LA-UR-13-26288
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Title: Detonation Waves: models & experiments

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Intended for: LANL talk

Issued: 2013-08-08

Detonation Waves: models & experiments

National Security Energetics council: summit series talk

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HE model regimes

Regime	Reactive mode	Model or experiment	Pressure scale	Time scale
Design mode	Shock Initiation	Ignition &Growth hot spots	Pshock > few GPa	< 1 μs
	Propagation	Programmed burn pseudo-reaction rate	Pcj ~ 30 GPa	10s μs
Safety issues and Accident scenarios	Non-shock initiation	Low velocity impact shear heating	Impact P < 1 GPa	few ms
	Thermal ignition	Cookoff expt. ODTX chemical reactions	< 100 MPa	seconds to hours

- Dominant physics depends on regime
- Need different model for each regime

HE burn model

- **Equations of state**
  - Reactants
  - Products
- **Mixture rule**
  - Homogenized PBX

    Average over grains, binder and pores
  - λ products mass fraction

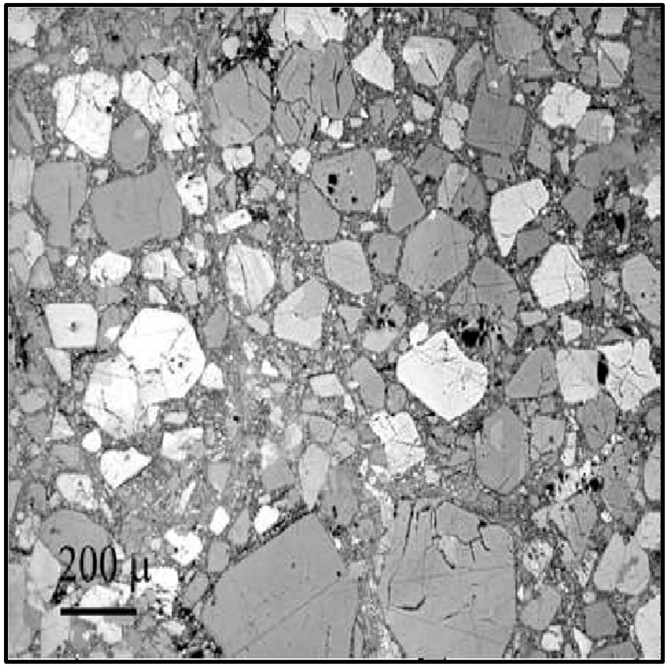
    P(V,e,λ) for partly burned HE
  - Typically P-T equilibrium

    Thermodynamically consistent
- **Burn rate**
  - Volume averaged rate

    Account for temperature fluctuations

    Hot spots dominate – chemical rate temperature sensitive
  - Empirically calibrated

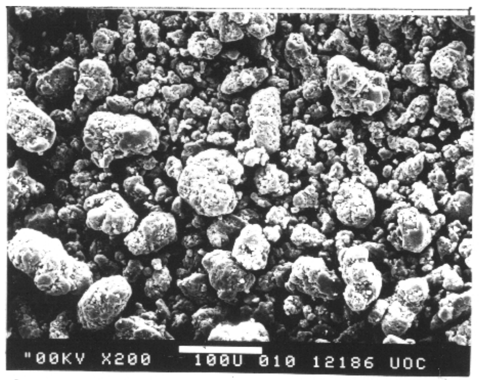
PBX 9501 (HMX)



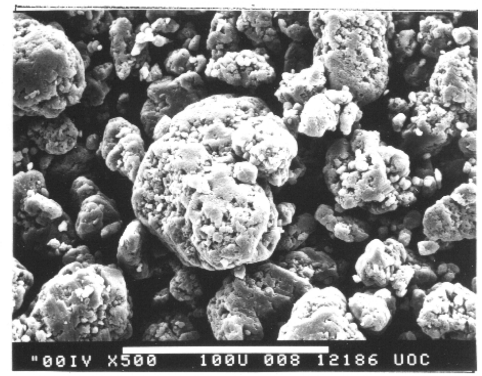
Polarized light micrograph
Cary Skidmore, 1998

TATB crystals (dry animated)

- **Scanning electron micrograph**
  - Pores (worm holes) within crystal



Pantex 12-11-82-0906-489, US Dry Sent to UK
200 x Mag.



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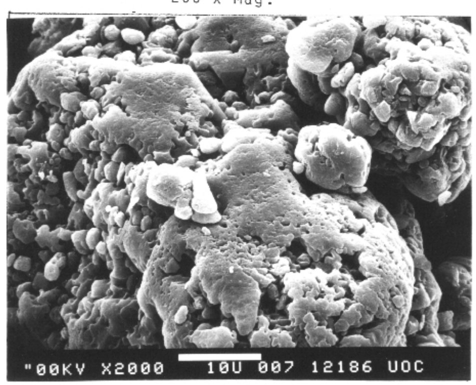

Pantex 12-11-82-0906-489, US Dry Sent to UK
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TATB used in PBX 9502
Insensitive HE

Ignition & Growth concept

- **Shock front triggers hot spots**

  Void collapse on fast time scale

- **Burn centers**

  Competition between heat conduction & reaction
  - Small hot spots quench
  - Large hot spots become burn centers

- **Reactive wavelets**

  Deflagration waves from burn centers

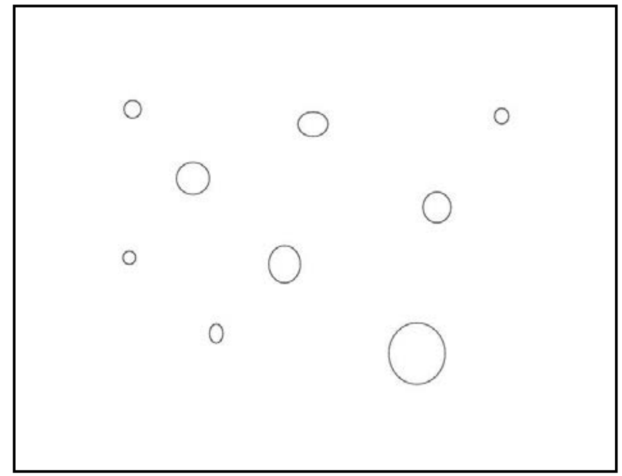
  Burn rate = (front area) $*$ (deflagration speed)

- **Depletion of reactants**

  Overlap of reactive wavelets

  Geometric effect on front area

Potential hot spot sites



For PBX:
Pores between gains
Inclusions within a grain
Cracks in grain when pressed

Ignition & Growth concept – 1

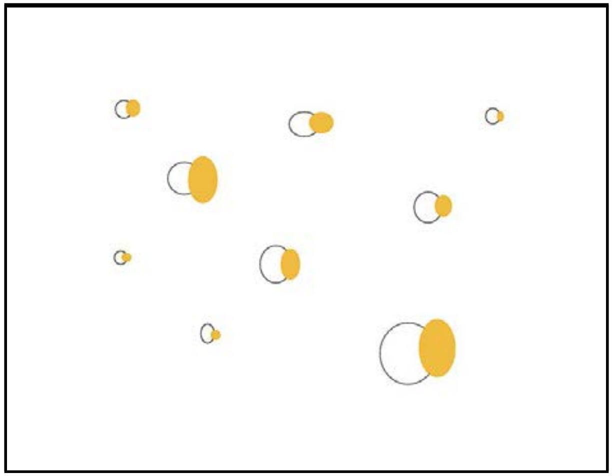
- **Shock front triggers hot spots**
  Void collapse on fast time scale

- **Burn centers**
  Competition between heat conduction & reaction
  - Small hot spots quench
  - Large hot spots become burn centers

- **Reactive wavelets**
  Deflagration waves from burn centers
  Burn rate = (front area) ∗ (deflagration speed)

- **Depletion of reactants**
  Overlap of reactive wavelets
  Geometric effect on front area

Shock sweeps over pores



Hot spots require
dissipative mechanism

Ignition & Growth concept – 2

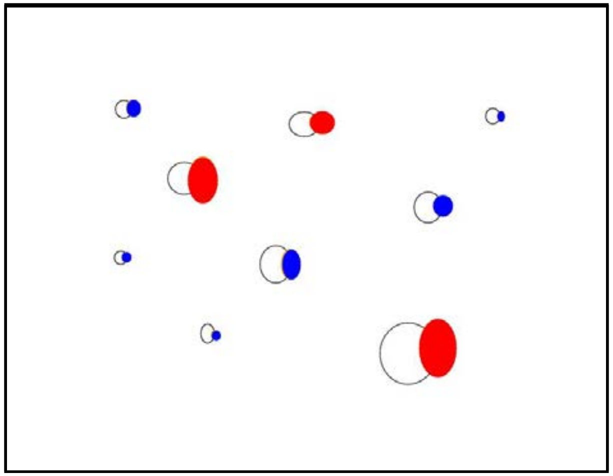
- **Shock front triggers hot spots**
  Void collapse on fast time scale

- **Burn centers**
  Competition between heat conduction & reaction
  - Small hot spots quench
  - Large hot spots become burn centers

- **Reactive wavelets**
  Deflagration waves from burn centers
  Burn rate = (front area) ∗ (deflagration speed)

- **Depletion of reactants**
  Overlap of reactive wavelets
  Geometric effect on front area

