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Title: Modeling of Detonation Propagation

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Abstract

Modeling of Detonation Propagation

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Summary:

A simple methodology for propagation of detonation waves, Detonation Shock Dynamics (DSD), is presented. Theory, experiments and computational issues regarding DSD will be addressed. Detonation Shock Dynamics is based on a weak curvature, quasi-steady analysis of the compressible reactive Euler equations. See [1] for a recent review of the field. The key result from DSD is that to a first order approximation, a detonation wave will propagate normal to itself at a velocity related to its local curvature. This is expressed as a D_n-K relation. This D_n-K relation is an intrinsic propagation rule (i.e. all that is needed to propagate the detonation front is its current shape).

Results and Discussions:

To be a useful theory, one must perform a calibration of the D_n-K relation for each high explosive (HE) of interest. Typically this calibration procedure uses data obtained from a series of rate stick experiments. These experiments measure the steady propagation speed of the detonation wave along a long cylindrical charge of HE, in addition to the shock “break-out” at the end of the charge. Knowing the “break-out” time and propagation speed of a steady traveling wave allows one to determine the shape of the detonation wave. Knowing the shape and speed then allows one to determine detonation normal velocity and curvature along the detonation wave. Many rate sticks experiments are generally performed at various radii, and a global fit to all the rate stick data is used to determine D_n-K [2].

This D_n-K relation can then be used for more general detonation propagation modeling. Details of numerical implementation, coupling to hydrodynamic codes and validation experiments will be presented.

References:

[1] J. B. Bdzil, D. S. Stewart, “The Dynamics of Detonation in Explosive Systems,” Annual Review of Fluid Mechanics, 39 263-292 (2007).

[2] L. G. Hill, T. D. Aslam, “Detonation Shock Dynamics Calibration for PBX 9502 with Temperature, Density, and Material Lot Variations,” Proceedings of the 14th International Detonation Symposium, 2010, pp.779-788.

Modeling of Detonation Propagation

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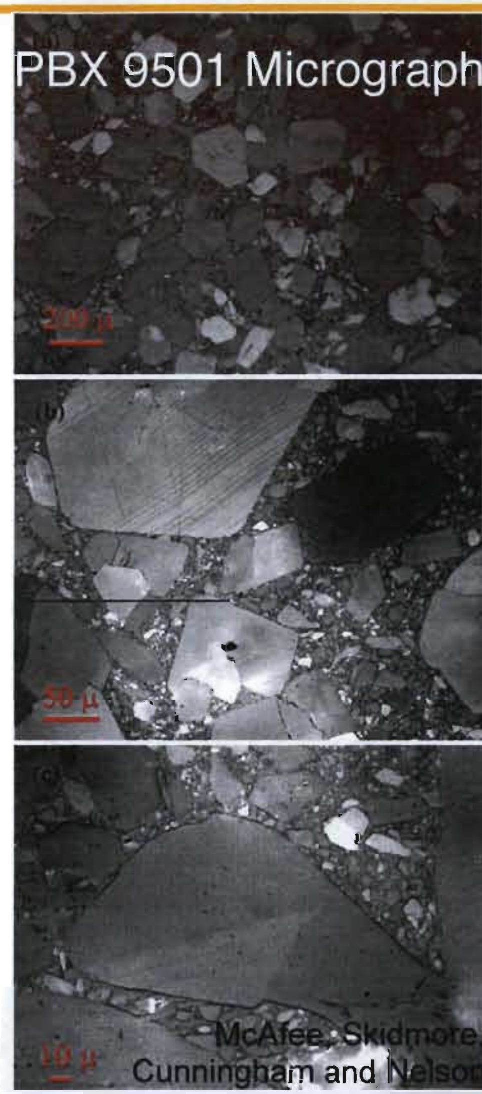
Outline

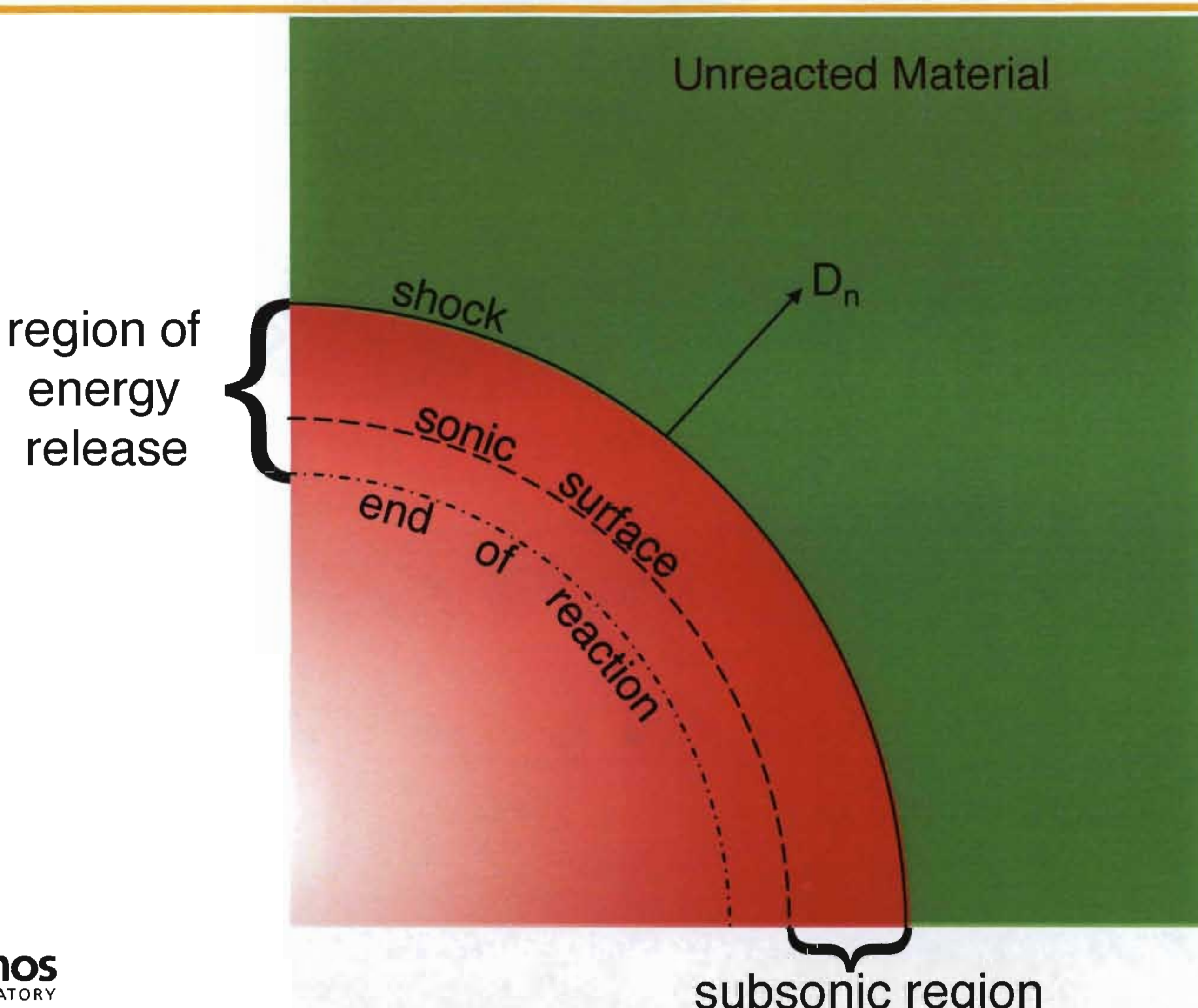
- High Explosive Modeling Issues / Detonation Propagation
- Overview of Detonation Shock Dynamics (DSD)
- High Explosive Detonation / Inert Interaction
- DSD Calibration
- DSD Implementation
- DSD Validation Experiments

