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Analysis of PBX 9502 Rate Stick Data

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EXTENSIONS TO DSD THEORY: ANALYSIS OF PBX 9502 RATE STICK DATA*

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Recent extensions to DSD theory and modeling argue that the intrinsic front propagation law can depend on variables in addition to the total shock-front curvature. Here we outline this work and present results of high-resolution numerical simulations of 2D detonation that verify the theory on some points, but disagree with it on others. Chief among these is the verification of the extended propagation laws and the observation that the curvature is infinite at the HE boundary. We discuss how these results impact the analysis of PBX 9502.

I-INTRODUCTION

The benefits of using insensitive high explosives (IHE) like PBX 9502 (9502) have been well documented [?]. These desirable features come at a price. The reaction zone is longer for IHEs is more nonideal. In real world applications, this translates into significant performance problems, such as problems with detonation wave spreading. The speed of detonation propagation is affected over large regions. To be realistic, calculations of performance must include reaction zone effects.

To capture these effects on propagation with direct numerical simulation (DNS) as we show later, requires roughly 50 cells in the streamwise direction of the reaction zone to get an error of no more than 50m/s for the detonation speed. Considering only the volume occupied by the reaction zone in a 3D DNS, $V_{rz} = a \cdot \mathcal{L}^2 \cdot \eta_{rz}$, where $\mathcal{L} \approx 200\text{mm}$ is the system dimension, $\eta_{rz} \approx 1\text{mm}$ is the reaction-zone length and a is an $O(1)$ geometry factor. For 50 cells in the reaction zone,

this estimate yields $O(10^{10})$ cells just in the reaction zone at any instant. A time of 10^{-4}s is required for one cell update for a modern high-order algorithm running on a Silicon Graphics (SGI) R10K processor. With a time step of roughly $\Delta t = 4 \times 10^{-3}\mu\text{s}$, a physical time of $50\mu\text{s}$ corresponds to 1.25×10^4 time steps. This corresponds to a single processor computation time of

$$T_{\text{cpu}3D} = (10^{-4}\text{s}) \cdot (10^{10}\text{cells}) \cdot (1.25 \times 10^4\text{steps}) \quad (1) \\ = 1.45 \times 10^5\text{days}.$$

With perfect parallelization over 1000 cpus, this becomes $T_{||3D} = 145\text{days}$. Because this estimate includes only one aspect of an engineering simulation and we do not achieve perfect parallel performance, this is an under estimate.

In place of DNS, we have advanced using detonation shock dynamics (DSD), a strategy in which the effects of the reaction zone are captured by a subscale front model [?]. Then detonation propagation is described by an analytical expression for the normal detonation speed, D_n that depends on only intrinsic front related variables such as shock curvature, κ , yielding $D_n(\kappa)$. Fine zoning to simulate the reaction zone effects is then not required. With this approach, grid con-

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FIGURE 1. 3D Huygens and DSD wave spreading calculation for a 9502 simulant. The DSD wave is shown clearly lagging Huygens at late time. An algorithm based on level-set methods was used.

verged solutions of detonation propagation can be obtained in about an hour. Displayed in Fig. 1 is the results of such a calculation performed using level-set implementation of DSD [?]. The problem is 3D (due to the hole) and considers the "point" initiation of detonation in a shell of IHE. The offset between the two fronts at late time, shows the difference between Huygens and DSD for a 9502-like material.

In Sec. II of this paper, we briefly outline the derivation of an extended DSD front law that includes the effects of front acceleration, DD_n/Dt and transverse flow, $\partial^2 D_n / \partial \xi^2$, where ξ measures the arclength along the shock. This extends previous work of Jao & Stewart [?], Aslam & Stewart [?] and Short [?]. We explore the consequences that the modifications to $D_n(\kappa)$ bring. DSD is an asymptotic theory, based on perturbations about the reference state of an unsupported ZND detonation. To both verify the efficacy of the theory away from D_{ej} and more fully define the phase plane in which multi-D detonations live, we report the results of high-resolution DNS on the steady rate stick problem in Sec. III. This comparison indicates that, although the base $D_n(\kappa)$ gives a reasonable leading order description, the contributions of the extended theory are needed for high-fidelity results. Further we find when the phase velocity, D_0 difference between sticks is small, then D_n vs κ along the corresponding shocks is small. Surprisingly, we also find that κ is singular (although integrable) at the edge of unconfined sticks. Finally, in Sec. IV we carry all of our findings over to the analysis of 9502 curvature data, where the measured phase velocity differences are indeed small. We find that different D_n vs κ forms are needed along different shocks;

FIGURE 2. A grayscale rendering of DNS of a 2D rate stick. The detonation travels upwards, and $r = 0$ marks the plane of symmetry.

although not very different. Because of the smallness of the differences, uncertainties in the data at high κ and possible singularity in κ , no clear indication exists in the data on what direction the extensions should take. We argue that $D_n(\kappa)$ can provide a good average description.