Ignition regime

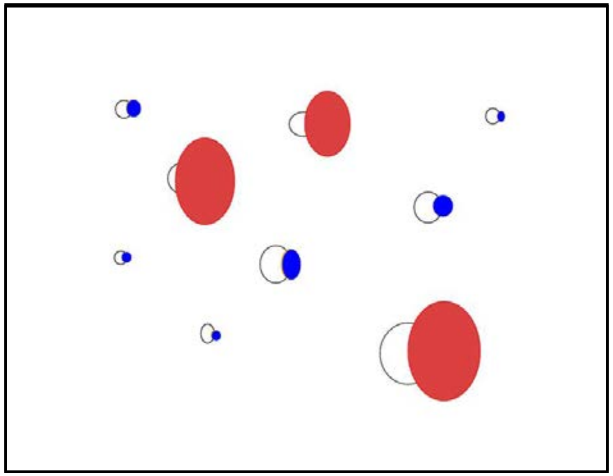


Number density of burn centers
Increases with shock pressure

Ignition & Growth concept – 3

- **Shock front triggers hot spots**
  Void collapse on fast time scale
- **Burn centers**
  Competition between heat conduction & reaction
  - Small hot spots quench
  - Large hot spots become burn centers
- **Reactive wavelets**
  Deflagration waves from burn centers
  Burn rate = (front area) $*$ (deflagration speed)
- **Depletion of reactants**
  Overlap of reactive wavelets
  Geometric effect on front area

Early growth regime



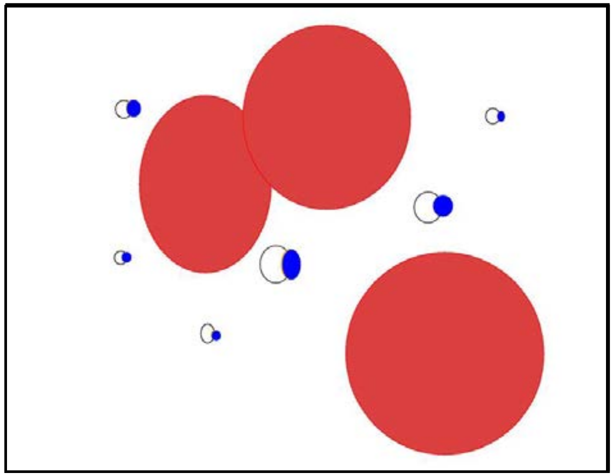
Burn front area increasing

Reactants & products
are phase separated

Ignition & Growth concept – 4

- **Shock front triggers hot spots**
  Void collapse on fast time scale
- **Burn centers**
  Competition between heat conduction & reaction
  - Small hot spots quench
  - Large hot spots become burn centers
- **Reactive wavelets**
  Deflagration waves from burn centers
  Burn rate = (front area) ∗ (deflagration speed)
- **Depletion of reactants**
  Overlap of reactive wavelets
  Geometric effect on front area

Late growth regime



Burn front area decreasing

Burn front area model scales as function of λ and proportional to number of burn centers

Burn front area scaling

- **Hot spot assumptions**
  - Spherical hot spots
  - All same radius
  - Large number
  - Randomly distributed
- **Al Nichols derivation, 2002**

  r_{hs} = hot spot radius

  d_{hs} = av distance between hot spots

  N = number of hot spots

  Vol = total volume = N d_{hs}^3

- **Key results**
  1. λ is function of r_{hs}/d_{hs}
  2. Burn front area is function of λ

$$1-\lambda = \prod_{hs}\left[1-\frac{r_{hs}^3}{Vol}\right] = \left[1-\frac{r_{hs}^3}{Vol}\right]^N$$

$$= \left[1-\frac{1}{N}\left(\frac{r_{hs}}{d_{hs}}\right)^3\right]^N$$

$$\rightarrow \exp\left[-(r_{hs}/d_{hs})^3\right] \quad \text{as } N \rightarrow \infty$$

$$\frac{d\lambda}{dt} = 3(1-\lambda)\cdot\left[\frac{r_{hs}}{d_{hs}}\right]^2 \cdot \frac{1}{d_{hs}}\frac{dr_{hs}}{dt}$$

$$\propto (1-\lambda)\left[-\ln(1-\lambda)\right]^{2/3}$$

$$\approx \lambda^{2/3}(1-\lambda)^{2/3}$$

Ignition & Growth assumptions

- **Wave width**

$$width = \int d\,\boldsymbol{\lambda}\,\frac{D-u}{Rate}$$ in stationary frame of wave

deflagration speed < CJ detonation speed

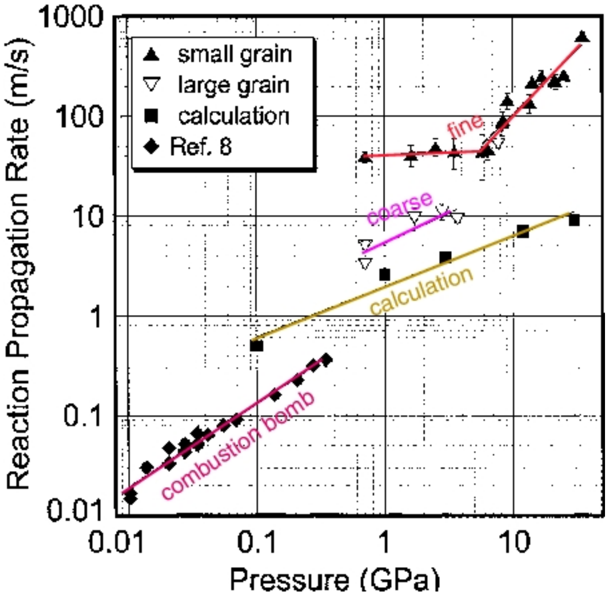
- **Hot spots**

deflagration width < **hot spot size** < detonation width

  - Hot spot triggers deflagation wave
    but not detonation wave
  - Collective effect of many hot spots

- **Deflagration speed**
  - Deflagration speed $\propto P^n$
  - Much lower than detonation speed
  - For fixed pore volume
    Need many small hot spots

HMX / PBX 9501
Esposito et al. 2003



HE burn models (pressure dependent rate)

- **Ignition & Growth model** (Lee & Tarver, 1980/Tarver, Hallquist & Ericson, 1985)
  - Rate is sum of three terms

    switch on $\lambda =$ mass fraction of products

    1. Ignition, $0 \le \lambda < \lambda_i$ small, $Rate(\lambda,\rho) \propto (\rho/\rho_0 - a)^n$
    2. Growth, $\lambda_i \le \lambda < \lambda_g$ $Rate(\lambda,P) \propto (1-\lambda)^q \lambda^r P^n$
    3. Burn out, $\lambda_g \le \lambda \le 1$ added for slow rate in TATB

- **WSD model** (Wescott, Stewart & Davis, 2005)

  Variation of Ignition & Growth

  - Smooth transition between terms in λ
  - Two coefficients for growth term: ignition & propagation regimes

    Switches on shock density (ρ_s from hydro code)

  - Ad hoc extension for shock desensitization

    Adds timer variable to cut off reaction

HE burn models (rate dependent on lead shock strength)

- **SURF model** (Shaw & Menikoff, 2010)

  L2 milestone (2010) : Reactive flow model for IHE

  - Transformed variable

    $\lambda = g(s)$ and s is scaled reactive variable = $\dfrac{\text{hot spot radius}}{\text{av dist between hot spots}}$

    $\dfrac{d}{dt}s = \mathrm{f}(\mathrm{P_s})$ where $\mathrm{P_s}$ is lead shock strength, $\mathrm{f} \propto \mathrm{D\ x\ (hs\ number\ density)}^{1/3}$

  - Rate function of lead shock pressure

    $$Rate(\lambda,\mathrm{P_s}) = \frac{d}{dt}\lambda = \frac{d}{ds}\,g \cdot \frac{d}{dt}\,s$$

    Naturally accounts for shock desensitization

  - Algorithm to detect lead shock

    Local, based on Hugoniot equation: $\mathrm{e} = \mathrm{e_0} + \tfrac{1}{2}(\mathrm{P}+\mathrm{P_0})(\mathrm{V_0}-\mathrm{V})$

  - Some aspects similar to other models
    - CREST (AWE, 2006)
    - History Variable Reactive Burn model (Kerley, 1992)

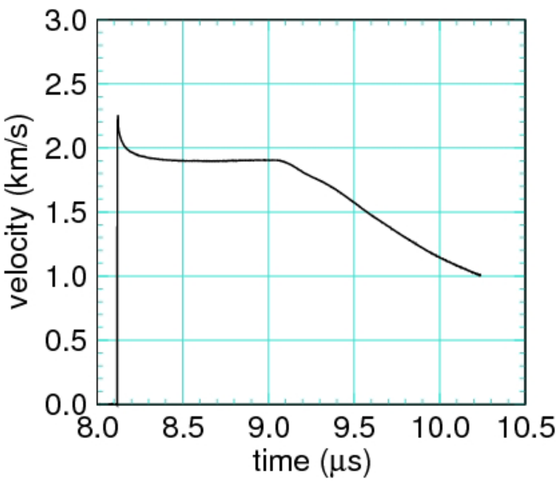
HE burn models (two-step reaction)

