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A Computational and Experimental Investigation of Violence in a Thermal Explosion Test

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USA

What is a thermal explosion?

Long-time exposure to fire

- A situation where if the heat transfer rate cannot keep pace with the rate of heat produced, then the temperature will rise at a greater and greater rate

$$\rho C(dT/dt) = \lambda \nabla^2 T + \rho Q Z e^{-E/RT}$$

- Ignition of an explosive by direct thermal heating from its environment
- Specific tests that a munition must pass to meet specified safety standards and the manner in which these tests are conducted
- It cannot be confidently modeled by separating the process into a thermal/chemical phase and a hydro/chemical phase

We want to gain knowledge in these areas

- Thermal response of HE under thermal explosion situation
  - Time to explosion
  - Ignition temperature
- Mechanical response of HE under thermal explosion conditions
  - Slow / fast strain rates
  - Fracture / fragmentation of structural (casing) materials
- Violence prediction of HE compounds such as
  - RDX and HMX based explosives
  - Other HE's of DOE/DoD interest

We develop predictive models!

Some issues with modeling HE Thermal Explosion are

- Thermal Explosion splits naturally into two stages based on the timescale

  <u>Pre-ignition</u>

  Involves both physical (e.g. melting) and chemical changes in hours to days

  <u>Post-ignition</u>

  Characterized by a reaction spread in hundreds of microseconds

- Can we simulate this problem in two separate steps (like some others in the field) and still reproduce the experimental records?
- How can we improve our predictive modeling capability?

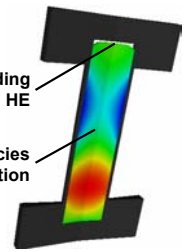
Outline of this talk is as follows

- ✓ Brief background on HE thermal explosion
- ✓ Brief description of experiments involved:
  - Scaled Thermal Explosion Experiment (STEX)
  - One-Dimensional-Time-to-Explosion (ODTX)
  - High Pressure Strand Burner
- ✓ Description of thermal explosion model for LX-10, LX-04
- ✓ Comparisons of 1D and 2D simulations with available measurements
- ✓ 3D fracture and fragmentation simulation
- ✓ Work in progress

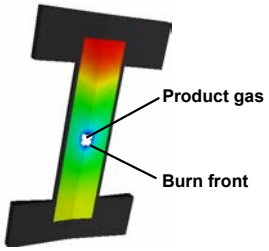
HE Thermal Explosion 101

Pre-ignition process (Chemical / Thermal)

- Long time exposure to heat for hours to days until ignition
- Slow non-linear decomposition chemistry
- Slow physical change (phase transition)
- Slow thermal transport
- Slow pressurization of system
- Multiphase material transport
- Deformation



Post-ignition process (Hydro / Thermal)

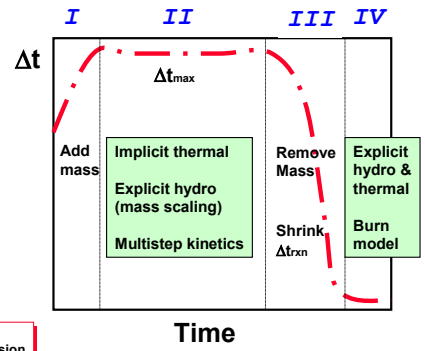


- Microsecond timescale event during the burn phase
- Fast non-linear multiphase chemistry
- High-strain rate deformation
- Fast pressurization
- Flame (deflagration) propagation
- Fracture and fragmentation of metal vessel

Compressive waves may coalesce into shocks leading to detonations (DDT)

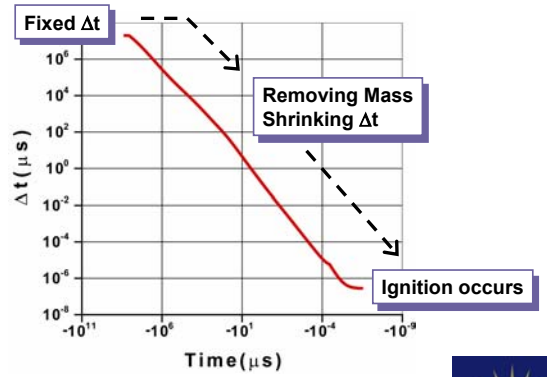
Time-step sizes of each phase are illustrated

- Four distinct phases of the thermal explosion simulation
  - Slow (*I & II*)
  - Fast (*III & IV*)
- In *I*, mass scaling lowers the sonic speed and further raises hydro time step size (fixed CFL)
- In *II*, the maximum time step size is specified during the thermal heating phase
- In *III*, the calculation proceeds in the reaction time scale
- In *IV*, burn model is used



