the outer dimensions of the boxes were varied to account for the number of cylinders contained, see Figure 2 ((a) compared to (c)). A critical PVF was defined as the maximum global PVF that does not initiate a DDT when thermally ignited. In Section 4.2 we show that the initial spatial layout of the explosives greatly influenced the probability of a DDT and that there was not a critical PVF for all packing configurations. This realization led to the hypothesis that varying the number of explosive cylinders in a “box” can increase the critical PVF and decrease the amount of space needed to package 320 PBX-9501 cylinders safely. In this study the only packing configuration examined was the Base configuration, Figure 2 (a and c). The number of “boxes” simulated varied in order to contain ≈320 cylinders. Two variables were varied in the parametric study: (1) the number of cylinders per box and (2) the distance between the boxes. Table 1 shows the simulations nearest to the critical PVF threshold for each configuration. This is a small representation of the >65 simulations examined. Figure 3 shows the PVF of all

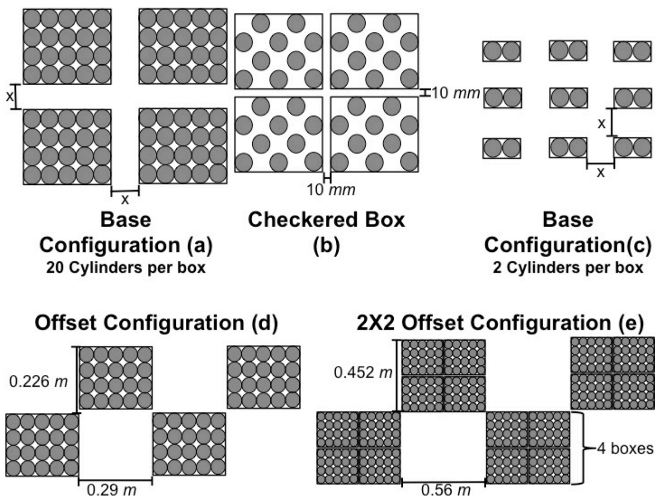

Figure 2. Initial packing configurations.

Table 1. Initial conditions for the simulations near the critical PVF (defined in Section 4.1) for each configuration.

Simulation Name	# of Cylinders per box	Spacing between boxes (x)	Configuration (Described in Figure 2)	Global PVF	DDT Initiation Mechanism
Transportation Accident	20	10 mm	Base	0.739	Inertial Confinement
Base_20_200mm	20	200 mm	Base	0.298	-
Base_20_190mm	20	190 mm	Base	0.31	IDT
Base_20_136mm	20	136 mm	Base	0.387	IDT
Base_16_150mm	16	150 mm	Base	0.26	-
Base_16_120mm	16	120 mm	Base	0.301	IDT
Base_12_104mm	12	104 mm	Base	0.37	-
Base_12_90mm	12	90 mm	Base	0.404	IDT
Base_9_90mm	9	90 mm	Base	0.367	-
Base_9_34mm	9	34 mm	Base	0.497	-
Base_9_30mm	9	30 mm	Base	0.54	IDT
Base_6_34mm	6	34 mm	Base	0.524	-
Base_6_30mm	6	30 mm	Base	0.547	Inertial Confinement
Base_4_30mm	4	30 mm	Base	0.505	-
Base_4_24mm	4	24 mm	Base	0.548	Inertial Confinement
Base_2_20mm	2	20 mm	Base	0.503	-
Base_2_10mm	2	10 mm	Base	0.62	Inertial Confinement
Base_1_16mm	1	16 mm	Base	0.598	-
Base_1_14mm	1	14 mm	Base	0.615	Inertial Confinement
Offset	20	-	Offset	0.385	-
2X2_Offset	20	-	2X2 Offset	0.375	Inertial Confinement
Checkered_Box	10	-	Checkered Box	0.393	-

simulations as a function of the number of explosives in a "box." The green line and points show the critical PVF for each configuration and the red points are simulations which resulted in a detonation. Below the critical PVF (blue points) detonation did not occur due to adequate spacing. Above the critical PVF threshold the explosives were too densely packed and resulted in a detonation. This plot illustrates two ideas: (1) the fewer cylinders there were per "box" the larger the critical PVF, (2) there was a threshold at 9 cylinders per "box" where the critical PVF dramatically increases from 0.37 to 0.497.

