Experimental and Modeling Analysis of Detonation in Circular Arcs of the Conventional High Explosive PBX 9501

Mark Shorta, Eric K. Andersona, Carlos Chiquetea, Scott I. Jacksona

aLos Alamos National Laboratory, Los Alamos, NM 87544, USA

Abstract

We examine the diffraction dynamics of a two-dimensional (2D) detonation in a circular arc of the conventional HMX-based, high performance, solid explosive PBX 9501, for which the detonation reaction zone length scale is estimated to be of the order of 100-150 µm. In this configuration, a steady propagating detonation will develop, sweeping around the arc with constant angular speed. We report on results from three PBX 9501 arc experiments, exploring the variation in linear speed on the inner and outer arc surfaces for the steady wave, along with the structure of the curved detonation front, as a function of varying inner surface radius and arc thickness. Comparisons of the properties of the motion of the steady wave for each arc configuration are then made with a spatially-distributed PBX 9501 reactive burn model, calibrated to detonation performance properties in a 2D planar slab geometry. We show that geometry-induced curvature of the detonation near the inner arc surface has a significant effect on the detonation motion even for conventional high explosives. We also determine the detonation driving zone structure for each arc case, and thus the subsonic regions of the flow that determine the influence of the arc geometry on the detonation propagation. In addition, streamline paths and reaction progress isolines are calculated. We conclude that a common approximation for modeling conventional high explosive detonation, wherein the shock-normal detonation speed is assumed equal to the Chapman-Jouguet speed, can lead to significant errors in describing the speed at which the detonation propagates.

Keywords:
Detonation, Condensed-phase, Arc geometry, Curvature, Diffraction

*Corresponding author:
Email address: short1@lanl.gov (Mark Short)
1. Introduction

Geometry-induced diffraction of a detonation in a condensed-phase high explosive (HE) affects the detonation propagation dynamics due to the resulting modification of the structure of the finite-length detonation reaction zone. An ideal geometry to examine the primary effects of diffraction is the two-dimensional (2D) circular arc [1–3], shown schematically in Fig. 1. In particular, after relaxing from an initiation transient, a steady detonation sweeping around the arc with constant angular speed will develop in the circular arc configuration. The energy release within the subsonic detonation-driving-zone (or DDZ), i.e. the region bounded by the non-planar detonation shock and sonic flow locus (relative to the frame of the steady rotating shock), controls the propagation properties of the detonation [4]. The circular arc configuration is also important in gaseous explosive systems to the understanding of the diffraction mechanisms of detonation propagating in a rotating detonation engine [5–7].

A number of physical insights on the dynamics of a steadily propagating, diffracting detonation in a 2D circular arc of HE have been recently been uncovered in [1, 2]. For example, the authors found that for a fixed inner arc surface radius, beyond a critical arc thickness, the angular speed of the detonation limits to a constant, independent of either further increases in the arc thickness or changes in the type of confinement on the outer arc surface. This is a result of the subsonic DDZ flow detaching from the outer arc surface, with supersonic flow now surrounding the DDZ. Also, the authors of [1, 2] found that a small radial layer of the arc attached to the inner arc surface played a disproportionate role in controlling the angular speed of the detonation propagation. In this layer, there is a strong influence of both the detonation curvature and the material confinement properties on the inner arc surface.

In addition to the theory-based studies [1, 2], Short et al. [3] describe an experiment in a circular section of the insensitive high explosive (IHE) PBX 9502 (95 wt.% TATB (2,4,6-triamino-1,3,5-trinitrobenzene)/5 wt.% Kel-F 800 poly(chlorotrifluoroethylene-co-vinylidene fluoride)) designed to measure the structure and speed of a 2D steady detonation in a circular arc geometry. The arc section had an inner radius of \( R_i = 64.98 \) mm, an outer radius of \( R_e = 89.97 \) mm and was 200 mm wide to ensure that the hydrodynamic flow along the centerline of the arc remained two-dimensional during the course of the experiment (Fig. 2). Associated reactive burn modeling showed that the sonic flow locus of the DDZ largely lies at the end of, or within, the fast reaction stage of the PBX 9502 detonation [3] for the 64.98x89.97 mm arc, with the largest area section of the DDZ lying close to the inner arc surface.