- **TATB – insensitive HE**
  - Excess carbon due to stoichiometry

    $C_6H_6N_6O_6 \rightarrow 3\ H_2O + 3\ N_2 + 1½\ CO_2 + 4½\ C$
  - Carbon clustering

    $C_n + C_m \rightarrow C_{n+m}$

    C-bonds release energy
  - Experimental evidence for fast & slow reactions
  - Recovery experiments find nanometer size diamonds



Shot 4f112
Vorthman et al.
1999

- **SURFplus model** (Menikoff & Shaw, 2012)
  - SURF model for fast reaction

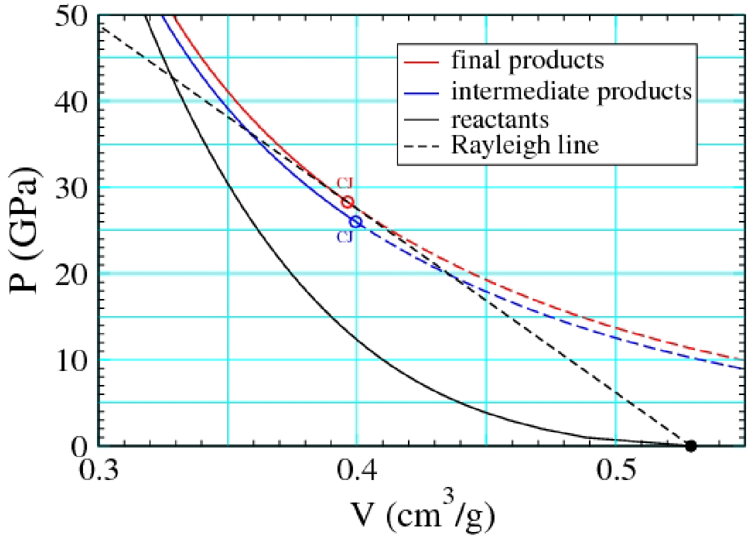
    Hot spot model
  - Plus second slow reaction for carbon clustering

    Based on analysis of Shaw & Johnson (1987)

    Diffusion process for cluster formation, hence slow rate

Effect of fast-slow rate

- **Carbon clustering energy release**
  - Shifts detonation locus and release isentrope



- Final products
  Equilibrium with carbon clustering
- Intermediate products
  Without carbon clustering energy

- **Slow approach to steady state**
  - Shock initiation to CJ state of intermediate products
  - Detonation speed increases to CJ state of final products
  - Slow transient due to sonic condition

Equations of state

- **Reactants**
  - Hugoniot data
  - Diamond anvil cell data (HE grains)
- **Products**
  - Overdriven detonation
  - Release isentrope
  - Cylinder test wall velocity
- **EOS fitting form**
  - Mie-Gruneisen form

    Ref curve: $P_{ref}(V)$, $e_{ref}(V)$
    - Principal Hugoniot or isentrope for solid
    - CJ release isentrope for products
  - Common fitting forms

    JWL, HOM, Davis, Shaw table for products

$$P(V, e) = P_{ref}(V) + \frac{\Gamma(V)}{V}\left[e - e_{ref}(V)\right]$$

Thermodynamic consistent

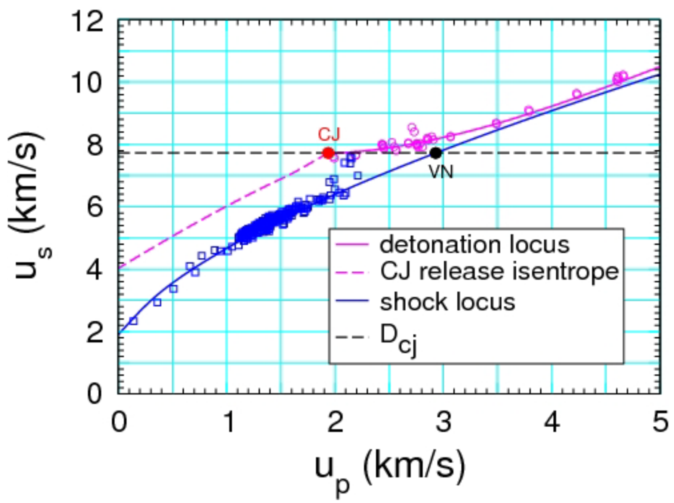
T based on Γ and C_v

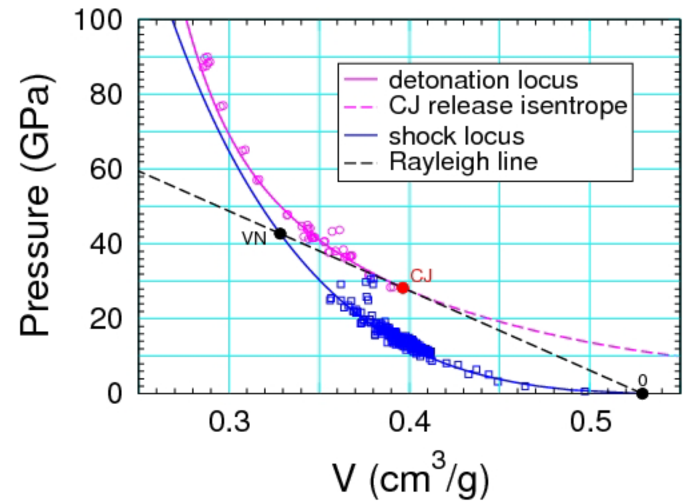
$$C_v(T, V) = C_v(T/\theta(V))$$

$$\Gamma(V) = -V\frac{d\ln\theta}{dV}$$

PBX 9502 – Hugoniot & detonation loci

- **Principal Hugoniot and release isentrope**

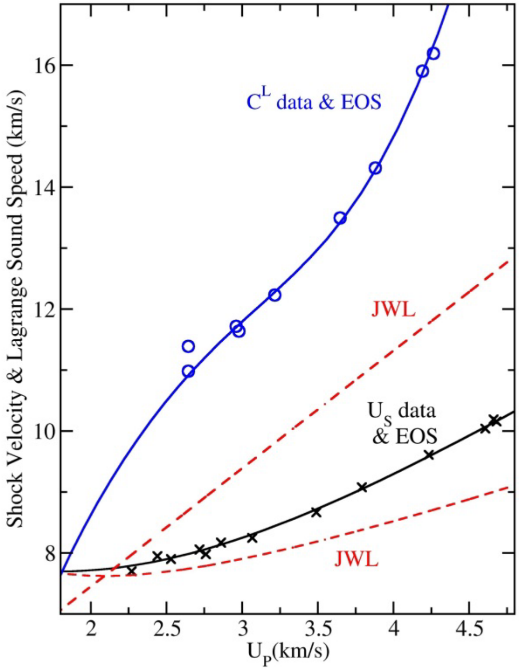




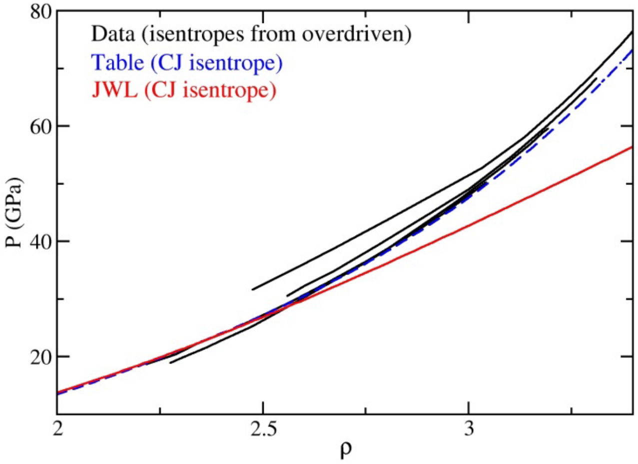
- ***Γ*(V) difficult to measure**
  - Need sound speed or 2 reference curves
- **Little temperature data**
  - Cv solid based on phonon spectrum
    from MD simulations or Raman scattering and infrared spectrometry

PBX 9502 – overdriven detonation & release wave

- **Uncertainty in CJ state**



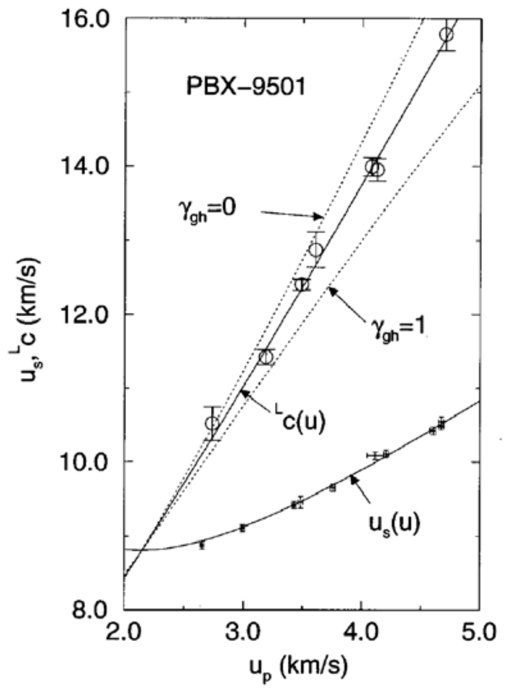
Courtesy Sam Shaw, 1999
Fritz, Hixson, Vorthman, Anderson