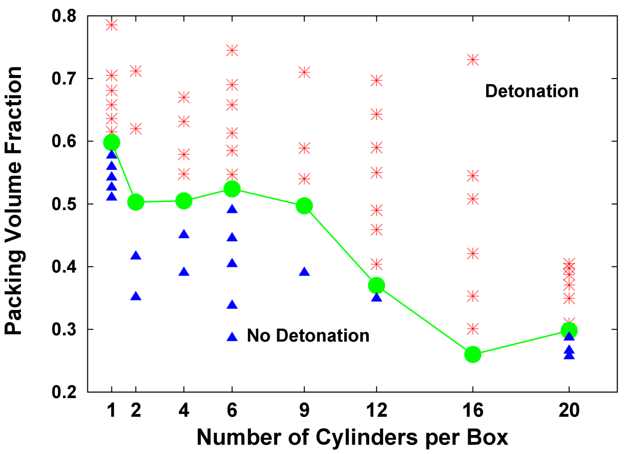

Figure 3. The PVF for each of the >65 simulations using between 1 and 20 cylinders per box. The green circles and line represent the critical PVF for each configuration. The red asterisks depict simulations that detonated while the blue triangles represent simulations that never detonated because they had a PVF below the critical one.

The explanation behind the two postulations illustrated in Figure 7.3 are very similar. The observed average pressure was lower in "boxes" containing fewer cylinders, 2 GPa compared to 3-4 GPa. When more explosives were packaged together the interior devices were "confined" by the surrounding cylinders, thus restricting the expansion of product gases and increasing the localized pressure. When the number of cylinders per box was increased from 9 to 12, in order to ensure safe deflagration the spacing between the "boxes" needed to be doubled, from 50 mm to 104 mm. This was due to a "box" with 12 cylinders reaching a higher pressure, from the confinement of the surrounding cylinders, than was seen in boxes containing 9 cylinders. Figure 4 shows that the pressure in the Base_12_90mm simulation was 1-1.5 GPa higher than the pressure reached in the Base_9_90mm simulation, Figure 5. Figures 6 and 7 show the position the data was extracted from, shown by the white line. The only difference between these two simulations was the number of explosives in a "box." A result of the elevated pressure was increased particle velocities. The observed particle velocities were over 100 m/s faster than those seen in the Base_9 simulation. This forced the boxes to be spaced further apart in order for the impact of deflagrating particles and pressure waves to not initiate an IDT event. Thus the more explosives packed together the higher the localized pressure, the higher the particle velocity, and the further the boxes must be separated

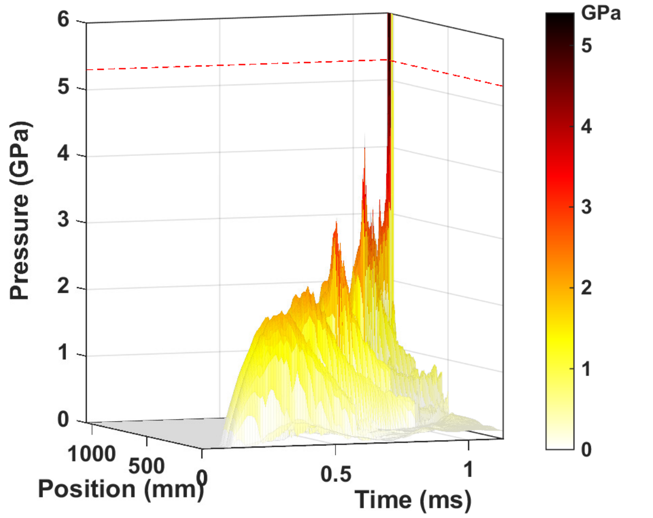

Figure 4. Pressure profile verse position and time for the Base_12_90mm simulation. The red dotted line represents the pressure threshold for a detonation. Position of extracted data is shown in Figure 6 by the white line.