A number of other experiments with either the circular arc section or rib geometry in TATB-based (insensitive) explosive formulations have also been conducted [8–10], although all had arc section widths smaller than both the inner and outer arc circumferential distances. Two-dimensional reactive burn simulations of the arc configurations in [8–10] have been conducted by Tarver and Chidester [11] and Ioannou et al. [12]. To date, the diffraction dynamics of a 2D steady detonation in a circular arc configuration of a conventional high explosive (CHE) have not been examined. Given the extensive use of CHEs in precision munition applications, it is important to demonstrate that we can accurately simulate and understand CHE detonation dynamics in geometries other than simplified 2D planar slabs or 2D axisymmetric.

![Figure 1: The 2D circular arc geometry and its polar coordinate representation. A schematic detonation shock surface is shown in blue. Here, BIL is the detonation breakout imaging line, while IL is the initiation line.](image1)

![Figure 2: Schematic of the circular arc section explored both in [3] and the current study. A region of 3D flow propagates from the left and right outer edges of the section toward the arc center plane. However, the 200 mm arc section width is such that the flow along the inner and outer surface centerlines remains two-dimensional, where the time-of-arrival and detonation front shape measurements are taken.](image2)
shock curvature of a given size will more significantly affect the longer reaction zone structure of a PBX 9502 detonation. In particular, the reaction progress along the DDZ sonic flow surface will be smaller than that for a PBX 9501 detonation. The failure thickness for a PBX 9502 detonation is significantly larger than for PBX 9501, in the region $3.5 < T < 3.75$ mm for PBX 9502, and smaller than $T = 0.8$ mm for PBX 9501 [13]. A comparison of the detonation shock shapes for the same slab geometry thicknesses are shown in Fig. 4, revealing some significant features. While the PBX 9501 detonations are flatter in the center of the charges than for the equivalent PBX 9502 detonations, significantly larger shock curvatures exist near the charge edges for PBX 9501. The near-edge curvature variation is significant since, as noted above, a detonation in a circular arc configuration is largely controlled by the shock curvature variation in a layer near the inner arc surface [1–3].

In the current study, three experiments are described examining the variation in speed and shock shape of the steady rotating detonation as a function of varying inner arc surface radius and arc thickness. The arc results are then used to validate a new PBX 9501 reactive burn model, calibrated via the slab geometry detonation properties in Figs. 3 and 4. Physical insights about the effects of the circular arc geometry on the PBX 9501 detonation reaction zone structure and speed are explored through the reactive burn model. This includes an examination of the DDZ structures to determine the subsonic flow region in each of the arcs influencing the detonation propagation.

2. PBX 9501 Circular Arc Section Experiments

Three different PBX 9501 arc section experiments were conducted with dimensions as follows (see Figs. 1-2): for arc 1, $65.35$ mm ($R_1$) x $67.35$ mm ($R_2$) x 200 mm (width); for arc 2, $65.47$ mm ($R_1$) x $69.97$ mm ($R_2$) x 200 mm (width); and for arc 3, $100.35$ mm ($R_1$) x $120.35$ mm ($R_2$) x 200 mm (width). The angular extent of each of the arcs was $\approx 3\pi/4$ radians. The densities of arcs 1 and 3 were 1.841 g/cm$^3$, while arc 2 was 1.840 g/cm$^3$. Polycarbonate (PC) supports of 9.2 mm nominal thickness were glued to the inner arc surfaces for stability during machining (Fig. 5). Time-of-arrival (ToA) wire diagnostics were located around the centerline of the outer arc surface (Fig. 2), while ToA shorting pins were inserted through the PC supports along the centerline of the inner surface. The ToA diagnostics are used to measure the linear detonation speed on the inner and outer surface centerlines. Their respective circumferential positions relative to the first pin or wire that triggered on each centerline are shown in Fig. 6. The breakout times of successive sections of the detonation shock as a function of radial coordinate along the centerline of the arc
Table 1: Linear speeds of the steady detonation motion along the inner \((r = R_i)\) and outer \((r = R_e)\) arc surfaces for the 3 arc tests showing a comparison between experimental (Exp.) measurements and the reactive burn (MWSD) model.