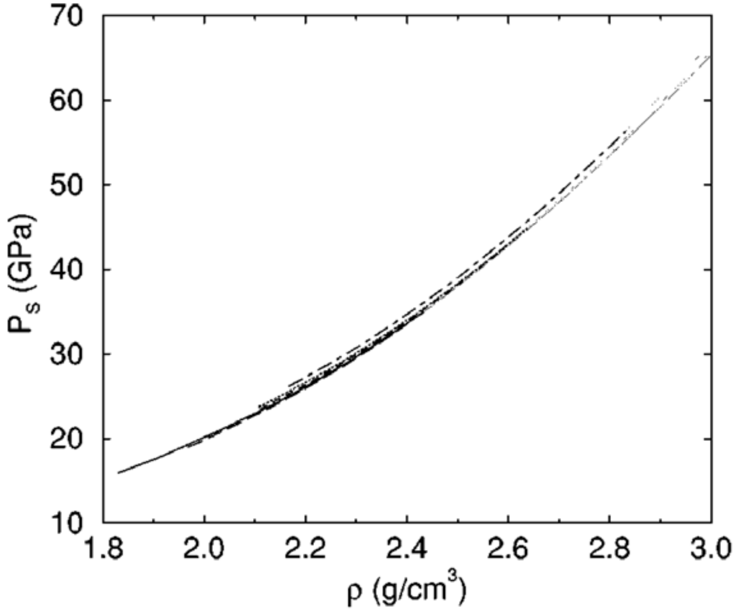
- **Anomalous behavior of isentropes**
  - Likely due to carbon clusters
    Possibly diamond/graphite transition
    Or surface molecules on cluster
  - Limits accuracy of EOS model

PBX 9501 – overdriven detonation & release wave

- **Fast reaction, no carbon clustering**
  - Expected behavior



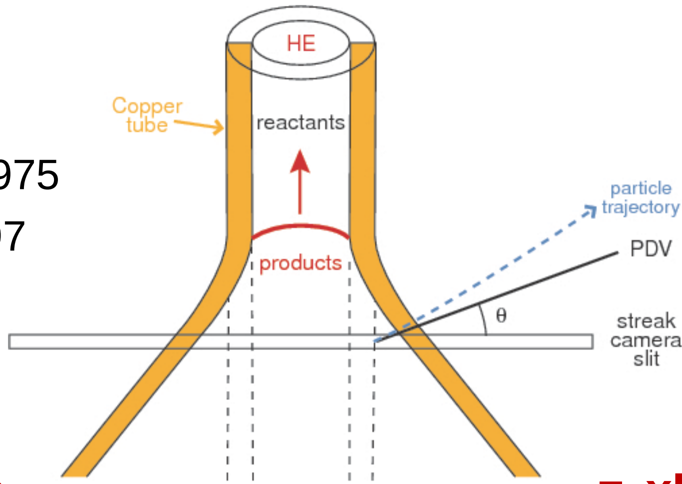
Fritz et al, 1996



Hixson et al, 2000

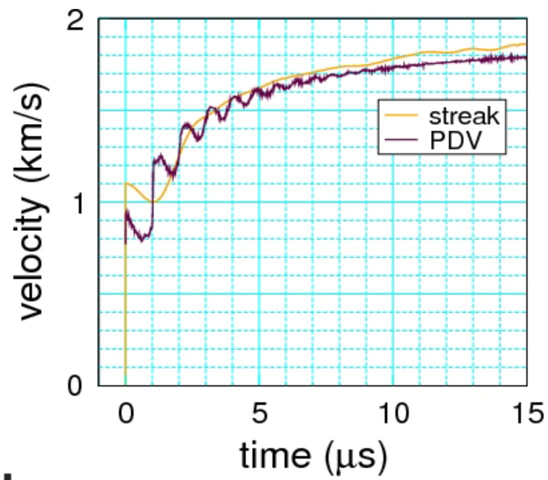
PBX 9501 – CJ release isentrope

- **Cylinder test**
  - Streak experiment
    Campbell & Engelke, 1975
    Reanalyzed by Hill, 1997
  - PDV experiment
    Pemberton, 2011

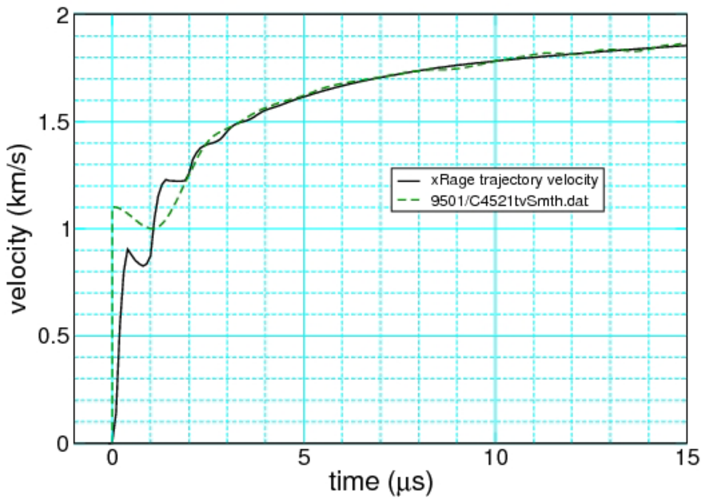


LLNL, early 1970s
Originally used to calibrate JWL EOS for HE products

- **Wall velocity data**



- **xRage simulation**



Data to calibrate & validate burn rate

- **Pop plot data**
  - Distance of run-to-detonation as function of initial shock pressure
- **Shock-to-Detonation Transition data**

  1-D experiments, gas gun – embedded velocity gauge data or PDV probes
  - Sustained shock
  - Short shock
  - Double shock – shock desensitization
- **2-D experiments**
  - Rod impact
  - Corner turning
  - Initiator/booster

    Onion skin, Mushroom, Hockey puck
  - Curvature effect and failure diameter

PBX 9502 – Pop plot

- **Sensitive to initial temperature**
  - Hot more sensitive
  - Cold less sensitive

    Also dependence on lot

- **Sensitive to initial density**
  - Lower density (increased porosity)

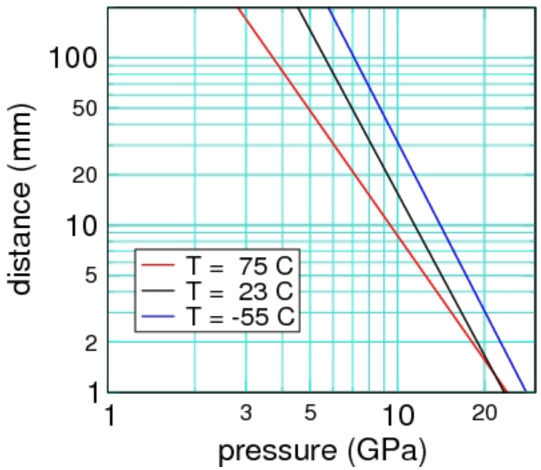
    More shock heating, $\Delta e = \frac{1}{2} P \Delta V$
  - CJ detonation speed varies with initial density

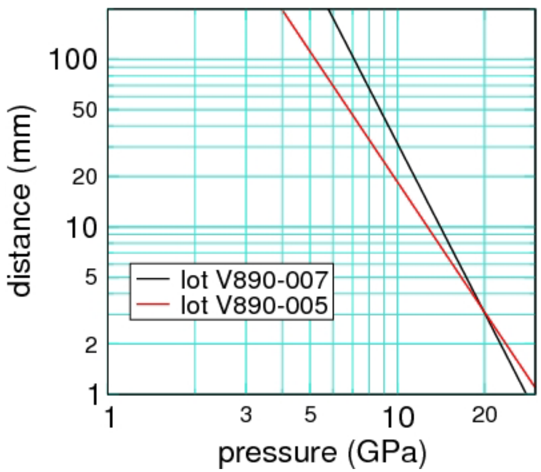
    Roughly ΔD = 2 to 3 (m/s) / (mg/cm^3)

    Thermal expansion $\frac{\Delta V}{V \Delta T} = 1.4 \times 10^{-4}$ / K

- **EOS issues**
  - PBX density measured at room temperature
  - Thermal expansion not accurate