II-EXTENDED DSD THEORY

Consider the steady, detonation rate stick shown in Fig. 2. With a simple geometric argument, it is easily shown that the time rate of change in the shock normal direction, $D()/Dt$ of D_n is

$$\frac{DD_n}{Dt} = -(D_0 \sin \phi)^2 \kappa_s, \quad (2)$$

where D_0 is the phase velocity, κ_s is the slab component of the total curvature

$$\kappa \equiv \kappa_s + (\sin \phi)/r, \quad (3)$$

with ϕ the shock angle and r the local radius to a point on the shock. The basic tenants of DSD theory are: (1) the shock curvature is small measured on the scale of the 1D ZND reaction zone (*i.e.*, $\kappa_s = O(\epsilon)$ with $\epsilon \ll 1$) and (2) the flow is quasisteady (*i.e.*, time variations are slow). From Eq. (2) it then follows that where ϕ and $\sin \phi$ are order one (*i.e.*, $O(1)$), then $DD_n/Dt = O(\kappa_s)$. Given the assumed slow time variations (say, with a scaled time, $\tilde{t} \equiv \epsilon t$), the departure of D_n from

D_{cj} would need to be $O(1)$. Then the perturbations κ_s and DD_n/Dt would enter the theory at the same order, off of a base state that is far from CJ. This is the limit considered by Yao & Stewart [?].

Here we do something different. We adopt the "traditional" DSD scalings [?], where $\kappa_s = O(\epsilon)$, $D = \epsilon \tilde{D} = (D_n - D_{cj})/D_{cj}$ and

$$\phi = \epsilon^{1/2} \tilde{\phi}, \tilde{t} = \epsilon t, \tilde{\xi} = \epsilon^{1/2} \xi, \quad (4)$$

where tilded variables are order one, ξ is shock arc length and $\kappa_s = \epsilon \tilde{\phi}_{,\xi}$. Then $DD_n/Dt = O(\epsilon^2)$, and time dependence enters the theory at one higher order than does κ_s . Here we briefly outline the steps in the formal asymptotic analysis that leads to the higher-order propagation law

$$\bar{\kappa} = \mathcal{F}(\mathcal{D}) - A \frac{D\mathcal{D}}{D\tilde{t}} + B \frac{\partial^2 \mathcal{D}}{\partial \tilde{\xi}^2}, \quad (5)$$

where the bared variables are dimensionless. We will study the properties of this law in some detail.

The basic physics that we study is described by the 2D Euler equations

$$\frac{\partial \rho}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u}) = 0, \quad (6)$$

$$\frac{\partial \rho \bar{u}}{\partial t} + \bar{\nabla} \cdot (\rho \bar{u} \bar{u} + \bar{I} P) = 0, \quad (7)$$

$$\frac{\partial \rho e}{\partial t} + \bar{\nabla} \cdot [(\rho e + P) \bar{u}] = 0, \quad (8)$$

where $e = E + (\bar{u} \cdot \bar{u})/2$, ρ is density, $\bar{u}$ is particle velocity, P is pressure and the the internal energy, $E(P, \rho, \lambda)$ is taken as the polytropic form

$$E(P, \rho, \lambda) = \frac{P/\rho}{\gamma - 1} - q\lambda, \quad (9)$$

with q the heat of detonation and λ the reaction progress variable ($\lambda = 0$ is unreacted), which is governed by

$$\frac{d\lambda}{dt} \equiv R = k\sqrt{1-\lambda} \left(\frac{P}{P_{cj}} \right)^n, \quad (10)$$

where k is the rate premultiplier and n is an integer. We carry forward the analysis using the shock-based, intrinsic coordinates we've described and used before (*i.e.*, the Bertrand coordinates given in [?], [?]). The cartesian coordinates (r, z)