Modeling Issues for High Explosives

- Real heterogeneous solid explosives are complex
- Equations of state not well known under detonation conditions
- Reaction zone is order of a O(1)-O(10) grains in width
- Empirical reaction rates are not “physically” correct, but generally need to be tuned
- An alternative is detonation front models, empirically calibrated to experiment



Detonation Propagation – Continuum Level



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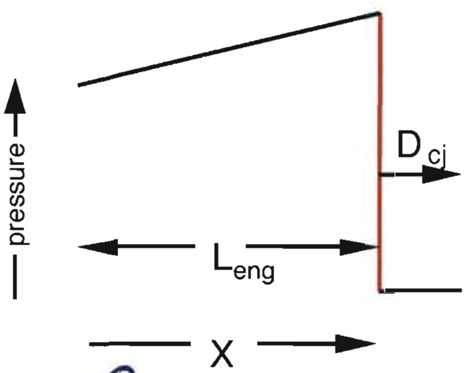
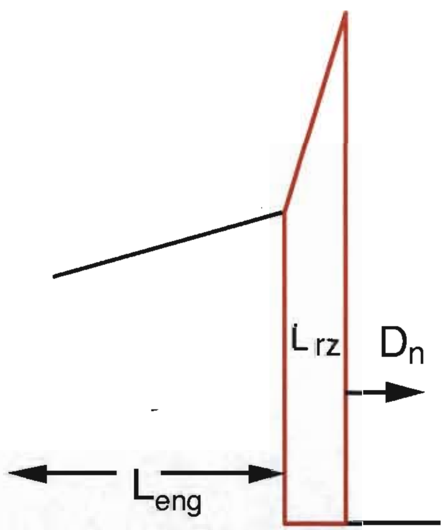
Overview of Detonation Propagation Models

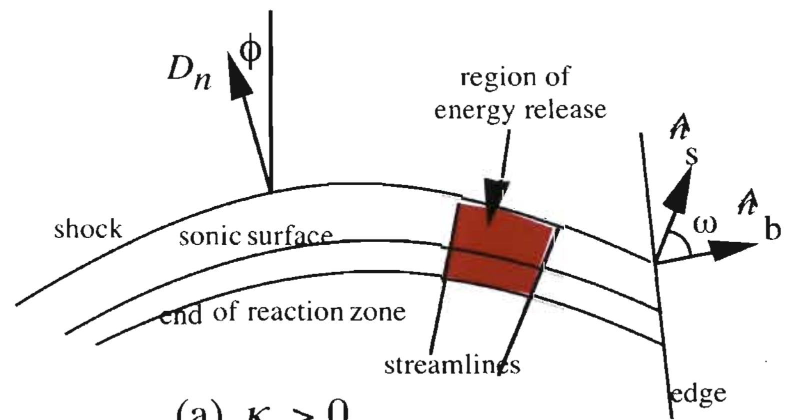
Chapman
Jouguet
(**CJ** Theory, 1900)
- 1D
- Steady
- Instant Reaction
- Huygens Construction



Zeldovich
von **N**uemann
Doering
(**ZND** Theory, 1940s)
- 1D
- Steady
- Finite Rate Reaction



Detonation **S**hock
Dynamics (Bdzil-Stewart)
(**DSD** Theory, 1980s)
- Quasi-1D
- Quasi-Steady
- Finite Rate Reaction
- O(ε): $D_n(\kappa)$, κ = curvature



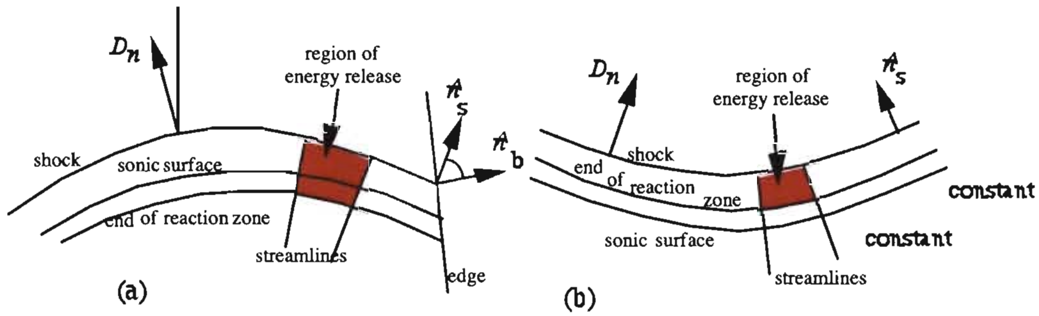
(a) $\kappa > 0$

Detonation Shock Dynamics (DSD)

Asymptotic Theory based in Euler Equations with Reaction

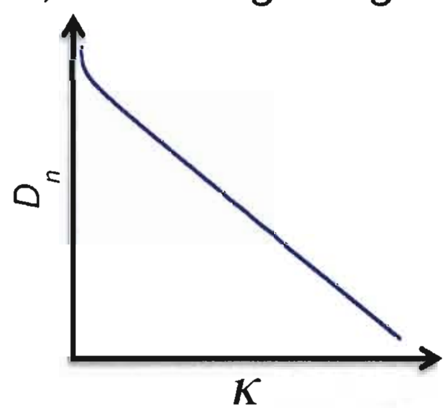
- Quasi-steady
- Weakly Curved
- Key Result: $D_n(\kappa)$