    Change in pore volume fraction



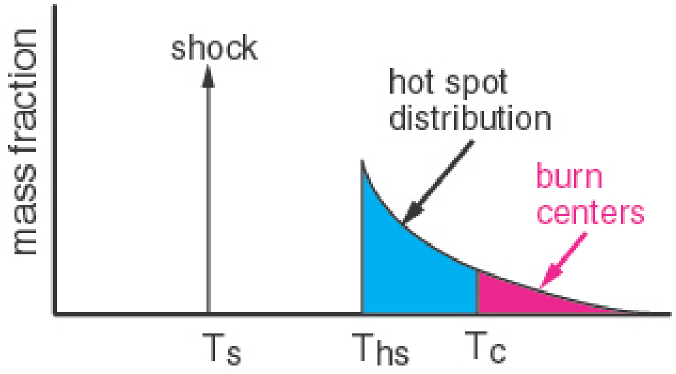


Ignition & Growth concept – shock sensitivity

- **Burn centers**
  - Tail of hot spot distribution

    Initial temperature shifts distribution

    Hence affects number of burn centers



- **Shock desensitization**

  Campbell & Travis, 1985

  - Weak shock closes pores

    Eliminates potential hot spot sites
  - Limiting case

    Pure crystal (no pores) very insensitive

    Detonation wave in PBX 9404 failed to initiate HMX crystal

    Detonation wave in HMX crystal can be initiated by flyer plate

    – Thermal rate at von Neumann spike temperature

PBX 9502 – shock-to-detonation transition - 1

- **Sustained shock**
  - Embedded velocity gauges

    Shot 2s58

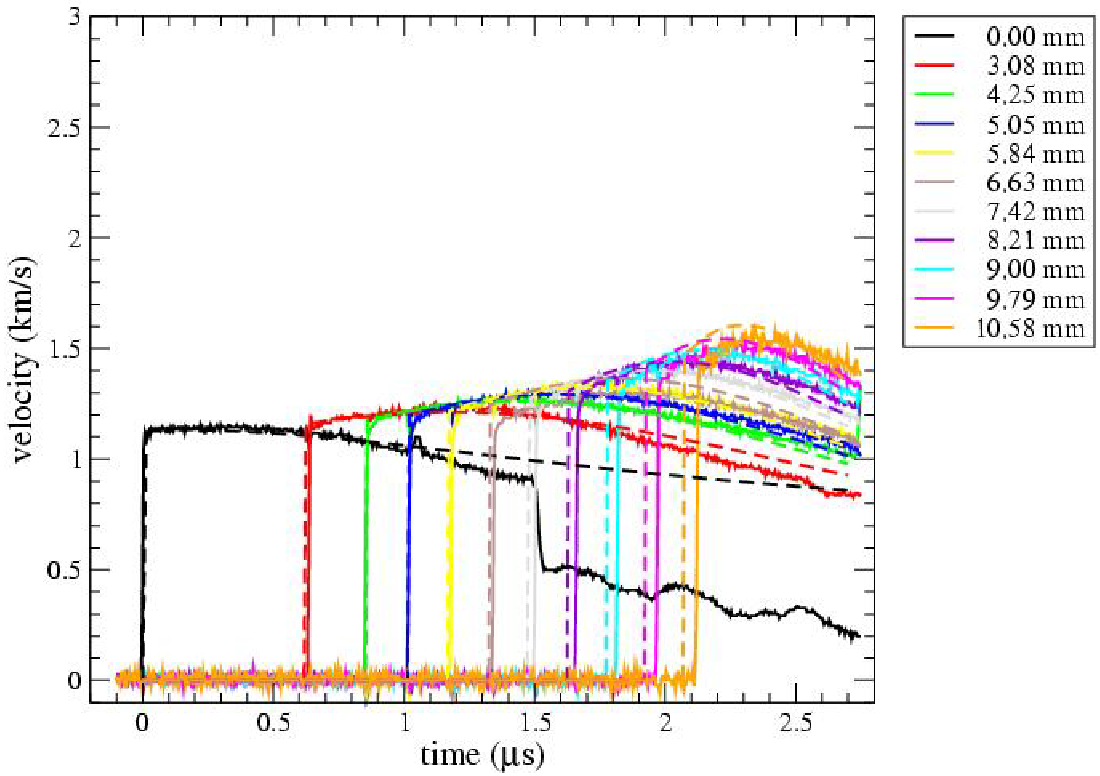
    P_s = 10.9 GPa
    - Solid, experiment
    - Dashed, simulation

Gas gun experiments
- Rick Gustavsen et al

Simulations
- **Amrita** environment by James Quirk

Lagrangian equation set and patch integrator for Amr_sol computational engine

SURF model simulation



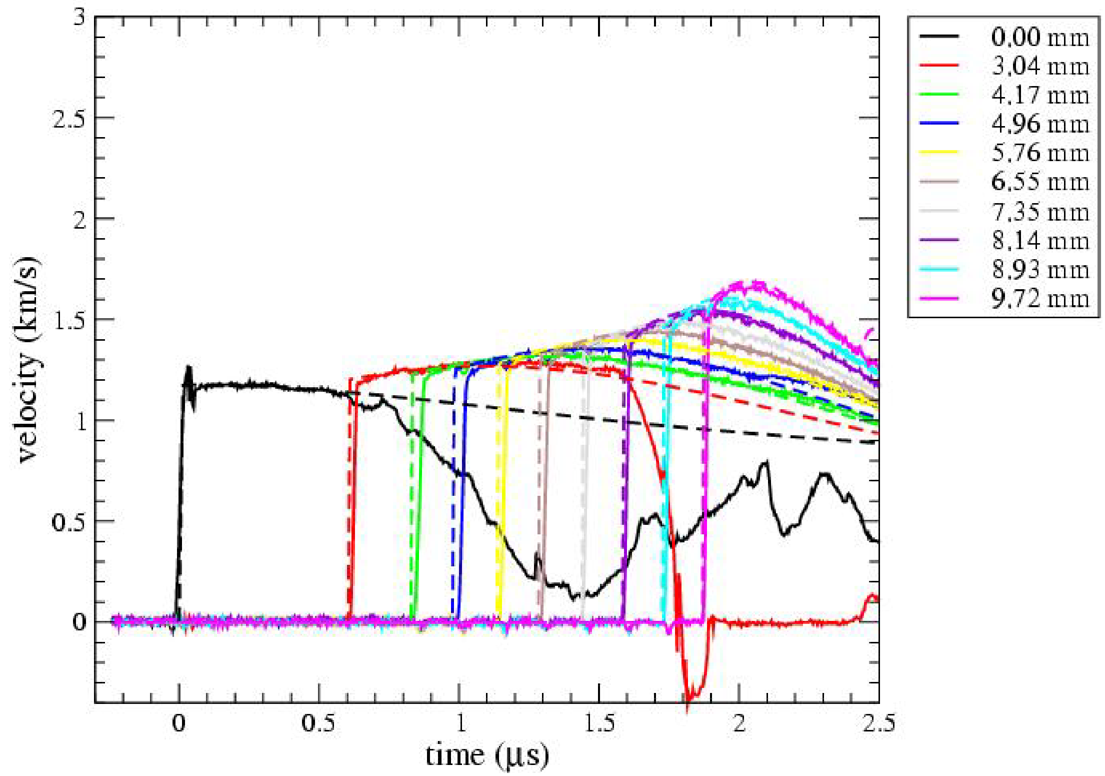
PBX 9502 – shock-to-detonation transition - 2