are replaced by shock arc length, ξ and the distance the distance along the local shock normal into the reaction zone, η . We further transform to (ξ, λ) as independent variables (*i.e.*, $(r, z) \Rightarrow (\xi, \eta) \Rightarrow (\xi, \lambda)$). Written in these variables and expressed in quasi-conservative form, the 2D Euler equations become

$$[\rho(D_n - u_\eta)]_{,\lambda} = -\frac{A}{(R - \mathcal{L}(\lambda))}, \quad (11)$$

$$[\rho(D_n - u_\eta)^2 + P]_{,\lambda} = \frac{B}{(R - \mathcal{L}(\lambda))}, \quad (12)$$

$$\left[E + 1/2(D_n - u_\eta)^2 + \frac{P}{\rho} \right]_{,\lambda} = \frac{C}{(R - \mathcal{L}(\lambda))}, \quad (13)$$

$$[u_\xi]_{,\lambda} = \frac{\mathcal{E}}{(R - \mathcal{L}(\lambda))}, \quad (14)$$

where

$$A = (D_n - u_\eta) \cdot (\mathcal{G} + \mathcal{L}(\rho)), \quad (15)$$

$$B = (D_n - u_\eta) \cdot ((u_\eta - D_n) \cdot \mathcal{G} + \rho \mathcal{H}) \quad (16)$$

$$+ \mathcal{L}(\rho(u_\eta - D_n)) + \rho \cdot \mathcal{L}(D_n)), \quad (17)$$

$$C = (D_n - u_\eta) \cdot (\mathcal{H} + \mathcal{L}(D_n)) + \frac{1}{\rho} \mathcal{L}(P) \quad (18)$$

$$+ -\mathcal{L}(E + 1/2(D_n - u_\eta)^2 + \frac{P}{\rho}), \quad (19)$$

$$\mathcal{E} = -\frac{P_{,\xi}}{\rho(1 - \eta\kappa_s)} + \frac{u_\eta}{u_\xi} \mathcal{H} - \mathcal{L}(u_\xi), \quad (20)$$

$$\mathcal{G} = \frac{\rho}{(1 - \eta\kappa_s)} (\kappa_s u_\eta + u_{\xi,\xi}), \quad (21)$$

$$\mathcal{H} = \frac{u_\xi}{(1 - \eta\kappa_s)} (D_{n,\xi} - \kappa_s u_\xi), \quad (22)$$

and where through $O(\epsilon^2)$

$$\mathcal{L}(\) = \epsilon \frac{D}{D\tilde{t}} + \epsilon \frac{D\lambda^{(1)}}{D\tilde{t}} \frac{\partial}{\partial \lambda} + O(\epsilon^{2+\delta}), \quad (23)$$

with $D(\)/D\tilde{t}$ the scaled intrinsic, shock fixed time derivative (called the "dot" derivative, herein) and $\delta > 0$. Note, that we have used $_{,x}$ to indicate partial derivative with respect to x in some places. To reiterate, Eqs. (12-14) are simply a rewrite of the complete, 2D, time-dependent Euler equations.

In forming the perturbation expansions of the dependent variables, we break with previous practice and take $\epsilon = D/\tilde{D}$ as the expansion or order parameter in place of κ and expand

$$\kappa_s = \epsilon \kappa^{(1)} + \epsilon^2 \kappa^{(2)} + \dots \quad (24)$$

This motivated by two things: (1) $\kappa_s(\mathcal{D})$ is single valued and (2) we anticipate an asymptotic expansion to have a larger range of validity. The remaining dependent variables are expanded as

$$Y = Y^{(0)} + \epsilon Y^{(1)} + \epsilon^2 Y^{(2)} + \dots, \quad (25)$$

$$u_\xi = \epsilon^{3/2} u_\xi^{(3/2)} + \dots, \quad (26)$$

where $Y = (\rho, u_\eta, P)^T$. We now trace the basic steps of the analysis.