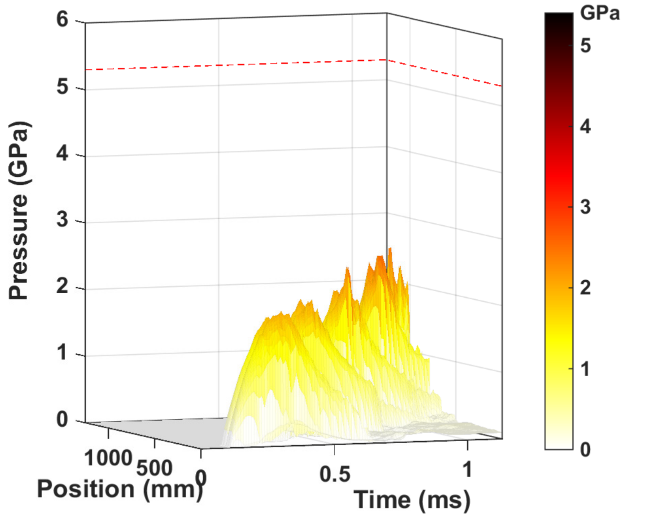

Figure 5. Pressure profile verse position and time for the Base_9_90mm simulation. The red dotted line represents the pressure threshold for a detonation. A detonation was not observed in this simulation. Position of extracted data is shown in Figure 7 by the white line.

to avoid a detonation.

The same explanation can be used to understand why decreasing the number of cylinders per box resulted in an increase of the critical PVF. It was observed when there were 4 or fewer cylinders per "box" the gases easily expanded resulting in low localized pressures. As a result the only observed DDT mechanism was inertial confinement which occurred when the boxes were packed closely together (<30 mm). For the Base_1 configuration the "boxes" had to be packaged less than 16 mm apart to form inertial confinement. That is less than the space needed for one cylinder (54 mm). Thus packing fewer cylinders in a "box" increased the critical PVF, decreased the space occupied, and decreased the probability of a detonation.

4.2 Packing Configuration

The second strategy for safer transportation and storage of explosive devices (hypothesis two) was to change the packaging configuration while holding the global PVF constant. The arrangements are presented in Figure 2. In the four configurations considered, the box size was held constant at 0.27 m x 0.216 m resulting in global PVF ranging from 0.375 to 0.393, see Table 1.

The first layout analyzed was the 2X2_Offset configuration, which had a global PVF of 0.375. It

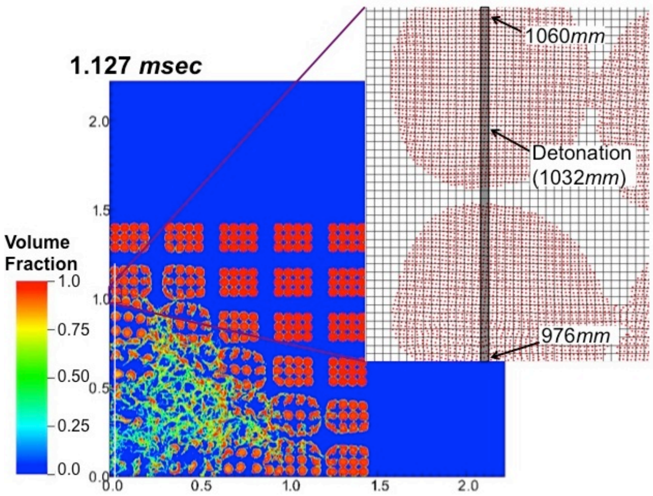

Figure 6. The volume fraction of PBX-9501 in each grid cell of the simulation domain, at the timestep at which an IDT initiation of a DDT was detected in the Base_12_90mm simulation. The white line illustrates where the data were extracted for Figure 7.4.

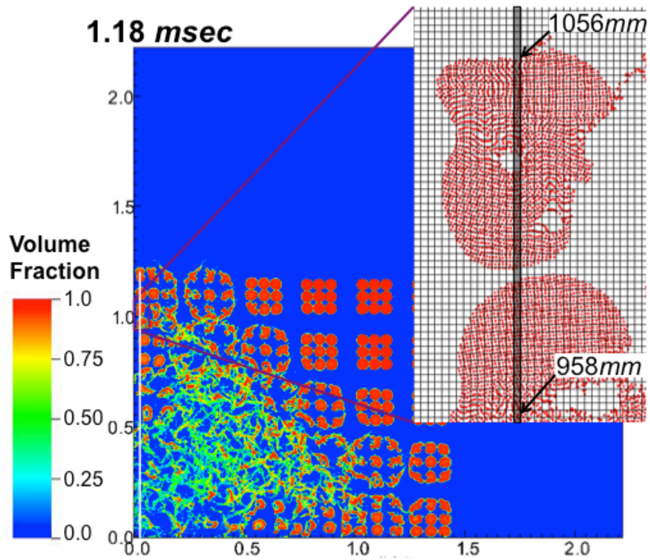

Figure 7. The volume fraction of PBX-9501 in each grid cell of the simulation domain in the Base_9_90mm simulation. The white line illustrates where the data were extracted for Figure 5.