- **Sustained shock**
  - Embedded velocity gauges

    Shot 2s42

    P_s = 11.2 GPa
    - Solid, experiment
    - Dashed, simulation

SURF model simulation



PBX 9502 – shock-to-detonation transition - 3

- **Sustained shock**
  - Embedded velocity gauges

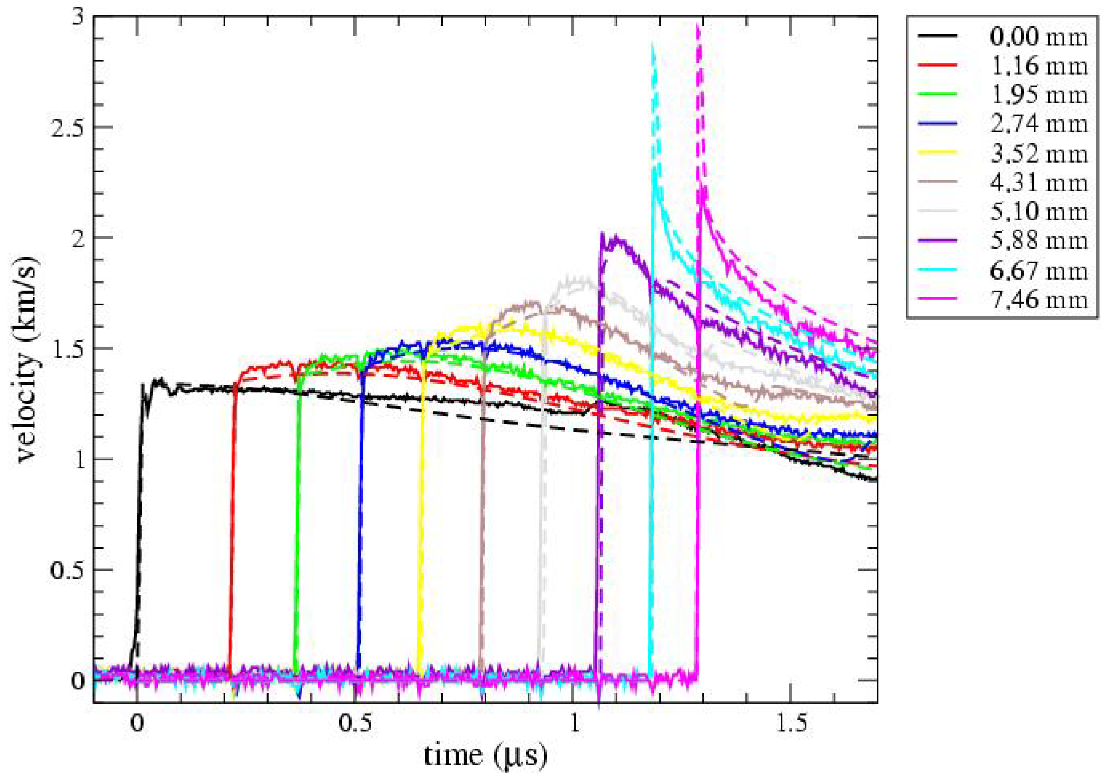
    Shot 2s40

    P_s = 13.5 GPa

    – Solid, experiment

    – Dashed, simulation

SURF model simulation



PBX 9502 – shock-to-detonation transition - 4

- **Short shock**
  - Embedded velocity gauges

    Shot 2s100

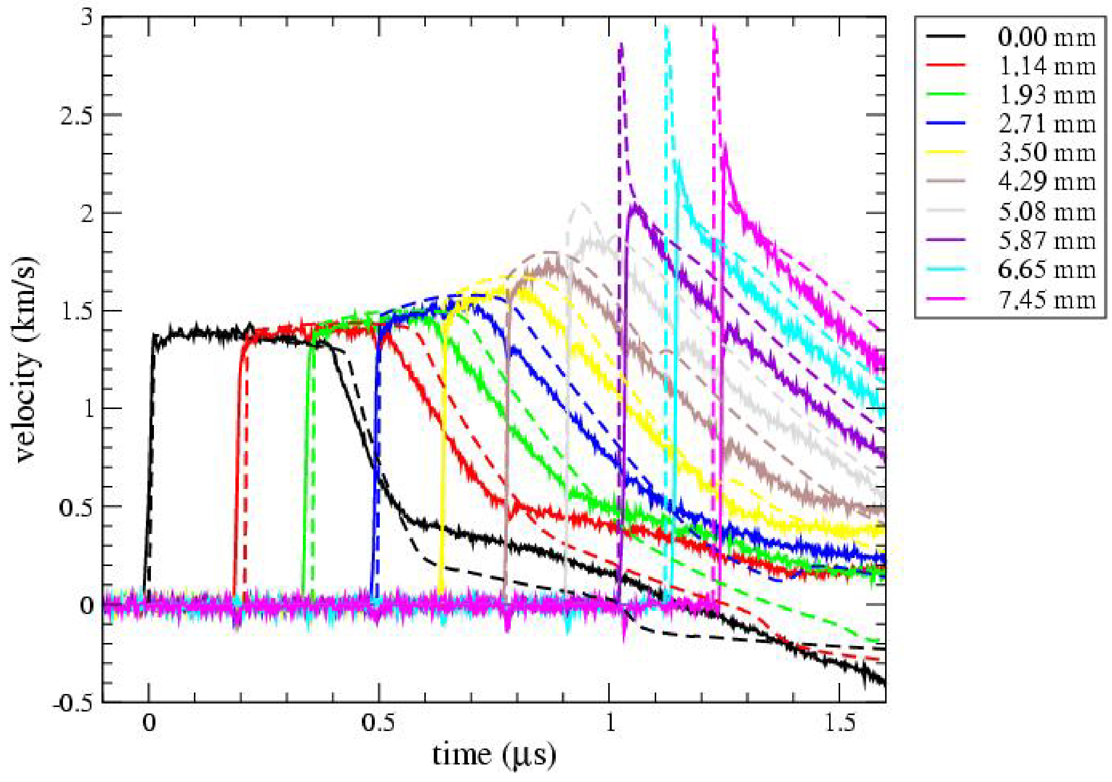
    $P_s = 14.0$ GPa

    $\Delta t = 0.35\ \mu s$

    – Solid, experiment

    – Dashed, simulation

SURF model simulation



PBX 9502 – shock-to-detonation transition - 5

- **Short shock**
  - Embedded velocity gauges

    Shot 2s105

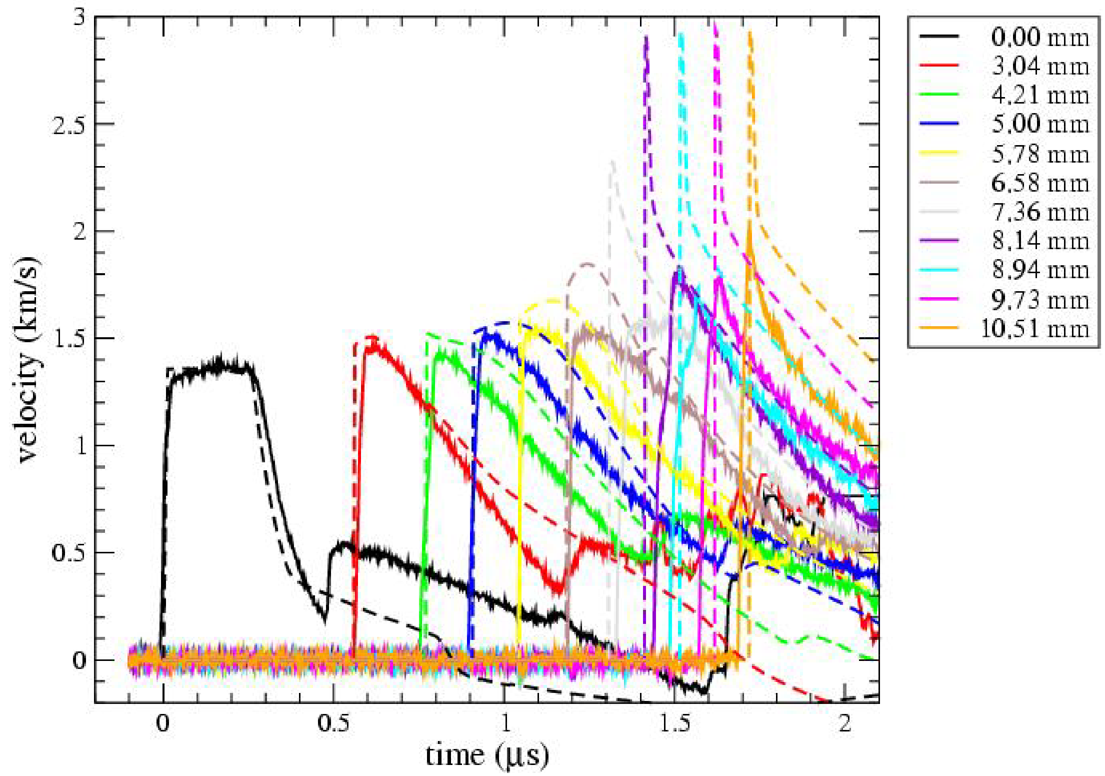
    $P_s = 13.9$ GPa

    $\Delta t = 0.27\ \mu s$

    – Solid, experiment

    – Dashed, simulation

SURF model simulation



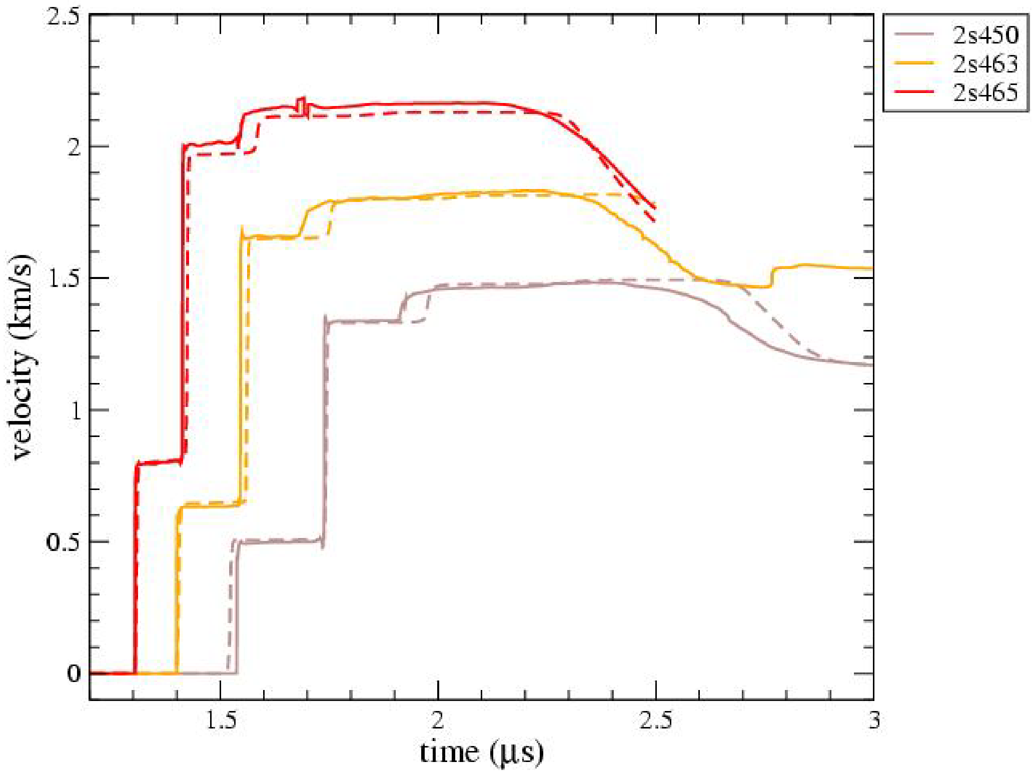
PBX 9502 – shock desensitization

- **Double shock**
  - PDV probes
    - Solid, experiment
    - Dashed, simulation