At $O(1)$, the right hand sides of Eqs. (12-14) make no contribution (since they are $O(\epsilon)$) and we simply get the steady, unsupported ZND wave. Substituting the $O(1)$ solution into the right hand side of Eqs. (12-14), expanding the left hand side through $O(\epsilon)$ and integrating with respect to λ , yields at $O(\epsilon)$ the linear algebraic system

$$\bar{M} \cdot \bar{Y}^{(1)} = \bar{N}^{(1)}, \quad (27)$$

where $\bar{M}$ depends only on the $O(1)$ solution. Solving for $\bar{Y}^{(1)}$, we encounter a solvability condition arising from a singularity in $\bar{M}^{-1}$ related to the sonic point of the base ZND problem. This condition returns the leading order eigenvalue relation similar to what we've presented before [?]

$$\frac{D_{cj}\kappa^{(1)}}{k} = -\frac{1}{2} \left(\frac{\gamma+1}{\gamma} \right)^2 \left(\frac{3-n}{2^{3-n}-1} \right) \tilde{\mathcal{D}}. \quad (28)$$

The next term in the expansion is $O(\epsilon^{3/2})$, from which we obtain

$$u_{\xi,\lambda}^{(3/2)} = -\frac{1}{R^{(0)}\rho^{(0)}} P_{,\xi}^{(1)} + \frac{D_{cj}u_\eta^{(0)}}{R^{(0)}} \tilde{\mathcal{D}}_{,\xi}, \quad (29)$$

which can be integrated to get $u_\xi^{(3/2)}$. The appearance of this term represents another point of departure from Yao & Stewart [?]; the inclusion of transverse flow. Going on to $O(\epsilon^2)$, which completes the analysis presented here, yields

$$\bar{M} \cdot \bar{Y}^{(2)} = \bar{N}^{(2)}. \quad (30)$$

With some help from Maple we can solve Eq. (30) and resolve the solvability condition to get

$$\kappa^{(2)}(\tilde{\mathcal{D}}^2, \frac{D\tilde{\mathcal{D}}}{D\tilde{t}}, \frac{\partial^2 \tilde{\mathcal{D}}}{\partial \tilde{\xi}^2}). \quad (31)$$

On combining this with $\kappa^{(1)}$, compressing the ϵ dependence and introducing the dimensionless variables

$$\bar{\kappa} \equiv \frac{\kappa_s D_{cj}}{k}, \bar{t} \equiv kt, \bar{\xi} \equiv \frac{k}{D_{cj}} \xi, \quad (32)$$

yields the extended intrinsic propagation law

$$\bar{\kappa} = \mathcal{F}(\mathcal{D}) - A \frac{D\mathcal{D}}{D\bar{t}} + B \frac{\partial^2 \mathcal{D}}{\partial \bar{\xi}^2} \quad (33)$$

where the function $\mathcal{F}(\mathcal{D})$ and the coefficients A and B depend on γ and n in a complex way. By scaling up the ϵ dependence of $\bar{\xi}$ and $\bar{t}$ (this can be viewed as a demagnification of the problem), we can systematically drop the "B" term and further drop "A" to get a higher-order $D_n(\kappa)$ theory. We define a shorthand with which to describe these various limits of the model: (1) DnK corresponds to including only the first term on the right hand side, (2) Dndot when the first two terms are included and (3) Dnxixi for the complete model. Equation (33) leads to a parabolic equation for the evolution of the front, which has an number of benefits. Next we examine the properties attendant to this front dynamics for some special cases.

The example we consider mimics 9502: $q = 4mm^2/\mu s^2$, $\gamma = 3$, $D_{cj} = 8.0mm/\mu s$ and $\rho_0 = 2gm/cc$. The parameters for Eq. (33) take the following values for this example: Case (1) $n=0$, $k = 2.5147\mu s^{-1}$, $\mathcal{F} = -0.3810 \cdot \mathcal{D} + 1.0126 \cdot \mathcal{D}^2$, $A = 3.821$, $B = 0.2148$ and Case (2) $n=2$, $k = 1.0061\mu s^{-1}$, $\mathcal{F} = -0.8888 \cdot \mathcal{D} - 1.2121 \cdot \mathcal{D}^2$, $A = 1.3319$, $B = 0.2024$. The rate premultiplier, k has been adjusted so that the 1D ZND reaction-zone length is 4 mm for both cases. We now ask, for a sequence of steady rate sticks: (1) what are the structural differences between the models, (2) what are the relative contributions of the DnK, Dndot and Dnxixi terms to the solutions and (3) what are the differences in the predicted functions D_n vs $\bar{\kappa}$ along the shocks for these models? We consider unconfined charges, which requires that the sonic, angle boundary condition be applied at the edge; $\phi_e = \arctan \sqrt{(\gamma-1)/(\gamma+1)} = 35.3^\circ$ for this example.