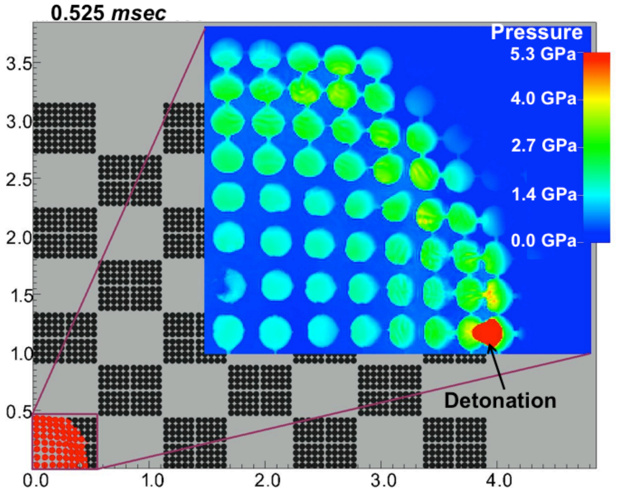

Figure 8. Contour plots of the progression of deflagration (red) and the pressure (upper right corner) in the 2X2_Offset configuration. This configuration transitioned to a detonation due to an inertial confinement initiation mechanism.

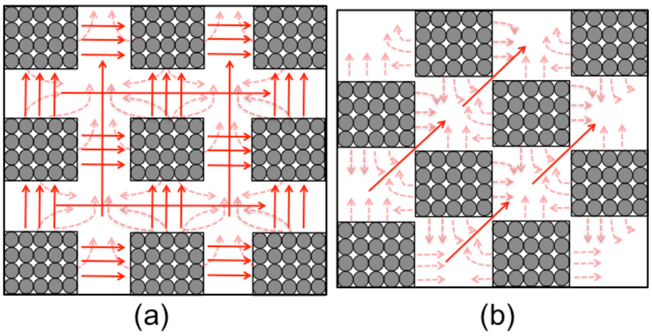

Figure 10. Schematic diagram of the idealized undeformed cylinders flow field for the Base_20_136mm (a) and the Offset configuration (b). The solid arrows represent the bulk flow and the dashed arrows the local flow field.

contained four boxes packed together surrounded by open space where four other boxes would have been, see Figure 2(e). Figure 8 shows the progression of deflagration (red) through the explosive cylinders (grey), an enlarged view of the pressure field as the DDT occurred is shown in upper right corner. These results showed that four "boxes" containing 20 cylinders should not be placed directly next to one another, to avoid a DDT.

The second packing configuration considered was the Base configuration, Figure 2(a). Here we present the results from the Base_20_136mm simulation, which had a global PVF of 0.387, similar to the previous test case. This simulation transitioned to detonation due to an IDT mechanism. Figure 9 shows a contour plot of the magnitude of the product gas velocities and the pressure field at the time of detonation. The pressure is shown in the upper right corner, focused where the DDT occurred. With this packing arrangement the particles and gases did not have sufficient room to expand causing the particles to impact surrounding deflagrating cylinders resulting in a transition to detonation. Figure 10 (a) is a schematic diagram of the flow field. Notice there is little impeding the flow of high velocity gases and explosive fragments from impacting the surrounding deflagrating cylinders. As illustrated in Section 4.1, in order for this packing configuration of 20 cylinders per box to be effective and not transition to detonation the "boxes" must be spaced ≥200 mm apart.