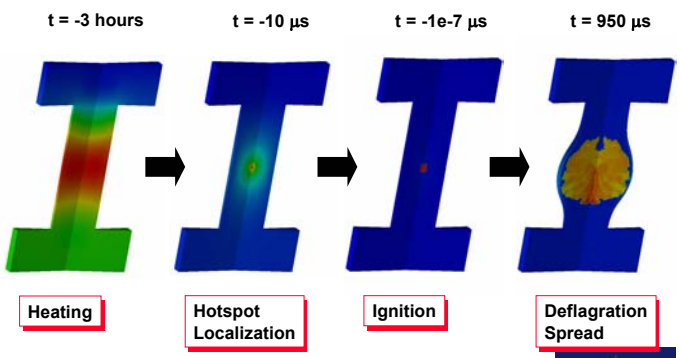
$\Delta t_{reaction} < \Delta t_{Courant} < \Delta t_{diffusion}$

Time step size undergoes 14 orders of magnitude change during the HE thermal explosion simulation

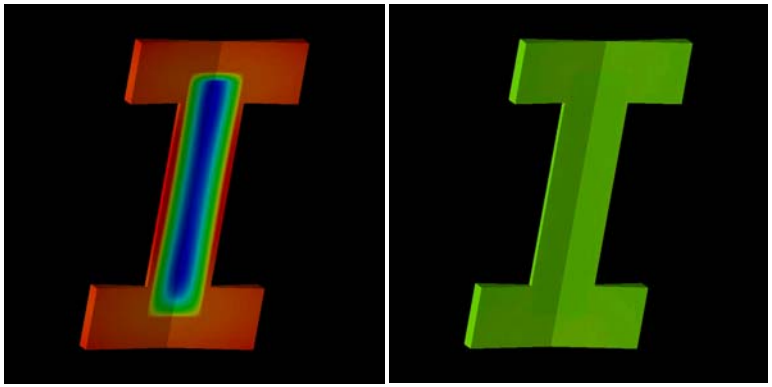


Final three hours before explosion shown

Four snapshots of temperature field at time t = -3 hours, -10 μs, -1e-7 μs, +950 μs. (1/4 million elements, Δx = 200 μm)



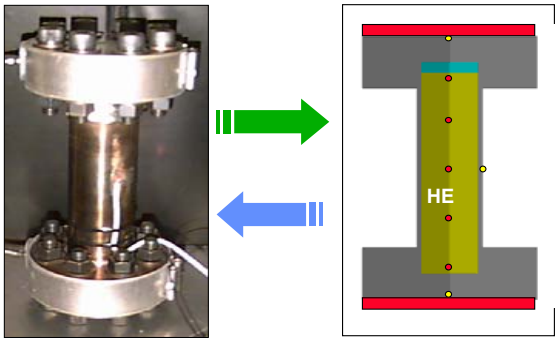
Computed on ASCI White using 32 processors



As an illustration of a typical cookoff simulation, PBXN-109 explosion process is shown in 2D (62 hours slow heating + 1400 μs rapid expansion)

Experiments

Scaled Thermal Explosion Experiment (STEX): Typical System vs. ALE3D Model System



LLNL-Experiment (PBXN-109)

ALE3D Simulation

We are preparing a slow cookoff (STEX) test with LX-10 and AerMet 100 steel

LX-10 (95% HMX, 5% Viton A)

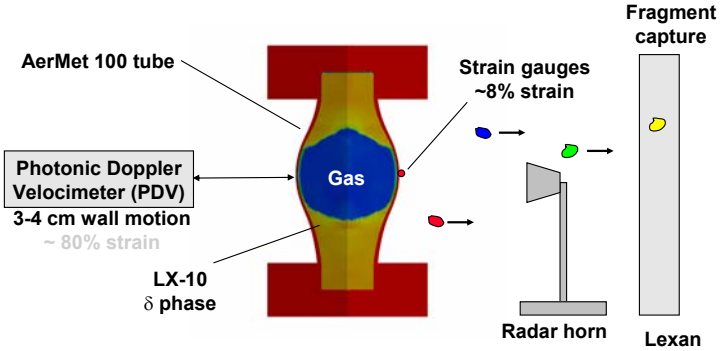
- Similar to Navy's PBXN-5
- Relatively simple
  - Mostly HMX
  - Non-reactive binder
- Exhibits wide range of violence

AerMet 100 steel
(71% Fe, 13.4% Co, 11.1% Ni, 3% Cr, other)

- Of interest to DoD
  High hardness and toughness
- Fragmentation models and materials characterization from T. Orzechowski's group

Our knowledge in LX-04 modeling is used

The LX-10/AerMet 100 STEX test will characterize violence at several stages of the explosion



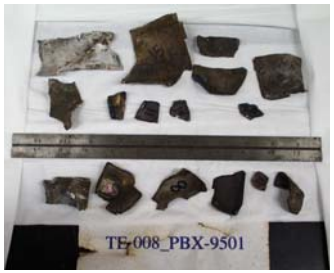
All measurements will be compared to ALE3D calculations

LX-10 STEX vessel is shown with instruments

Pipe dimension
(3 mm thick X 2 in. OD X 4 in. L)

STEX results for LX-10 are expected to be similar to a δ-phase STEX test with PBX-9501