Structurally, the DnK and Dnxixi limits lead to parabolic evolution for the fronts and always predict smooth shocks. Any value of ϕ_e can be applied as an edge boundary condition. The Dndot model generally leads to hyperbolic front dynamics and so can admit discontinuities in ϕ along the shock. However, the Dndot model has an upper limit for ϕ_{em} . For the $n = 0$ case, $\phi_{em} = 30^\circ$.

FIGURE 3. For case $n = 0$, a comparison of the contributions of $\mathcal{F}(\mathcal{D})$, $-A \cdot (DD/D\bar{t})$ and $B \cdot (\partial^2 \mathcal{D}/\partial \bar{\xi}^2)$ to $\bar{\kappa}$. As D_n is reduced $\mathcal{F}(\mathcal{D})$ is not the major contributor to $\bar{\kappa}$.

FIGURE 4. For case $n = 2$, a comparison of the contributions of $\mathcal{F}(\mathcal{D})$, $-A \cdot (DD/D\bar{t})$ and $B \cdot (\partial^2 \mathcal{D}/\partial \bar{\xi}^2)$ to $\bar{\kappa}$. $\mathcal{F}(\mathcal{D})$ is the major contributor to $\bar{\kappa}$ for all D_n 's. This case is very DnK-like.

The relative magnitudes of $(\partial^2 \mathcal{D}/\partial \bar{\xi}^2)$, $(DD/D\bar{t})$, $\mathcal{F}(\mathcal{D})$ and $\bar{\kappa}$ for the case $n = 0$ are shown in Fig. (3). The contributions of $(\partial^2 \mathcal{D}/\partial \bar{\xi}^2)$ and $(DD/D\bar{t})$ are comparable for this case. Importantly, although $\mathcal{F}(\mathcal{D})$ is the dominant contribution to $\bar{\kappa}$ for larger D_n 's, all three terms are roughly comparable for smaller D_n 's. For the $n = 2$ case, the situation is different (see Fig. (4)). Now $\mathcal{F}(\mathcal{D})$ makes the principal contribution to $\bar{\kappa}$, and the model is more DnK-like.

We compare how the models differ in their predictions of the shocks. To do this, we compare the computed D_n vs $\bar{\kappa}$ along the shocks as predicted by the DnK, Dndot and Dnxixi models. These results are shown in Figs. (5-6). All the models look more nearly alike for the case $n = 2$

FIGURE 5. For case $n = 0$, a comparison of D_n vs $\bar{\kappa}$ along a $D_0 = 0.77 \text{ cm}/\mu\text{s}$ shock. Results from the DnK, Dndot and Dnxixi models are shown. The large difference shown here suggests that large differences will be seen between the shocks for the various models.

FIGURE 6. For case $n = 2$, a comparison of D_n vs $\bar{\kappa}$ along a $D_0 = 0.77 \text{ cm}/\mu\text{s}$ shock. Results from the DnK, Dndot and Dnxixi models are shown. The smaller difference shown here suggests that the shocks for the various models will be more nearly alike.

than for $n = 0$. Finally, we examine how small changes in the phase velocity effect D_n vs $\bar{\kappa}$ along the corresponding shocks. We consider only the Dnxixi model and case $n = 2$ since it more nearly mimics 9502. Figure 7 shows that in the range of phase velocities observed for 9502, the differences in D_n vs $\bar{\kappa}$ along the shocks is small. If this behavior is obtained for the physical data for 9502, it will be hard to distinguish between the various modeling forms. We consider this issue in Sec. IV. Next we go on to describe the numerical simulations, the results they yield and compare these results with those for the models we have just described.

FIGURE 7. For case $n = 2$, a comparison (using the D_{nxi} model) of D_n vs $\bar{\kappa}$ along $D_0 = 0.75, 0.77, 0.79$ cm/ μ s phase velocity shocks. The small differences argue that when the phase velocity differences are small, it would be difficult to distinguish between the various models.

III-DIRECT NUMERICAL SIMULATIONS

Direct numerical simulations were carried out for unconfined rate sticks for the model described in Sec. II. Since the simulations were to be used to both validate the theory and expose new phenomena, we required the simulations to be very accurate. To get sufficient resolution of the reaction zone, the computational mesh was localized to the immediate vicinity of the reaction zone. Previously we had experienced problems with accuracy using standard shock capturing and interface algorithms. The shocks were either excessively thick (though smooth) for low order methods or noisy for higher-order methods. These artifacts produced $O(1)$ solution errors in things we care about such as an increase in the reaction-zone length and problems with reaction ignition. Consequently, existing algorithms were modified and new ones developed [?] [?] so as to enhance our ability to get higher-fidelity, grid converged solutions. A code was built around these algorithms for doing the rate stick problem.