<table>
<thead>
<tr>
<th>(R_i-R_e) (mm)</th>
<th>Speed ((R_i)) (mm (\mu)s(^{-1}))</th>
<th>Speed ((R_e)) (mm (\mu)s(^{-1}))</th>
<th>Speed ((R_i)) (mm (\mu)s(^{-1}))</th>
<th>Speed ((R_e)) (mm (\mu)s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exp.</td>
<td>Exp.</td>
<td>MWSD</td>
<td>Exp.</td>
<td>MWSD</td>
</tr>
<tr>
<td>65.35-67.35</td>
<td>8.582((\pm0.013))</td>
<td>8.572</td>
<td>8.831((\pm0.003))</td>
<td>8.834</td>
</tr>
<tr>
<td>65.47-69.97</td>
<td>(-)</td>
<td>8.582</td>
<td>9.186((\pm0.006))</td>
<td>9.172</td>
</tr>
<tr>
<td>100.35-120.35</td>
<td>8.664((\pm0.021))</td>
<td>8.630</td>
<td>10.411((\pm0.018))</td>
<td>10.350</td>
</tr>
</tbody>
</table>

Figure 5: Image of the 100.35x120.35x200 mm PBX 9501 arc test.

End surface was measured by streak camera imaging of the destruction time of an illuminated mirrored surface (see Fig. 1-2 and 5). The outer radius \((R_e)\) dimensions of each arc, listed above, were obtained by fitting a circle through an optical comparator measurement of the Cartesian locations of the ToA wires. Since there was no direct method of measuring the arc inner radius \((R_i)\) due to the PC support, the end-surface detonation breakthrough record for each test was used to determine the arc thickness, using a fiducial image to determine the position of the arc edges. The detonation is initiated uniformly along the width of each arc section with a line wave generator (LWG) placed in direct contact with the PBX 9501 arc (Fig. 5). The LWG generator thickness was 3.5 mm.

For each arc test, the relative trigger times for the ToA diagnostics along the inner and outer arc surface centerlines with circumferential distance along each line are shown in Fig. 6. The resulting detonation speeds are determined by a least squares fitting of a linear distance-time function once the detonation has relaxed to a steady rotating propagation mode. Steady-state propagation was determined by calculating where the standard deviation about a local mean in inter-ToA diagnostic speeds, marching backwards from the final ToA record on each surface, exceeded a threshold. The resulting speeds, with standard deviations, are shown in table 1, and the corresponding distance-time functions shown in Fig. 6. Note that we did not record a meaningful steady speed along the inner surface of arc 2 (65.47x69.97 mm), where inter-pin speed variations were consistently \(O(100)\) m/s along the surface. However, the front shape image for the arc 2 test showed the presence of jetting between the inner arc surface and the PC layer, likely caused by an air gap between the...
The relative breakout times $t_b$ from the end of the arc surface for each point on the detonation shock as a function of radial location are shown in Fig. 7 for the 3 arc tests. The heterogeneous microstructure of PBX 9501 is reflected in the observed noise levels, particularly for the scale of the arc 1 test. As a result, the first point of breakout, shifted to $t_b(r) = 0$, is obtained from the gradient of the breakout shapes $dt_b/dr$ using a Savitzky-Golay filter. For arc 1, the breakout shape is moderately symmetric across the arc thickness. Arcs 2 and 3 have features similar to those observed for the PBX 9502 arc [3]. The initial point of breakout occurs close to the inner arc surface. There is significant breakout surface curvature in the region of the inner arc, while the outer sections of the breakout surface are more linear.

3. PBX 9501 Reactive Burn Modeling

Reactive burn modeling allows the structure of the detonation driving and reaction zone in the PBX 9501 arc configuration to be explored. Using a newly calibrated reactive burn model for PBX 9501, we now describe computational simulations of detonation in the three circular arcs with inner and outer radii given in §2, with each of the arcs extending the angular region $0 \leq \theta \leq 3\pi/2$ in polar coordinates $(r, \theta)$. The PBX 9501 is surrounded by a low-density elastomer. This is a similar computational similar set-up to that used in [3], but with PBX 9502 replaced by PBX 9501. As in [3], we model the flow in both the arc-geometry explosive and elastomer with the compressible Euler equations,