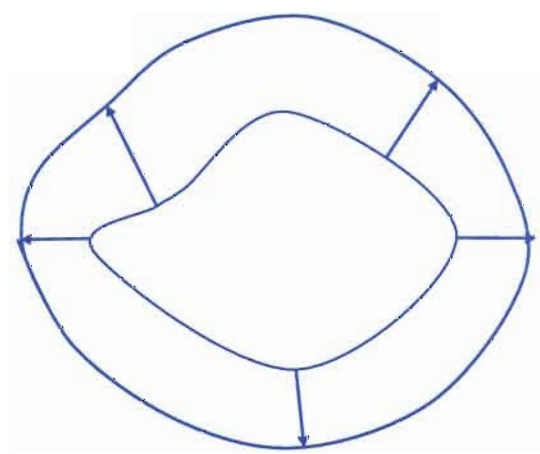
(no initiation, failure)



Practical Implementation Requires Calibration with Experiments

In addition, DSD "edge angles" are required at Inert Boundaries





DSD comparison with other detonation models

- Huygens' Construction (constant detonation velocity)

  Pros: Very Fast, Simple Model

  Cons: Doesn't take into account Reaction Zone Effects such as Diameter Effect, Initiation, Corner Turning & Detonation Failure

- Reactive Flow

  Pros: "Real" Physics & Chemistry

  Cons: Very Expensive if done correctly, Difficult/Expensive to Calibrate for practical HEs

High Resolution, 14μm finest grid, Ignition & Growth Simulation

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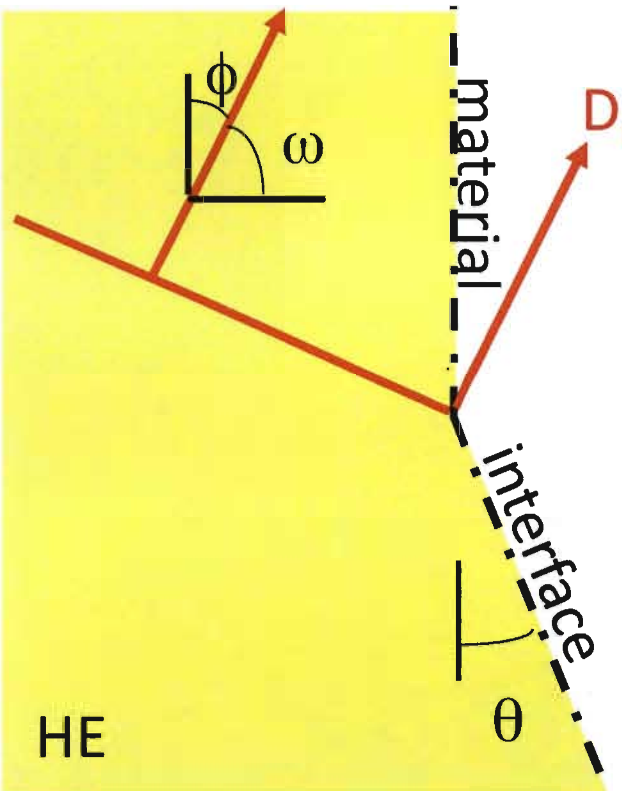
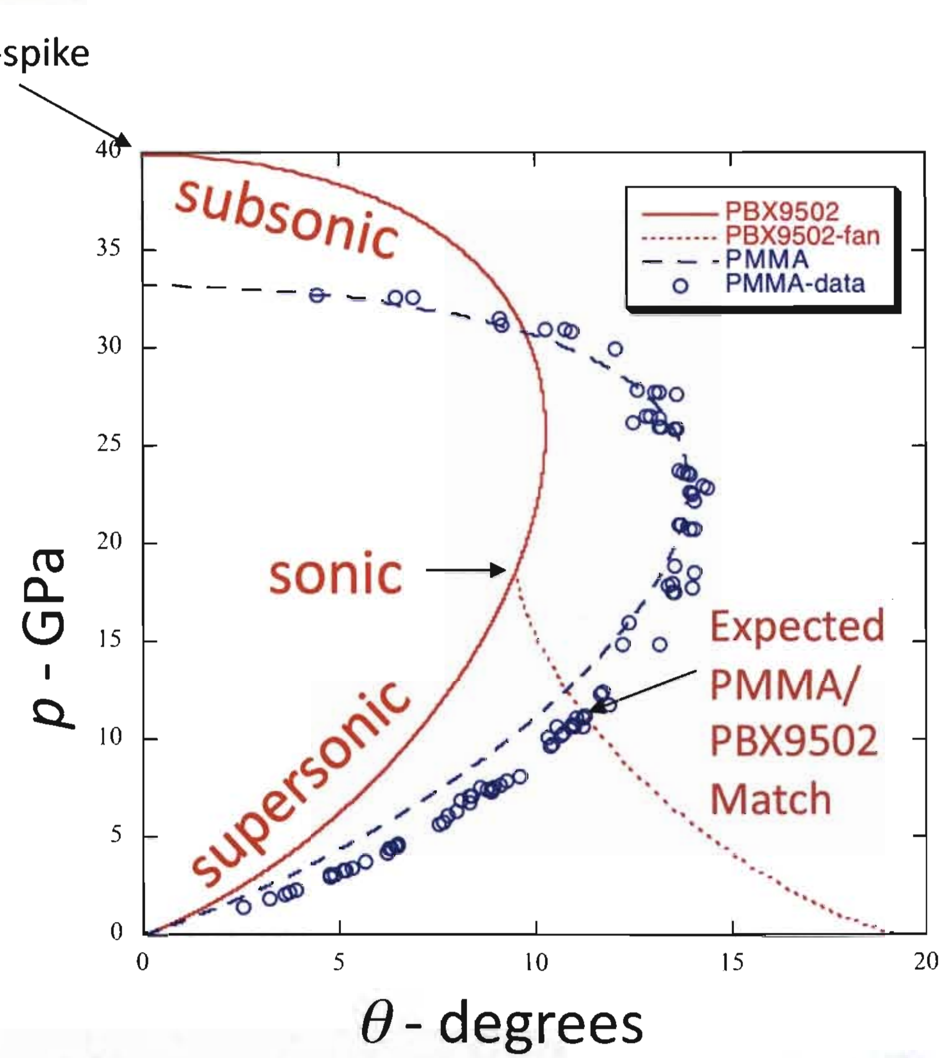
Boundary Conditions for DSD HE/Inert Interface: Shock Polar Theory