The interior algorithm was based on the Lax-Friedrichs scheme, principally because it doesn't suffer from stability problem when computing waves that are stationary on the grid, such as is the case here [?]. A variant of the essentially nonoscillatory (ENO) algorithm of Osher, et al. [?] was used. To get high order spatial accuracy in smooth regions of the flow and smooth profiles near shocks, the high order spatial interpola-

tion of the flux functions was obtained by using a convex combination of small stencil, local interpolants [?]. This had the property of smoothly transitioning to a monotone low order algorithm near shock waves. The shocks were still narrow, with 90% of the shock rise occurring monotonically in about 2 cells. A third order Runge Kutta method was used for the time integration.

A new interface algorithm (called the Ghost Fluid Method [?]) was developed that tracks the HE/confinement interface. It works by extending the calculation of fluid A across the interface into the region of fluid B (the virtual fluid is called the ghost fluid). This is done under the constraint of continuous pressure and normal particle velocity at the interface. This method essentially eliminates the smearing and overheating artifacts found at captured and volume of fluid reconstructed interfaces. It allows for perfect slip at the material interface, should that be desired. The location of the interface is then tracked with a level-set method based on solving an extended advection equation.

To keep the calculation on a restricted spatial domain, mesh was recycled from regions downstream of the reaction zone that no longer influenced the reaction zone to upstream of the detonation shock. The time at which the detonation crossed a given laboratory (z, r) point was recorded and saved as the array of values (t, z, r) , called the burntime table

$$t_b(z, r). \quad (34)$$

By appropriately differentiating (differencing) this data, front intrinsic quantities such as D_n and κ_s could be calculated

$$\vec{n} = \frac{\vec{\nabla}(t_b)}{|\vec{\nabla}(t_b)|}, |D_n| = \frac{1}{|\vec{\nabla}(t_b)|}, \kappa_s = \vec{\nabla} \cdot \vec{n}, \quad (35)$$

where $\vec{n}$ is the unit vector in the shock normal direction.

If no special care is taken in differencing $t_b(z, r)$, quantities like D_n can pose $O(1)$ errors and higher derivatives would diverge under grid refinement. By taking a stencil for the differencing that is greater than the minimum required, yet not so broad that spatial resolution is completely lost, grid converged values were obtained along most of the shock. Simple centered differences were used to compute the quantities in Eq.

FIGURE 8. For case $n = 0$, a grid convergence study for the computed value of ϕ_e and the phase velocity, D_0 for a 48 mm "radius" 2D HE charge. Good convergence is obtained for ϕ_e to the exact value of 35° . About 50 grid points are needed in the reaction zone to get D_0 good to $O(50 \text{ m/s})$.

(35). The stencil width, w was related to the order of the derivative, m being computed and the grid spacing, Δx

$$w \propto (\Delta x)^{\frac{1+m}{2+m}}. \quad (36)$$

Due to the w -step skipping of grid points, some of the higher derivatives could not be calculated within a few points of the HE charge boundary.

All the calculations on which we report were performed on an 8-cpu, SGI-Origin. The calculations were run in parallel mode over 7-cpus. By way of example, we show how well all this numerical technology works by examining the convergence of the computed shock edge angle, ϕ_e , a quantity for which we have the exact theoretical result of $\phi_e = 35.3^\circ$ for the equation of state of this problem. Figure 8 shows that under refinement, the computed ϕ_e is within 0.3° of the exact value (the number of grid points in the reaction zone was 8, 16, 32, 64 and 128). Also shown is the computed phase velocity (in $\text{mm}/\mu\text{s}$), where the errors are $O(50 \text{ m/s})$ even with 50 grid points in the reaction zone. These are the results for a simple easy to resolve problem. The situation is not nearly so "favorable" for more complex rate laws and problems. A surprising result was obtained in the resolution study for the computed value of κ_s at the edge of the charge; the grid convergence study indicates that κ_{edge} is diverging (κ_{edge} is singular). These results are shown

FIGURE 9. For case $n = 0$, a grid convergence study for the computed value of κ_e for a 48 mm "radius" 2D HE charge. As the grid is refined, the differences in κ_e grow ever larger. This implies that the curvature at the edge in an unconfined charge is singular.

in Fig. (9). This suggests that measuring curvature to the very edge of the charge in experiments would give poor results, since the very problem would be ill posed. We return to this issue in our discussion of the 9502 data.