The next arrangement considered was the Offset configuration, with a global PVF of 0.385. With this spatial layout detonation was not observed. Figure 11 shows a contour plot of the magnitude of the gas velocities and pressure. The large open regions allowed the product gases to expand. The pressure in this simulation never reached more than 3 GPa, well below the threshold needed for a detonation. In this configuration an IDT mechanism seemed likely due to the large gaps, allowing gases and particles to accelerate as was seen in the Base_20_136mm configuration. We hypothesize that this did not occur due to the arrangement of the boxes, allowing for the higher gas velocities to redirect the particles and pressure waves away from the deflagrating cylinders and into the small gaps between the corners of the boxes, as shown in Figure 11. This gas movement redirects the particles and pressure waves, which

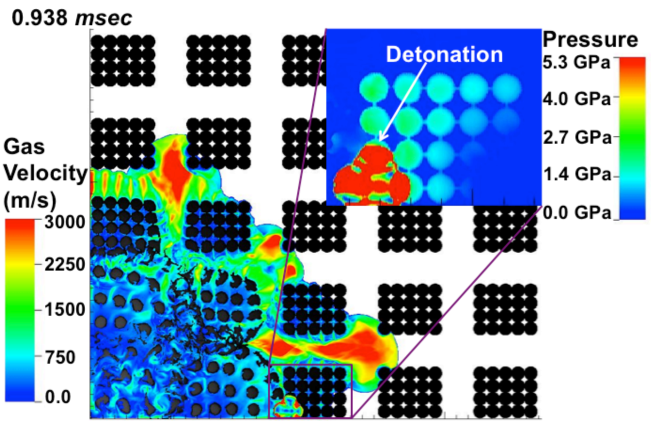

Figure 9. Contour plots of the magnitude of the gas velocity and the pressure in the Base_20_136mm configuration. A detonation occurred due to an IDT mechanism.

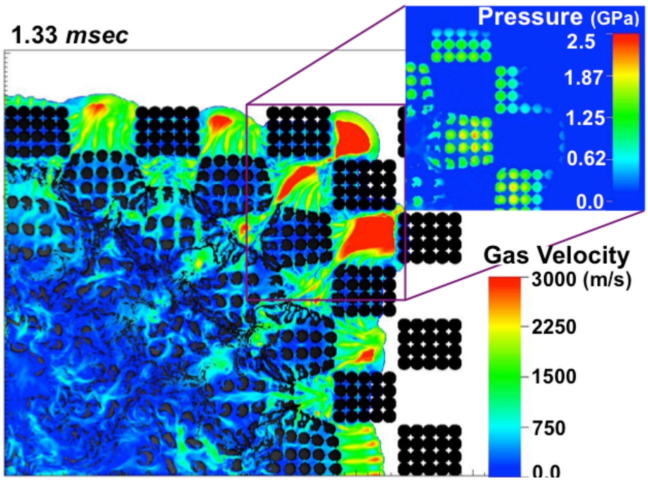

Figure 11. Contour plots of the magnitude of the gas velocity and the pressure in the Offset configuration. A detonation did not occur.

could cause an IDT, to an open area. Figure 10 (b) illustrates a schematic of how we believe the gas flow is altered by packing the "boxes" in an Offset configuration rather than the Base configuration. This configuration shifted the flow of gas and particles from directly toward the deflagrating cylinders 10(a) to in-between the "boxes" 10(b), preventing a detonation.

The last packing configuration considered was the Checkered Box configuration, Figure 2(b). In this loading arrangement every other cylinder was removed from the box, and the remaining cylinders were positioned in a checkered configuration so no explosives were directly on top of one another. Figure 12 shows the pressure field and magnitude of the gas velocity at t= 0.8 msec. The simulation results showed product gases easily expanded with minimal impedance, resulting in relatively low pressures. Since the pressures were low the particle velocities were ≈300 m/s, much lower than the ≥500 m/s seen in an IDT event. Inertial confinement was also not a possible mechanism for this distribution because there was substantial distance between each cylinder (>54 mm), making it difficult for them to compact into one another and form a barrier. Similar to the Offset configuration the pressure in the deflagrating cylinders never reached more than 3 GP a. An enlarged view of the pressure field is seen the upper right corner. This result suggests that this configuration has a low probability of a detonation.