shot	P1	P2
	GPa	GPa
2s450	5.3	19
2s463	7.0	25
2s465	9.0	33

CJ pressure 28 GPa
VN spike pressure 42 GPa

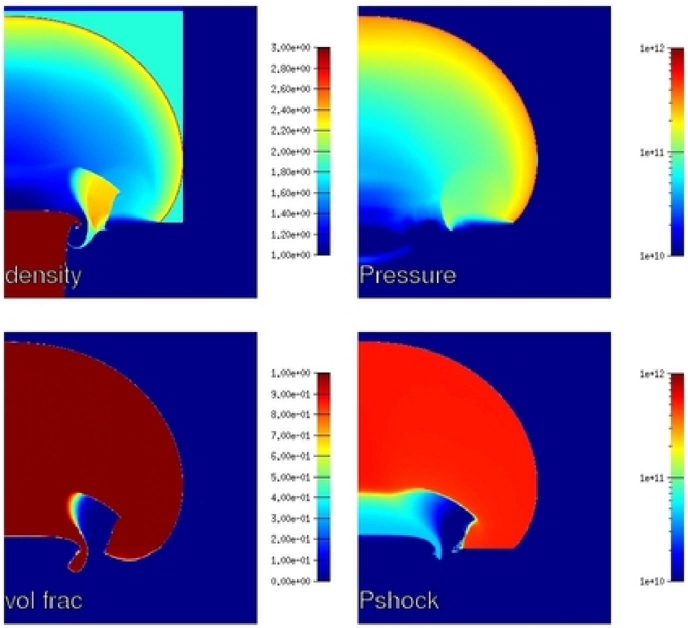
SURF model simulation



PBX 9501 – shock initiation & corner turning

- **Rod impact,** xRage simulations (click on plots to see movie)

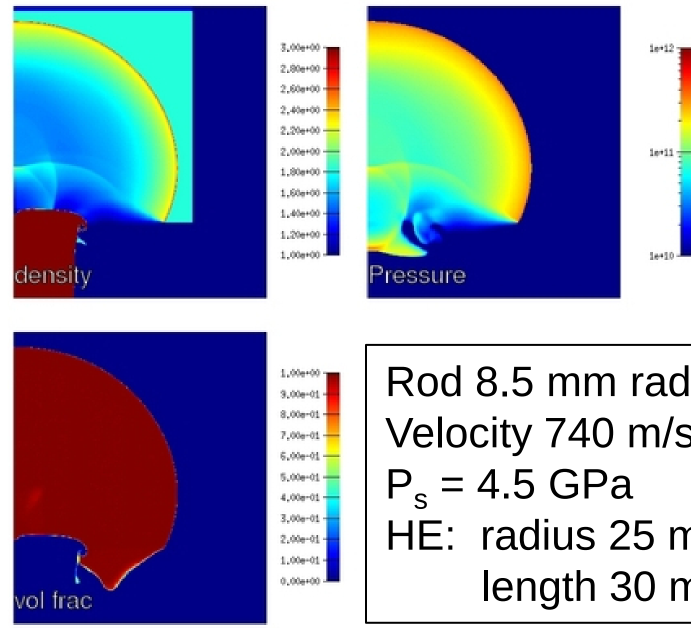
time 4.20 μs



SURF model

- Desensitized HE near corner of rod

time 4.20 μs



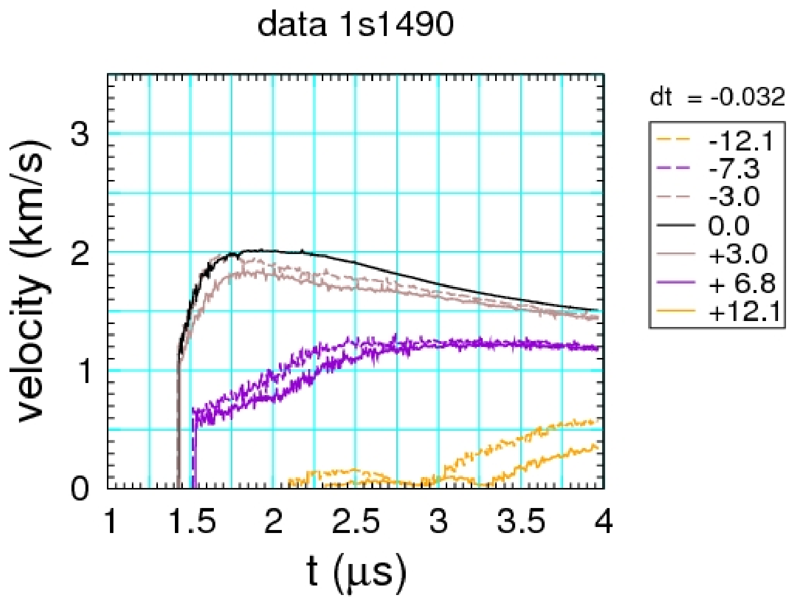
Ignition & Growth model

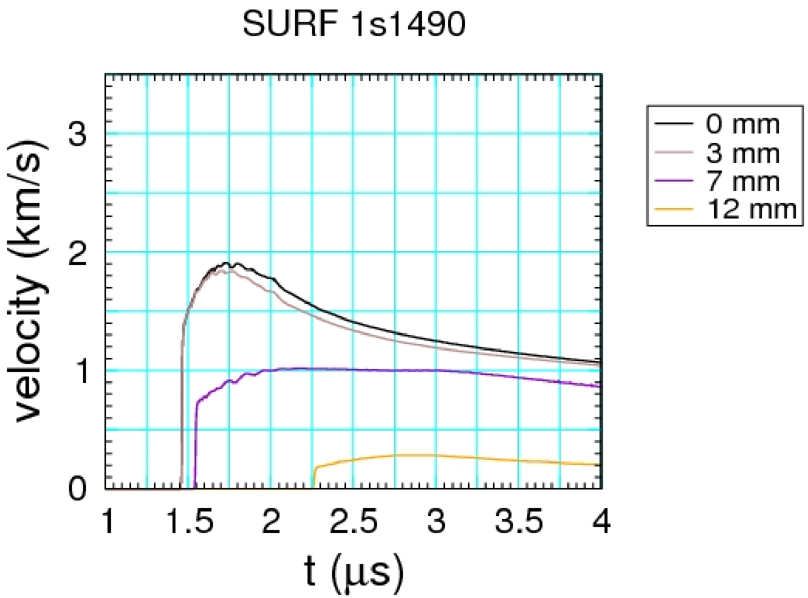
Rod 8.5 mm radius
Velocity 740 m/s
P_s = 4.5 GPa
HE: radius 25 mm
length 30 mm

- Initiation leads to reactive wave in precompressed HE

PBX 9501 Rod Impact Experiment: comparison 1

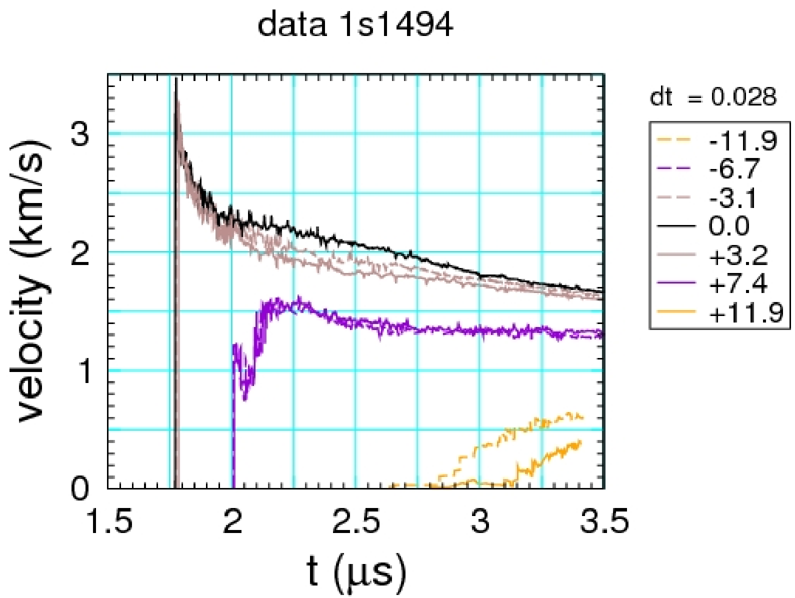
- **Shot 1s1490**
  - HE 6 mm thick
  - Below run distance on Pop plot
  - No shock-to-detonation transition