Next we examine some of the higher-order derivative intrinsic variables such as κ_s , (DD/Dt) and $(\partial^2 D / \partial \xi^2)$ and the relationships between them. Most of the results we show are from results having 128 points in the reaction zone. Displayed in Fig. (10) is a comparison of some intrinsic quantities obtained both from the DNS and the Dndot and Dnxixi theories. The Dndot's are all grouped together. Significantly, the Dnxixi from the DNS is very much larger in magnitude than is Dndot and also considerably larger in magnitude than is the result from the Dnxixi theory. Except for the fact that the Dndot theory doesn't have the term $(\partial^2 D / \partial \xi^2)$, which is shown by the DNS to be large, it agrees with the $\bar{\kappa}$ of the DNS quite well.

Displayed in Fig. (11) is $\mathcal{D}$ vs $\bar{\kappa}$ for the case $n = 2$. This example shows that although the phase velocities for the DNS and theories are about the same, all the theoretical curves resemble $D_n(\kappa)$ more so than they resemble the DNS. The initial slopes at D_0 are about the same, but as $\mathcal{D}$ drops the DNS becomes much more highly curved than any of the theories. This suggests two things. First, that a high curvature boundary

FIGURE 10. For case $n = 0$, shown is a comparison of $\bar{\kappa}$, $(D\bar{D}/D\bar{t})$ and $(\partial^2 D/\partial \bar{\xi}^2)$ vs D for the case of a 24 mm radius stick for the DNS and the Dndot and Dnxixi theories.

FIGURE 11. For case $n = 2$, shown is a comparison of D vs $\bar{\kappa}$ along a 24 mm shock for the DNS and Dndot and Dnxixi theories.

FIGURE 12. The interpretation of the functions $\mathcal{F}(D)$ and $A(D)$ of Eq. (37) vs D using the 18 mm and 24 mm shocks as data. The case is $n = 0$, and the DNS is compared to the theories.

layer is found in the DNS that none of the theories are capable of. Second, since the $A(D)$ for the $n = 2$ case is considerably reduced from the value found for the $n = 0$ case, the "spreading" angle is much larger (closer to 45°), so all the theories begin looking very diffusive and much more DnK-like.

Given that some level of discrepancy exists between the DNS and the near D_{cj} asymptotic theory, we now analyze the DNS results and those from the theory to ascertain what common relationship may exist between them. We make the ansatz that an intrinsic propagation law exists of the generic form

$$\bar{\kappa} = \mathcal{F}(D) - A(D) \frac{D\bar{D}}{D\bar{t}}, \quad (37)$$

where $\mathcal{F}(\)$ and $A(\)$ are considered to be unknown functions that are to be determined directly from the solution data sets given by the DNS and theories. Using only two shocks from the $n = 0$ case that have a significant overlap in D_n , we can uniquely determine these functions (these fits may not do well at reproducing an available third shock). We then ask, are the functions so determined consistent with our notions of what $\mathcal{F}(D)$ and $A(D)$ could possibly represent physically? Shown in Fig. (12) are the $\mathcal{F}(D)$ and $A(D)$ so determined. The theories and DNS all show the same trends. Viewed as the inverse of the square of the transverse speed function of Dndot theory, $A(D)$ predicts that the transverse wave

FIGURE 13. The analyzing mirrored surface used the 9502 curvature measurements. The edges of the mirror served to define the spatial scales.

speed should decrease as D_n increases, which is certainly counter intuitive.

Two possibilities present themselves. Either our notion of what $A(\mathcal{D})$ represents is flawed or the ansatz about the form of the propagation law is flawed. An answer to this question awaits the completion of a more complete DNS database. In the next section, we go on to consider how the ideas we have explored in Sec. II-III can be used to help analyze the physical data sets for 9502 collected by Davis, et al. [?].