4.3 Comparison of 2D versus 3D Computational Domain

A 3D simulation was run to confirm the results of the 2D Offset configuration. The 3D initial setup was the same as the 2D with the addition of 4 rows of "boxes" in the z dimension, giving more space for the product gases to expand, making it more difficult to build to the pressures need for a detonation. Due to the configuration of the boxes Adaptive Mesh Refinement

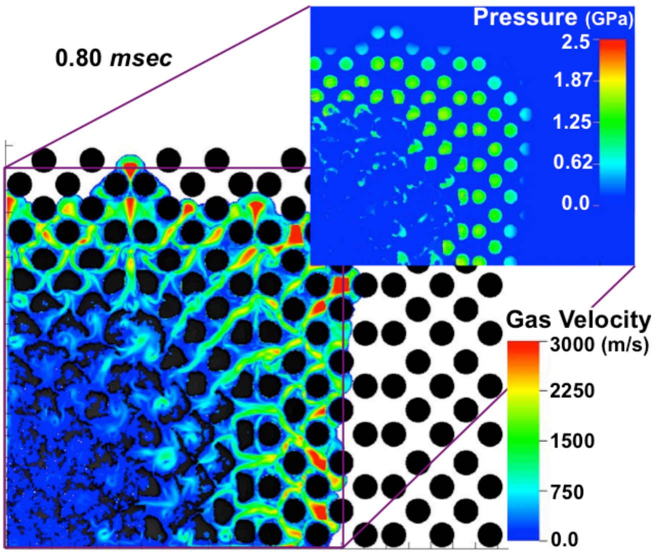

Figure 12. Contour plots of the magnitude of the gas velocity and the pressure in the Checkered_Box configuration. A detonation did not occur.

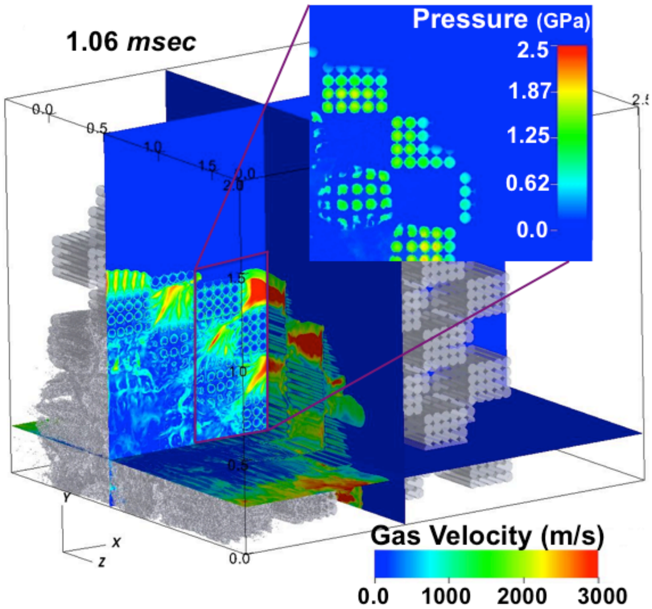

Figure 13. Contour plots of the magnitude of the gas velocity and the pressure in the 3D Offset configuration.

[26] could not be utilized, drastically increasing the computational costs (>6 million central processing units). Figure 13 shows a contour plot of the pressure and the magnitude of the gas velocity. Notice the pressure was well below 5.3 GPa. The pressure and gas velocities were qualitatively similar to those found in the 2D simulation, Figure 11. In both simulations we observed high velocity gases flowing between the corners of the boxes. Even though the 3D simulation did not run to completion, due to lack of resources, the similarities between the 2D and 3D simulations suggest that a detonation would not occur in this configuration.

4 Conclusion

The results from numerical experiments described here have shown that the number of cylinders packed in a "box" effected the probability of a detonation. An important factor in the Base configuration not leading to a detonation was adequate space for the explosive fragments and gases to expand. As fewer explosives were packaged together the mechanism for a DDT switched from IDT to inertial confinement. This allowed the cylinders to be packed closer together without transitioning to a detonation. IDT was less probable with fewer cylinders packed in a "box" because the explosives could not sustain the elevated pressures needed. Strong evidence also suggested that while holding the global PVF constant the packing configuration changes the probability of a detonation along with the DDT mechanism. Two configurations showed that detonation can be avoided while sustaining a global PVF ≈0.39, the Offset and Checkered Box configurations. The 2X2_Offset and Base_20_136mm configurations on the other hand exhibited two different mechanisms for DDT, and quickly transitioned to a detonation.

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