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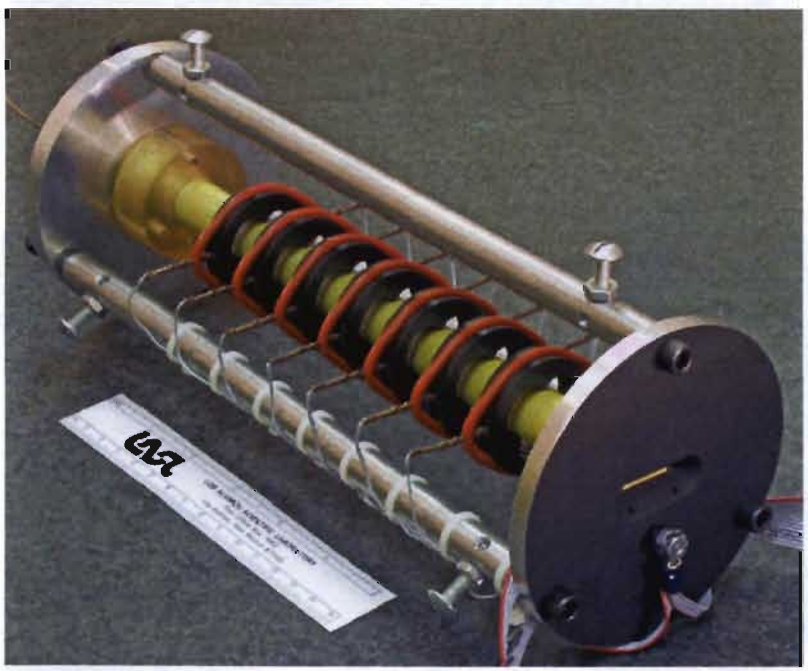
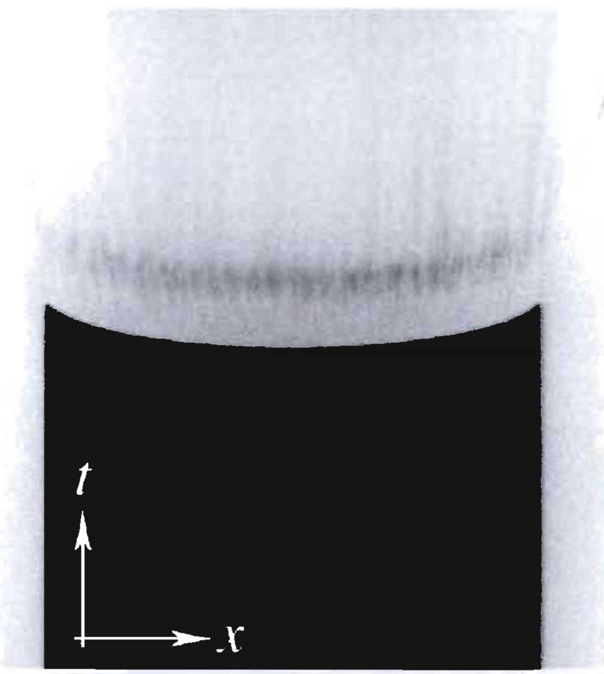
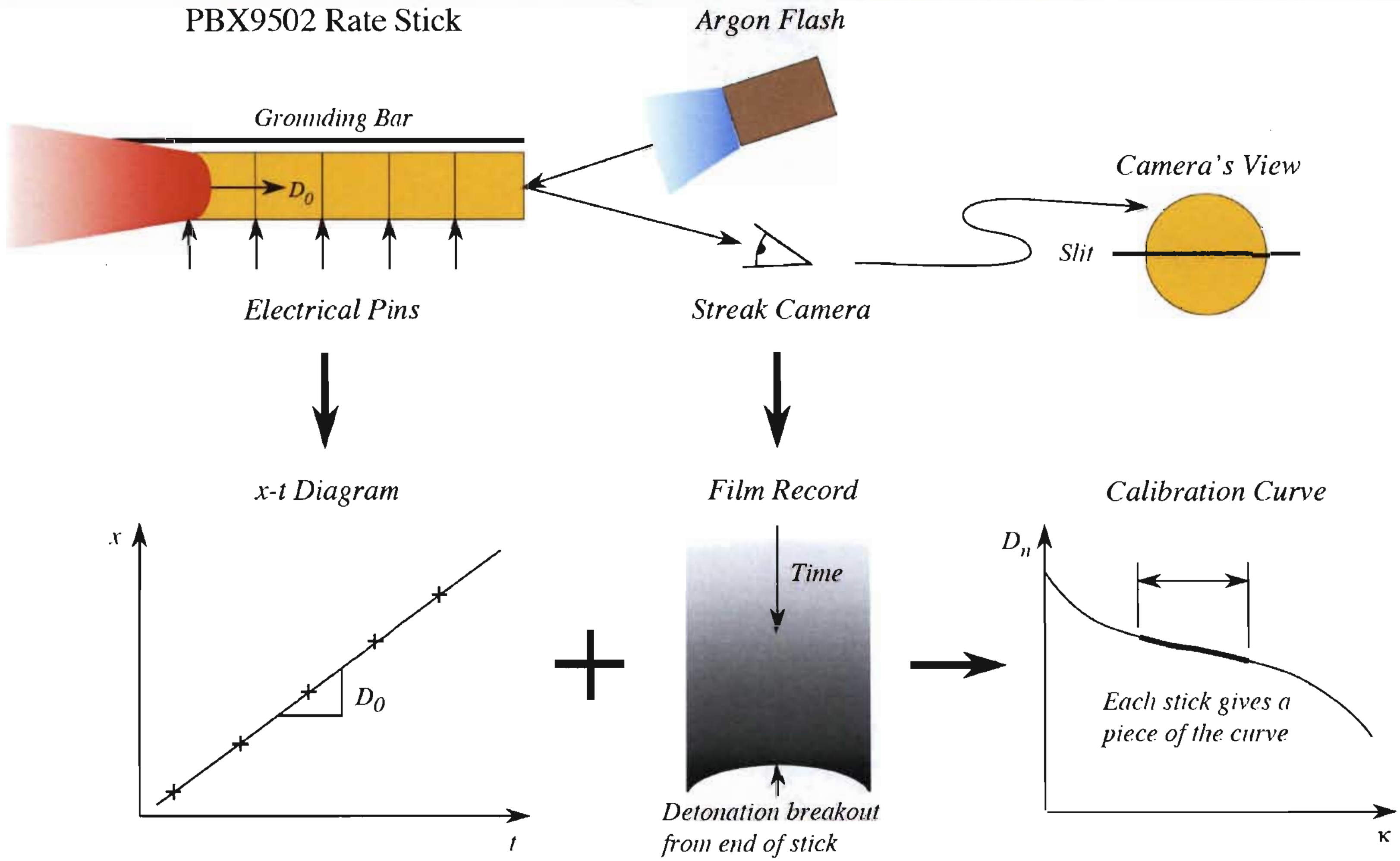
DSD Calibration Experiments

- Standard DSD experiment: the front curvature rate stick.
- Solid sticks are usually fired bare. Powders, putties, liquids must be fired in tubes. Foam tubes are ~unconfined.