ANALYSIS OF PBX 9502

The curvature measurements performed by Davis, et al. [?] were designed to yield high-quality data for the purpose of calibrating a $D_n(\kappa)$ -law for 9502. Special care was taken so as to collect reliable data to the very edge of the charge. This was accomplished by affixing a mirrored glass plate (containing its own centering mark and spatial scales) to the front face of the charge as shown in Fig. (13). Since the mirror extended beyond the edge of the charge, a clean record was obtained to the very edge of the charge. Measurements were made for 10, 12, 18 and 50 mm diameter cylindrical sticks. This wave-front shape plus the phase velocity data was analyzed by postulating the existence of a unique $D_n(\kappa)$ function, of the form

$$\mathcal{D} = C_1 \cdot ((\kappa_c - \kappa)^\mu - \kappa_c^\mu) - \frac{C_2 \kappa^\nu}{1 + C_3 \kappa^\omega}, \quad (38)$$

where the parameters C_1 , C_2 , C_3 , κ_c , ν and ω were constrained to be positive while $0 < \mu \leq 1$. The ansatz was that a single $D_n(\kappa)$ could be made to fit all the data and that ϕ_e and D_{cj} where parameters (same for all the shocks) also to be determined in the process. Under these assumptions, Eq. (38) could be integrated to get

FIGURE 14. $D_n(\kappa)$ for PBX 9502 @ 25C. Shown are the individual fits to the 10, 18 and 50 mm shocks along with a composite fit to all the data. The arrows indicate at what point we are within 1% of the charge boundary, beyond which the fits are probably not significant. The parameters for the composite fit are: $D_{cj} = 7.818 \text{ mm}/\mu\text{s}$, $C_1 = 0.2643$, $\kappa_c = 1.276 \text{ mm}^{-1}$, $\mu = 0.8042$, $C_2 = 0.1950$, $\nu = 0.5264$, $C_3 = 27.81$, $\omega = 1.279$ and $\phi_e = 43^\circ$.

both a diameter-effect curve and the family of shock shapes. These numerically generated solutions were then systematically fit to the above described experimental data set using a Levenberg-Marquardt, nonlinear least squares algorithm.

The shocks (and corresponding phase velocities) were fit both individually and as part of a composite data set. When fit individually, the (z vs r) shock data was fit with a total error of 0.5%, that was randomly distributed, and to within 10 m/s for the phase velocities. For the composite data set, the shock error increased to 4%, with systematic variations mostly localized near the charge boundary. The $D_n(\kappa)$ function obtained in this way are shown in Fig. (14). Considering the uncertainties in the data near the charge edge and in the light of the result that the curvature may be singular at the edge, the composite $D_n(\kappa)$ appears as a good representation of the data.

Based on the arguments presented in Sec. II and the observation that the phase velocities differ by only 250 m/s, we expect that this data can not be used to select between the modeling forms we have discussed. Nevertheless, the increase in error of fit for the shocks from 0.5% to 4% suggests that improvements could be made over $D_n(\kappa)$. Here we consider whether one of the new modeling assumptions that we have suggested would give a better fit to the data that at the same time was

FIGURE 15. The $A(\mathcal{D})$ of Eq. (37) plotted vs D_n . Dimensional units of mm and μs are used. The DNS and theories used $n = 0$ and differenced across the 18 mm and 24 mm radius charges.

physically plausible. Since the functions in the Dndot form can be adjusted so that two shocks can be fit exactly, we analyze the data, DNS and the theories in this way to see if a consistent picture emerges. The 10 mm and 50 mm $D_n(\kappa)$ fits for 9502 are used for this purpose. The results obtained for the $A(\mathcal{D})$ of Eq. (37) for the experiments, simulations and the various theories (for case $n = 0$) are compared in Fig. (15). The striking observation here is that the the $A(\mathcal{D})$ for the data has a sharp upturn for large D_n that the DNS and theories don't show. This does not seem plausible. The trend that $A(\mathcal{D})$ is an increasing function of D_n seems to be a shared property. However, the observation that the $A(\mathcal{D})$ for the data has a sharp upturn for large D_n that the DNS and theories don't show is a striking difference. This does not seem plausible.

What does this argue? Perhaps that the data is not sufficiently accurate to differentiate between various extended models. Clearly, if the curvature is singular at the edge (as the DNS indicates), then trying to measure and use curvatures near the edge is ill conceived. To build these higher-order effects into the propagation law in a way that is inconsistent with the results from DNS and theory would be an error. Thus, given the current state of understanding, we do not propose a high-order intrinsic propagation law for PBX 9502 at this time. Experiments are needed that probe parts of the phase plane for multidimensional detonations that are not accessible

with rate sticks. We are currently examining "rib" data and nonsteady experiments, such as detonation corner turning.