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0, \quad \frac{Du}{Dt} = -\nabla p, \quad \frac{De}{Dt} = \frac{p}{\rho^2} \frac{DP}{Dt}, \quad (1)$$

for density $\rho$, pressure $p$, particle velocity $\mathbf{u} = (u, w)$, specific internal energy $e$ and time $t$. The material derivative $D/Dt = \partial/\partial t + \mathbf{u} \cdot \nabla$. In the HE, assuming a reactant state burning to a product state, the internal energy $e$ and specific volume $v = 1/\rho$ for the reactant/product mixture is $e = (1 - \lambda) e_R(p_R, v_R) + \lambda e_P(p_P, v_P)$ and $v = (1 - \lambda)v_R + \lambda v_P$, where $\{\}$ refers to the state in the reactant material and $\{\}_P$ to the product. Here $\lambda$ represents the reaction progress variable in the conversion of reactants ($\lambda = 0$) into products ($\lambda = 1$). The reactant and product equations of state (EOS) have the same (Davis) form as in [3], except they are reparameterized here for PBX 9501, with the EOS parameters now taking the values given in tables 2 and 3. To
close the system, we invoke pressure equilibrium and volume (density) equality as in \[3\], i.e. $p = p_p = p_R$, and $v = v_p = v_R$.

For PBX 9501, the reaction rate is given by

$$\frac{D\lambda}{Dt} = r, \quad r = kp^\varepsilon(1 - \lambda)^\delta. \quad (2)$$

The rate parameters $k$, $n$, and $\varepsilon$ are calibrated to reproduce the detonation thickness effect and front shape data in a 2D planar slab geometry [13] using the merit-function-based fitting approach in [14], whereby $k = 0.0036010 \mu s^{-1} GPa^{-n}$, $n = 3.0$ and $\varepsilon = 0.76781$. Figure 3 shows the thickness effect variation obtained as part of the reaction rate parameter calibration process. We term this as a modified Wescott-Stewart-Davis model (MWSM) for PBX 9501. For an initial density $\rho_0 = 1.832 g/cm^3$, $D_{CJ} = 8.80 mm/\mu s$, while the ZND detonation reaction zone length is $\approx 96 \mu m$. The elastomer EOS is that used in [3]. For the arc calculations, the flow equations in the HE and elastomer regions are integrated with a cell-centered finite volume method on a Cartesian mesh [4]. Material interfaces are treated with a Ghost Fluid method as described in [15], where a local linearized Riemann solution is used to fill the real fluid states. With adaptive mesh refinement, we find that a mesh spacing of $3.125 \mu m$ is needed to ensure mesh converged solutions. The wave is initiated with a hot-spot as in [3] and allowed to relax to the steady rotating propagation mode.

Angular speeds of the steady detonation from the MWSM model computations are determined to be $\omega_0 = 0.13116 rad/\mu s$ for the $65.35x67.35$ mm arc, $\omega_0 = 0.13108 rad/\mu s$ for the $65.47x69.97$ mm arc and $\omega_0 = 0.08600 rad/\mu s$ for the $100.35x120.35$ mm arc. The MWSM model based calculation of $\omega_0$ can then be used to generate the linear speeds $\omega_0 R_i$ and $\omega_0 R_e$ on $r = R_i$ and $r = R_e$, respectively, shown in table 1. The agreement with the experiments is good, showing that the MWSM model is capturing the salient physical mechanisms of the detonation propagation. For the MWSM model of the $65.35x67.35$ mm and $65.47x69.97$ mm PBX 9501 arcs, the linear speeds on $r = R_i$ are almost equal, showing that even for a $2 mm$ thick arc with a fixed inner radius of $\approx 65 mm$, the detonation angular speed no longer depends on the arc thickness. For each arc, the linear speeds on $r = R_i$ depart significantly from $D_{CJ} = 8.8 mm/\mu s$, by $228 m/s$ for the $65.35x67.35$ mm arc and $170 m/s$ for the $100.35x120.35$ mm arc. Curvefit effects, particularly near the inner surface as we demonstrate below, have a significant influence on the propagation even for the CHE PBX 9501. Figure 7 also shows a comparison between the relative detonation shock breakout times from the MWSM modeling and the experiment for each arc geometry. In all cases, the agreement is excellent, further validating the MWSM PBX 9501 model across a range of arc sizes.

Figure 8 shows the detonation driving zone structure in steady flow for each arc simulation. The subsonic DDZ flow is bounded by the detonation shock and sonic flow loci [2]. Sonic flow is measured relative to a frame rotating with the detonation shock front, along which each location on the shock moves with speed $(r\omega_0 \sin \theta, -r\omega_0 \cos \theta)$, and is determined by the locus of points for which $M = [(u + r\omega_0 \sin \theta)^2 + (w - r\omega_0 \cos \theta)^2]^{1/2}/c_{HE} = 1$, where $c_{HE}$ is the frozen sound speed [2]. Also shown in Fig. 8 is a series of steady flow streamlines, representing the spatial paths obtained from the integration of $dx/dy = (u + r\omega_0 \sin \theta)/(w - r\omega_0 \cos \theta)$, along with HE/elastomer material interface locations and a series of reaction progress isolines for $\lambda = 0.5, 0.9$ and 0.99. Figure 9 shows the normal surface speed $D_\alpha$ and curvature $\kappa$ variations along the detonation shock front for each arc, obtained by interpolating a smooth function through the shock shapes and using geometric constraints [1] to obtain $D_\alpha$ and $\kappa$.