DSD Calibration Experiments



DSD Calibration for PBX 9502: Material Variability (material lot, $\rho_{pressing}$, T_0)

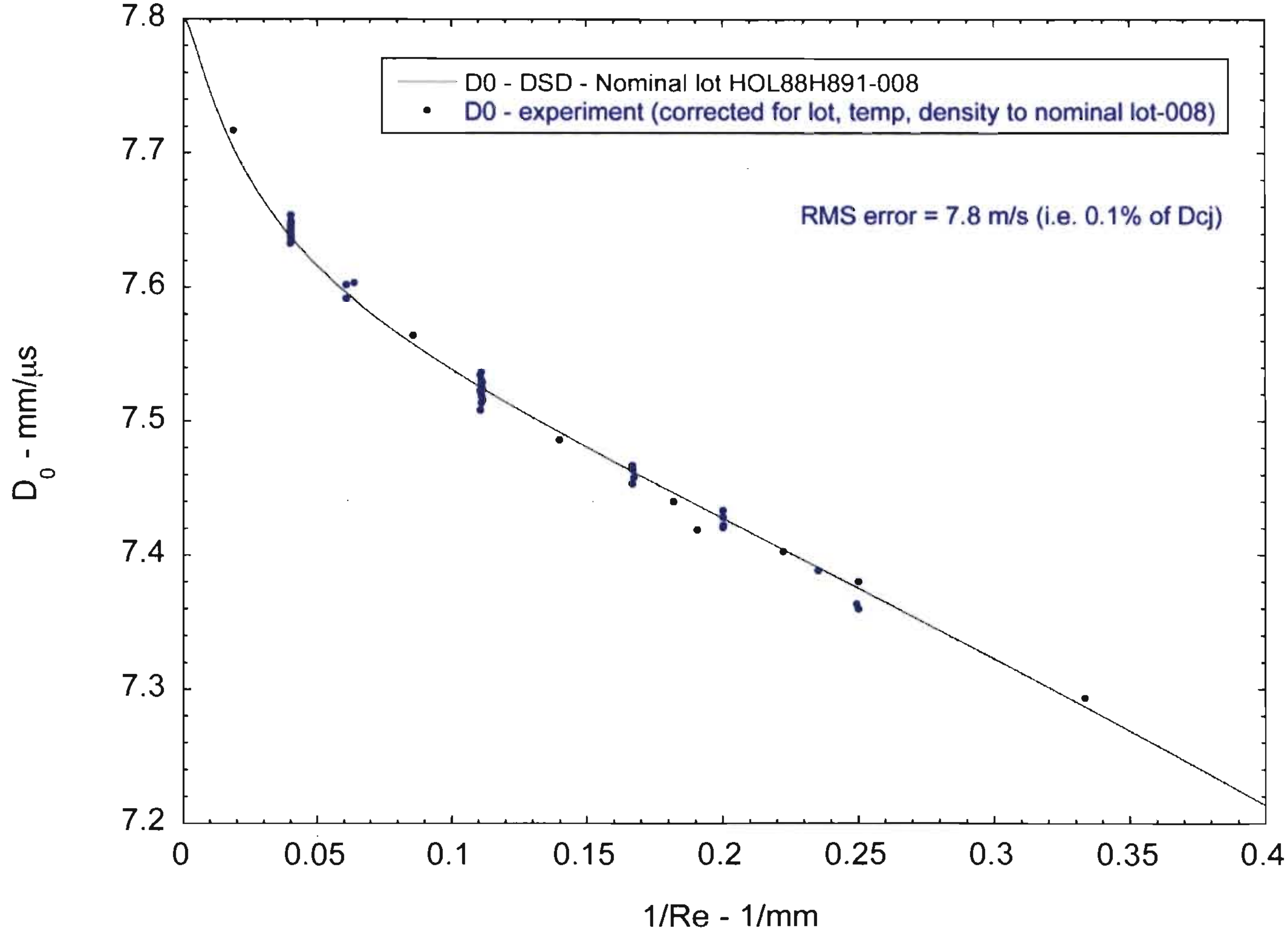
- Calibration Data
  - 50+ Rate Sticks
  - 4 material lots
  - Various Temp & Densities
- Calibration Technique
  - Steady Rate Stick DSD ⇒ ODEs
  - Constrained Downhill Simplex to calibrate DSD Constants:

$$\frac{D_n}{D_{cj}} = 1 - B\kappa\left(\frac{1 + c_1(B\kappa) + c_3(B\kappa)^2}{1 + c_2(B\kappa) + c_4(B\kappa)^2}\right)$$