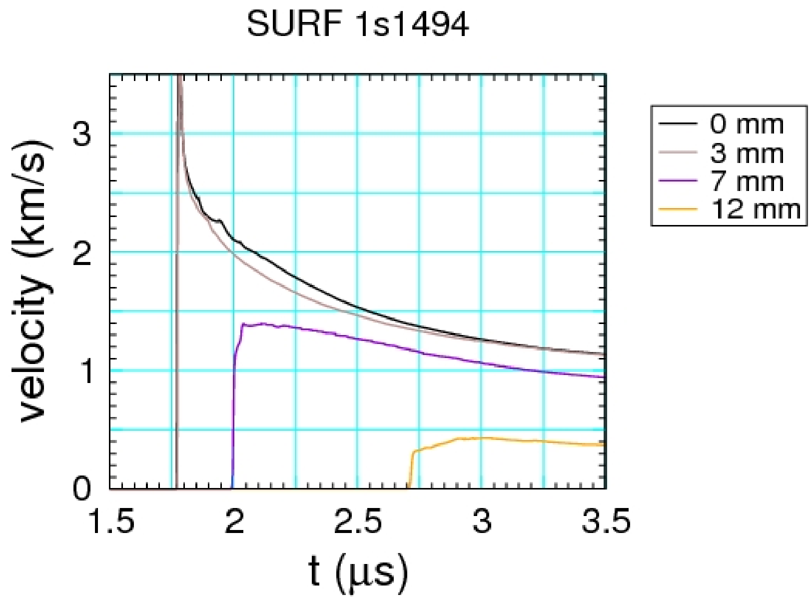




PBX 9501 Rod Impact Experiment: comparison 2

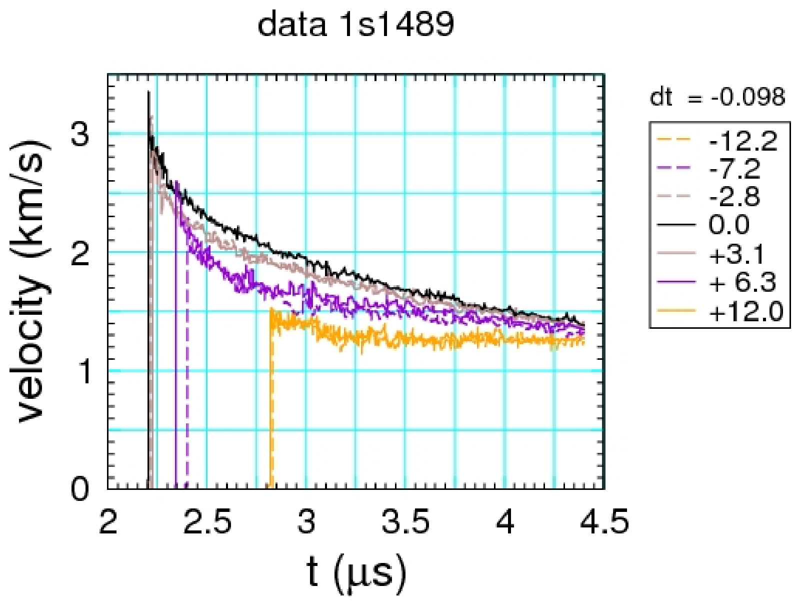
- **Shot 1s1494**
  - HE 8 mm thick
  - Shock-to-detonation transition on axis
  - Detonation does not spread transverse direction

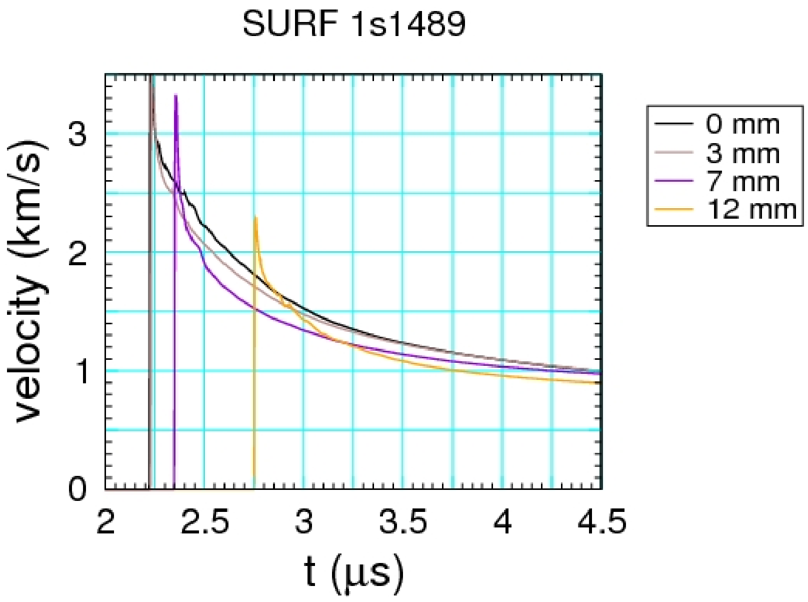




PBX 9501 Rod Impact Experiment: comparison 3

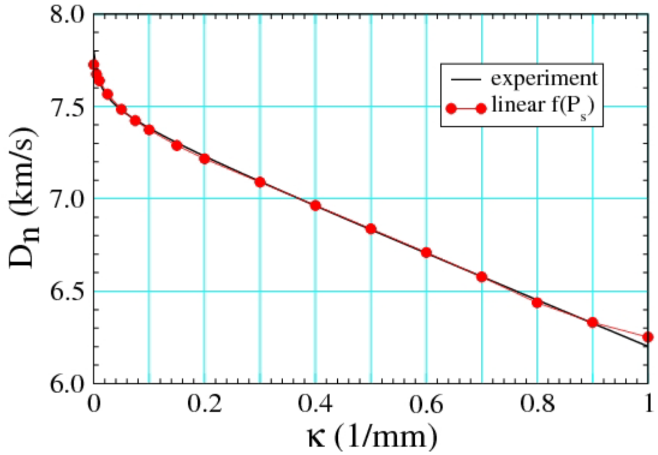
- **Shot 1s1489**
  - HE 12 mm thick
  - Shock-to-detonation transition on axis
  - Detonation spreads in transverse direction

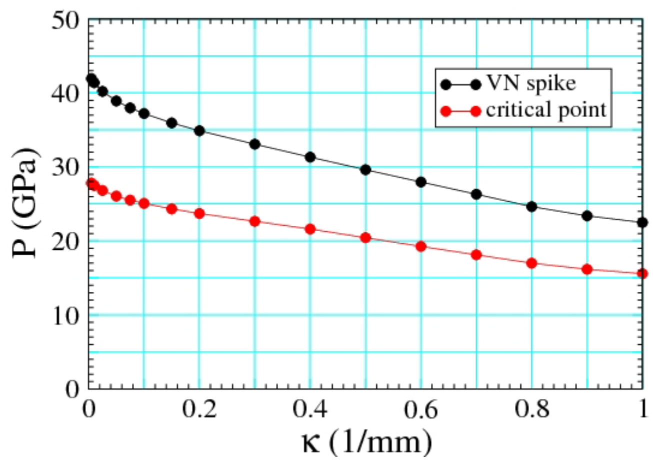


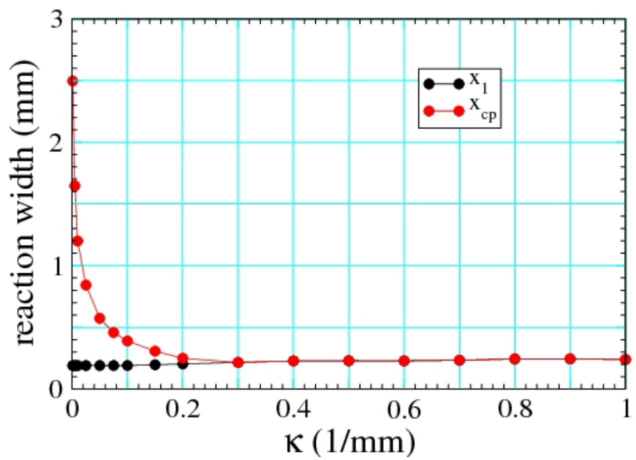


PBX 9502 – curvature effect

- **$D_n(\kappa)$ curve**
  D = Detonation speed
  κ = front curvature
- **SURFplus model**
  - Quasi-steady ODEs
  - Determines curved detonation state
  - Requires high resolution







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Model calibration

- **What data is available**
  - Small Scale Database

    Extension and replacement for High Explosive Database

    On line 4^{th}Q FY2013 (Scovel & Menikoff)

    Funded by V&V program (Wysocki)
- **Automate simulations**
  - Data file from Small Scale Database

    Header block with key experimental parameters
- **Fitting parameters**
  - Minimize metric for "*goodness of fit*"

    Weight function for data from many different experiments

    Shock arrival times & velocity profiles with uncertainties
  - Non-linear fit with many variables (up to 26 in WSD model)

    Need good initial guess to start iteration & fix inessential parameters

Computational issues

- **Mesh resolution**
  - Hot spot reaction zone width ~ 0.1 mm

    Comparable to grain size – smaller than needed for homogenization
  - Need mesh refinement to track detonation front (AMR)
- **Curvature effect**
  - Detonation speed as function of front curvature

    Affected by mesh resolution
  - Detonation state for curved front

    Depends on rate and reaction zone width

    Issue for programmed burn (DSD) model
- **Accuracy requirement**
  - Detonation speed, CJ state and release isentrope
  - Application simulations – typically not mesh converged

    Coarse mesh, reactive shock rather than ZND profile

Predictive capability

- **Validation of HE model**
  - Need good EOS for reactants and products
  - Need to compare with wide range of detonation phenomenon

    Large number of experiments to simulate
    - For each explosive
    - For each HE model (EOS + burn rate)
  - Need to automate simulations
- **Initiation sensitive to initial temperature and initial density**
  - Calibration for each T_0 and ρ_0

    Treated as distinct explosive – effectively, many more explosives
- **Shock desensitization**
  - SURF model

    Naturally accounts for desensitization, rate function of P_s

    Possibly account for sensitivity change with initial temperature