Figure 8a shows the DDZ for the $65.35x67.35$ mm arc. The DDZ has a broadly curved, crescent like appearance, with the shock front oblique to the incoming flow except in the central regions. The DDZ is spatially thin for PBX 9501 detonation, $\approx 80 \mu m$ wide in the central part of the arc. Significant $D_\alpha$ and $\kappa$ variations are observed in a layer within $\approx 0.5 mm$ of $r = R_i$ (Fig. 9), associated with limited reaction (Fig. 8a, 10). The shock curvature is smaller in the central part of the arc, where reaction progress is greater, before increasing again at the outer section of the arc. Flow streamlines enter the DDZ in a circular fashion, and are deflected both by the shock front and the onset of reaction. However, on the scale of the DDZ (Fig. 8a), the deflections are small. The DDZ structure for the $65.47 mm \times 69.97 mm$ arc is shown in Fig. 8b. The detonation rotates at a very similar angular speed, $\omega_0 = 0.13108 rad/\mu s$, to the $65.35x67.35$ mm arc, for which $\omega_0 = 0.13116 rad/\mu s$. Near $r = R_i$, we again observe a crescent-like structure.
reactant is almost depleted along the sonic flow line (Fig. 10), and the normal speed $D_n$ is close to $D_{CJ} (=8.8 \text{ mm/µs})$ [Fig 9a]. The shock front in this outer section is oblique to the incoming circular flow, allowing it to rotate at speed $\omega_0 = 0.13108 \text{ rad/µs}$, with its motion controlled by the inner layer DDZ structure, consistent with the asymptotic theory developed in [1]. Figure 11 shows an overlay of the DDZ structures for the 65.35x67.35 and 65.47x69.97 mm arcs. For a layer of size $\approx 1 \text{ mm}$ attached to $r = R_i$, the structures closely overlap. Given the similarity in the angular speeds, we conclude that the energy release in the quasi-1D section of the arc does not contribute to the propagation dynamics. Near $r = R_e$, the sonic layer moves internal to the reaction zone due to the presence of the Prandtl-Meyer fan on the outer boundary, meeting the detonation shock at $r = R_e$.

The DDZ structure for the larger 100.35x120.35 mm arc is shown in Fig. 8c. The overall properties are similar to those of the 65.47x69.97 mm arc, with the bulk of the oblique detonation outside of the inner layer being sweep around the arc by the controlling inner layer DDZ structure. Flow streamline deflections are more noticeable on the scale of Fig. 8c. Significant $D_n$ and $\kappa$
action progress contours. This analysis shows that for

variation in the inner layer, even for

variations are again present in the inner layer, even for the larger $R_i$. In the outer layer, the sonic locus is drawn into the reaction zone at a comparatively earlier stage relative to $R_i - R$ than the 65.47x69.97 arc (Fig. 10), due to the oblique flow.

4. Summary

We have described three experiments on 2D steady detonation of the high performance, HMX-based conventional high explosive (CHE) PBX 9501 in a circular arc geometry, measuring linear propagation speeds on the inner and outer arc surfaces, along with the detonation shock front shape. We have used this data to validate a MWS model, calibrated to 2D planar slab geometry data, demonstrating very good agreement. Using the MWS model, an extensive study of the detonation driving structure (shock and sonic flow loci) for the three arcs was undertaken, including analysis of flow streamlines and reaction progress contours. This analysis shows that for

PBX 9501, curvature variations in a layer near the inner arc surface, $r = R_i$, largely controls the propagation dynamics. We conclude that geometry-induced curvature effects have a significant influence on the detonation structure and dynamics even for CHEs, yielding speeds on the inner arc surface that can be significantly below $D_C^f$. Hence, for complex geometries such as the arc, assuming that the detonation runs at the Chapman-Jouguet speed can lead to significant errors for modeling detonation performance of CHEs.

References