Table of Experiments used in Calibration

Lot Number	Nom.Dia. (mm)	Meas. Dia. (mm)	Shot Temp. (C)	PressedDensity (g/cc)**	Det. Speed (mm/μs)
LANL 79-04	108	Not	24	1.886	7.716
(Recycled)	50	given	24	1.891	7.667
BET: 2.91 m²/g	50	"	24	1.892	7.672
"	31.5	"	24	1.892	7.630
"	23.3	"	24	1.891	7.589
"	18	"	24	1.890	7.556
"	18	"	24	1.889	7.549
"	12	"	24	1.887	7.493
"	10	"	24	1.888	7.469
"	9	"	24	1.886	7.443
"	8.5	"	24	1.893	7.430
"	8	"	24	1.886	7.408
"	50	"	75	1.892	7.654
"	33	"	75	1.893	7.623
"	18	"	75	1.892	7.554
"	12	"	75	1.887	7.491
"	10	"	75	1.890	7.478
"	8	"	75	1.892	7.446
"	6	"	75	1.893	7.387
"	50	"	-55	1.891	7.672
"	50	"	-55	1.891	7.667
"	33	"	-55	1.893	7.625
"	18	"	-55	1.889	7.543
"	14.3	"	-55	1.894	7.496
"	12	"	-55	1.886	7.452
"	11	"	-55	1.891	7.427
	10.5	"	-55	1.892	7.403
HOL85F000E-136 (Recycled)	50	50.00	22	1.892	----
BET: 1.43 m²/g	50	50.02	25	1.895	7.677
"	18	17.99	22	1.892	7.553
"	18	18.02	23	1.895	7.556
"	12	11.99	24	1.892	7.495
"	10	10.00	24	1.891	7.455
"	10	9.99	22	1.895	7.457
HOL80L890-007 (Virgin)	18	18.01	25	1.880	7.494
BET: 0.87	18	18.00	25	1.889	7.497
"	18	17.99	25	1.889	7.502
"	18	18.00	75	1.887	7.521
"	18	17.99	-55	1.889	7.465
HOL88H891-008 (Virgin)	50	50.0	25	1.886	7.641
BET: 0.62 m²/g	18	18.0	25	1.886	7.523
"	18	18.0	25	1.886	7.512
"	10	10.0	25	1.890	7.421
"	50	50.0	75	1.886	7.616
"	18	18.0	75	1.886	7.521
"	18	18.0	75	1.886	7.507
"	8	8.0	75	1.890	7.397
"	50	50.0	-55	1.886	7.637
"	18	18.0	-55	1.886	7.494
"	18	18.0	-55	1.886	7.489
"	12	12.0	-55	1.890	7.399

PBX 9502:
DSD Calibrated Diameter Effect & Data



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DSD Numerical Implementation: Level Sets and Narrow Band Methods

DSD package is "stand-alone"

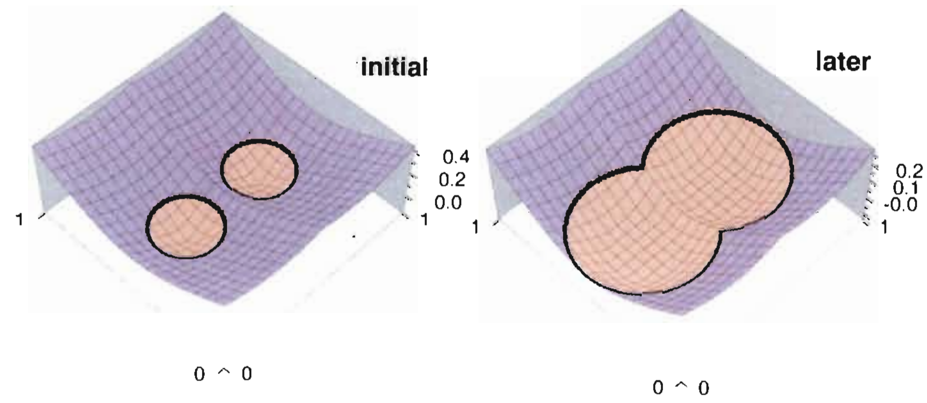
- Input geometry, materials from hydrocode. Outputs "burntable"

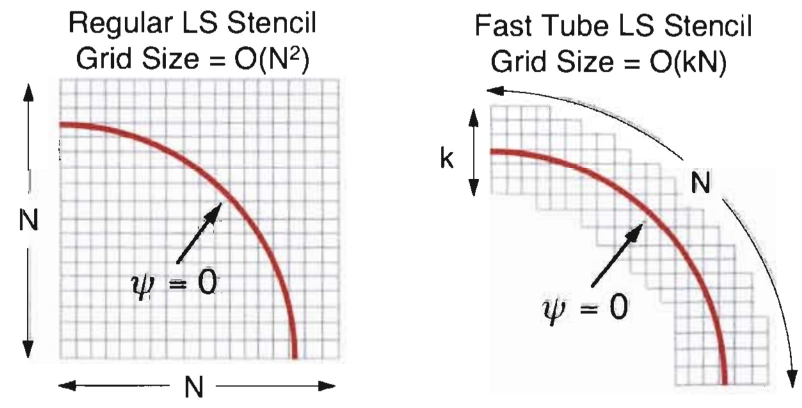
Level Set Methods

- Cartesian Grid
- Standard PDE Solvers
- Complex Geometry and Topology Changes are easily handled

Narrow Band Level Set Methods

- Focus Effort near $\psi = 0$
- Very Efficient, O(N) savings





Accuracy is easily predicted through Taylor Series

Care must be taken at edge of tube to maintain accurate solution

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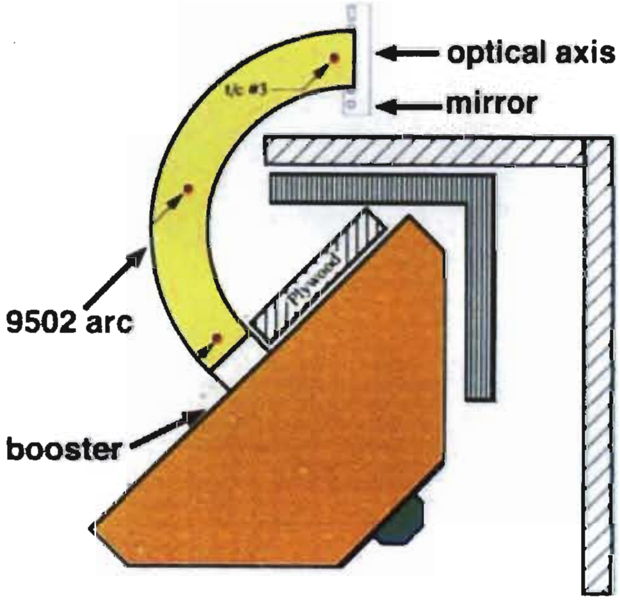
DSD Validation Tests:

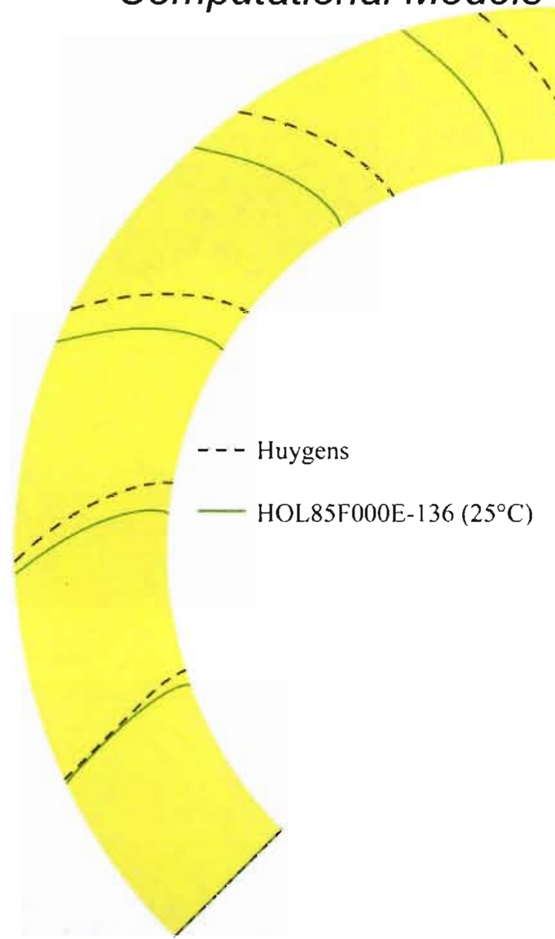
1. 135° PBX 9502 High Explosive Arc
2. NC/NG Barrel Test

DSD Validation Test:
PBX 9502 135° 2D Arc Experiment

Experimental Setup

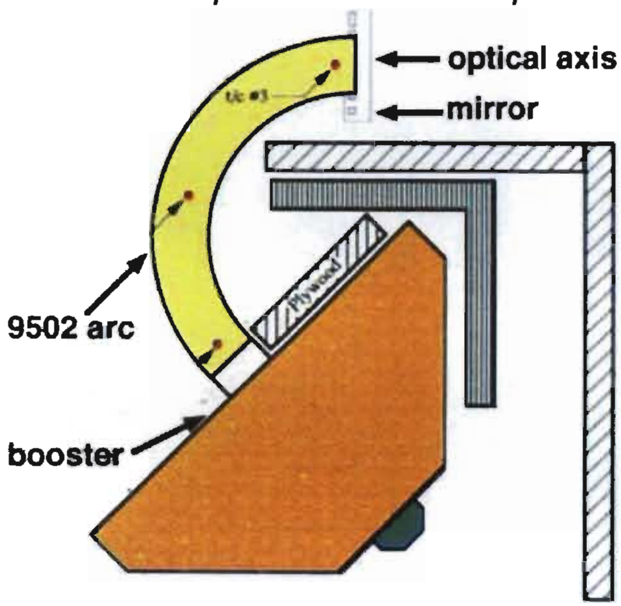


Computational Models



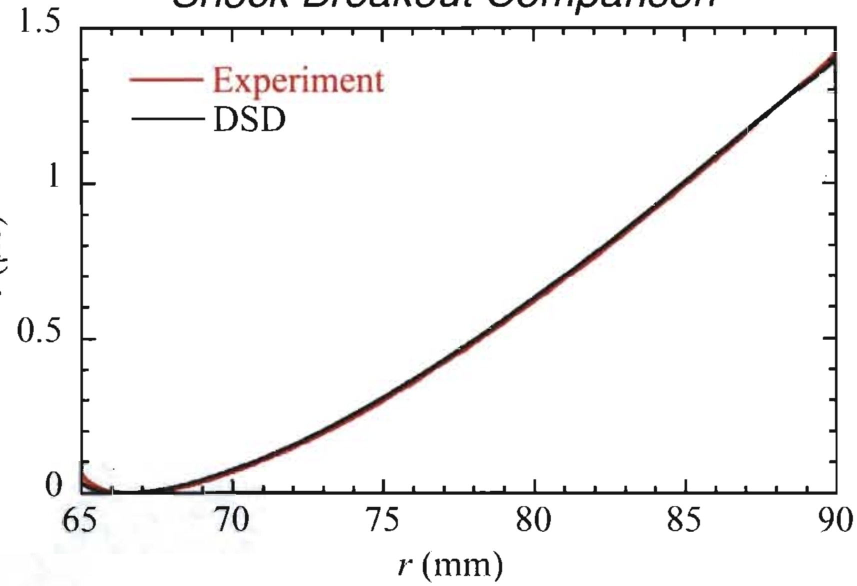
DSD Validation Test: PBX 9502 135° 2D Arc Experiment

Experimental Setup



	Inner Speed	Outer Speed
Experiment	7.188 mm/ms	9.953 mm/ms
DSD Model	7.192 mm/ms	9.958 mm/ms

Shock Breakout Comparison



DSD Validation Tests:

1. 135° PBX 9502 High Explosive Arc

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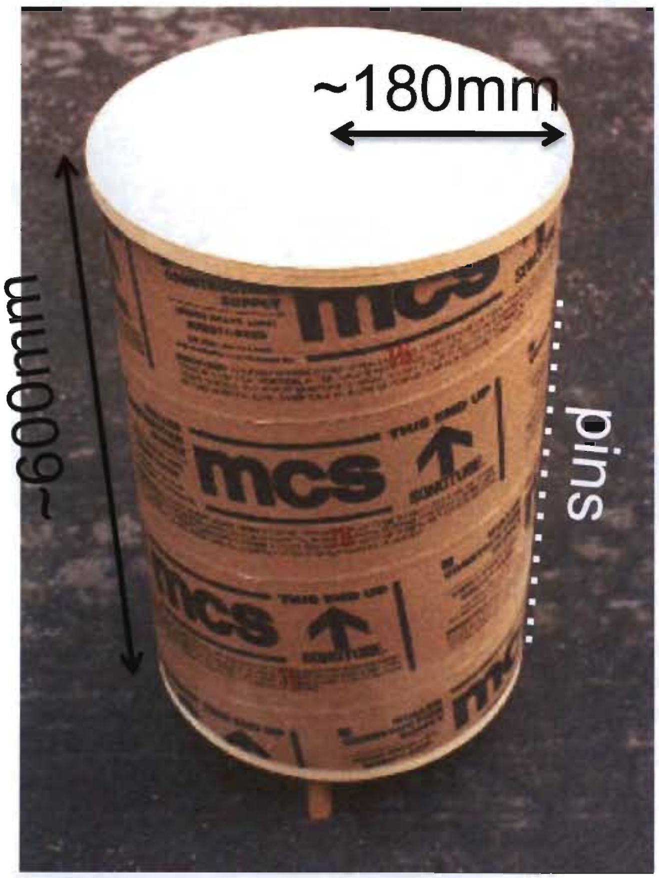
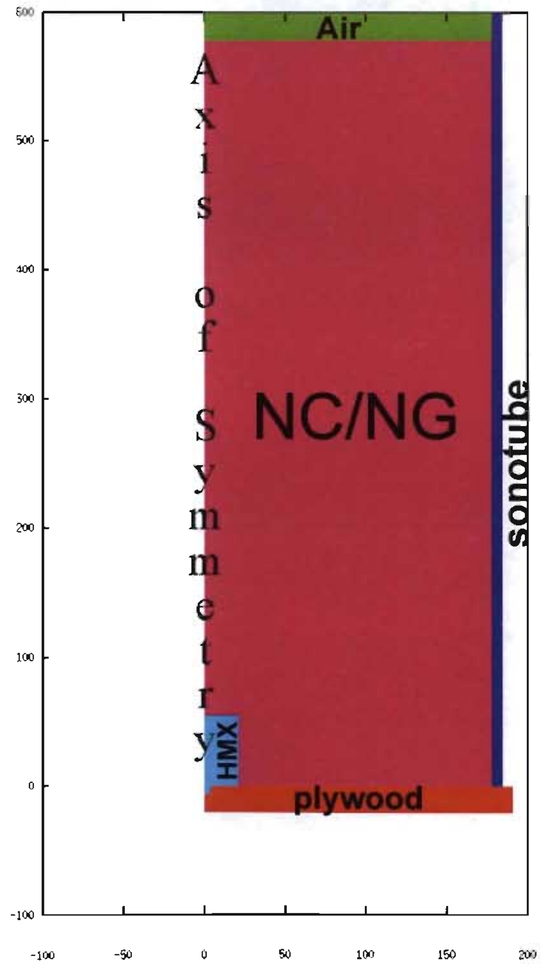
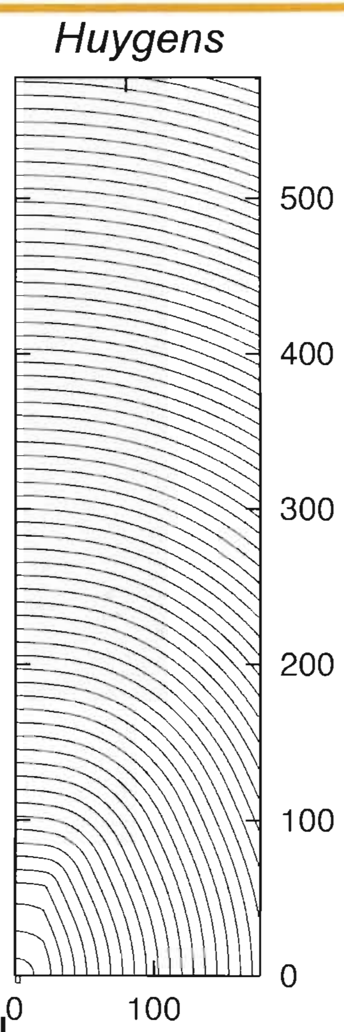
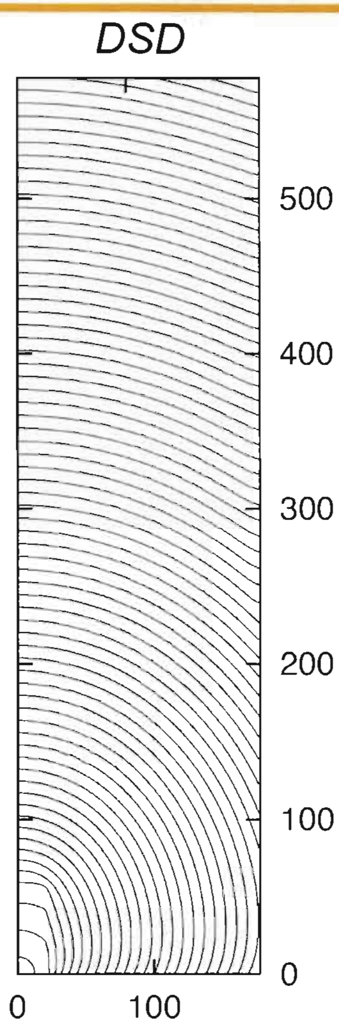
DSD Validation Test:
NC/NG Barrel Test

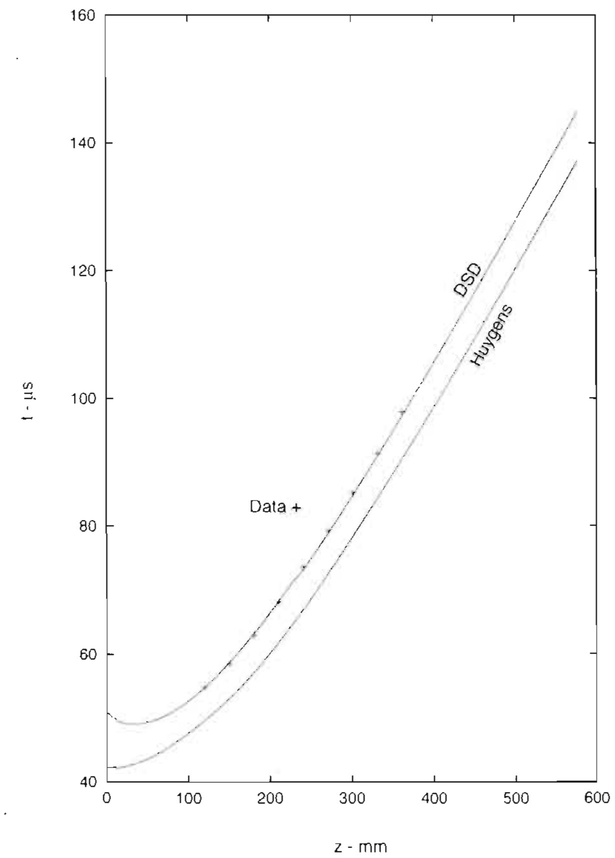




DSD Validation Test: NC/NG Barrel Test







Conclusions

- DSD is a practical approach to modeling detonation propagation
- A calibration for PBX 9502 is presented*
- Validation tests confirm applicability to other geometries
- DSD can be run:
  - independent from hydrodynamics code
  - a preprocessing step to hydrodynamics code with PRZ

*L Hill, T Aslam, "Detonation Shock Dynamics Calibration for PBX 9502 with Temperature, Density, and Material Lot Variations," Fourteenth International Detonation Symposium, August 2010