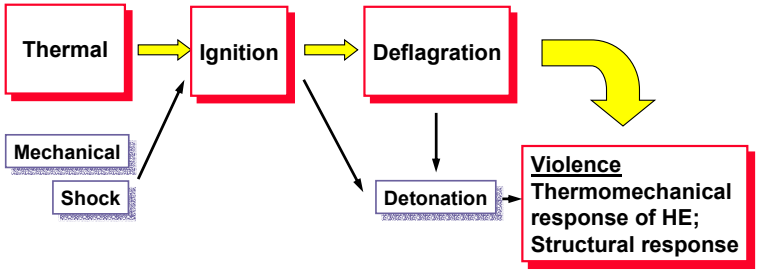
Delta phase, 2 kbar confinement, 1°C/h, no venting



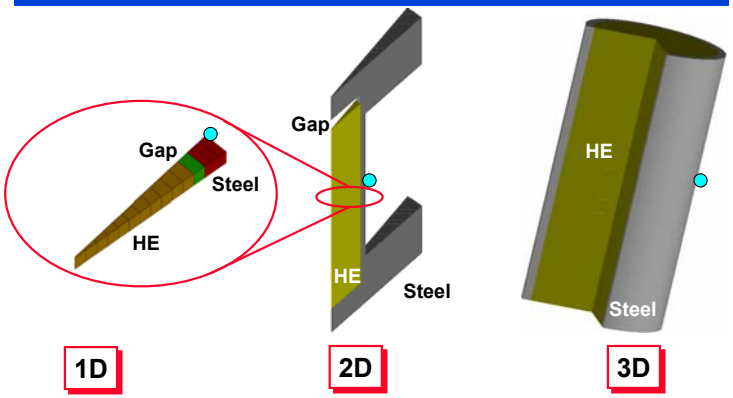
Mild violence
- Wall velocity 420 m/s
- Ignition temperature 170 °C

Modeling with ALE3D

Different violence initiation paths are analyzed

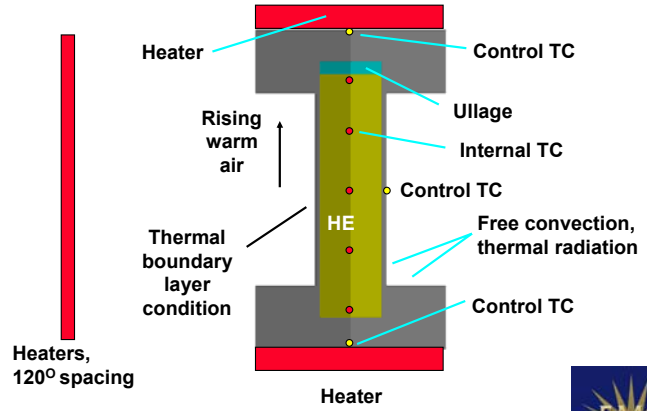


A 1D model problem is a subset of 2D and 3D problems



- Gauge locations

Modeled thermal boundary conditions (courtesy of M. McClelland)



Material models of HMX-based explosives (LX-04, LX-10) are as follows

LX-10 (95% HMX, 5% Viton)
LX-04 (85% HMX, 15% Viton)

Material properties

- Solid HE : 7-term poly. EOS with linear elasto-plastic model
- Product gases : gamma-law EOS

- Viton solid: no strength with 7-term poly. EOS
- Viton gas : gamma-law EOS

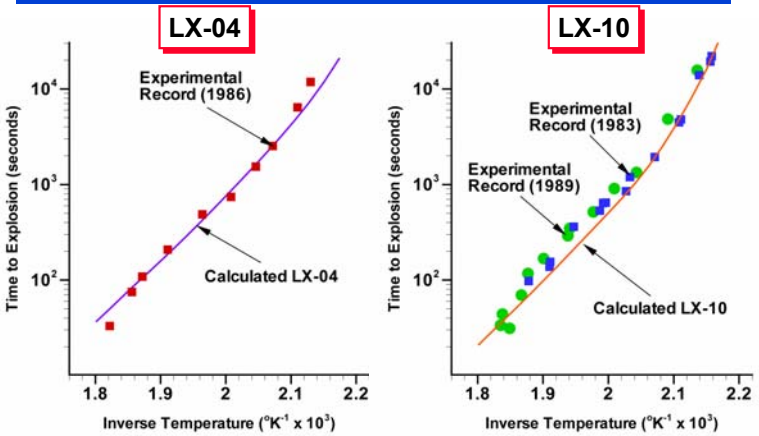
- Aermet100 : Steinberg-Guinen strength with Gruneisen EOS
- 4340 Steel : Steinberg-Guinen strength with 7-term poly. EOS

Chemical model uses four-step, five-species kinetics of HMX for LX-10 and LX-04

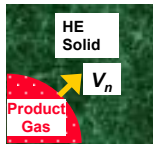
Shown decomposition and ignition kinetics of Tarver and Tran (2004)

HMX-β (A) → HMX-δ (B)	$r_1 = Z_1 \exp(-E_1/RT)\, \rho_A$
HMX-δ (B) → Int. solid (C)	$r_2 = Z_2 \exp(-E_2/RT)\, \rho_B$
Int. solid (C) → Gas int. (D)	$r_3 = Z_3 \exp(-E_3/RT)\, \rho_C$
Gas int. (D) → Product (E)	$r_4 = Z_4 \exp(-E_4/RT)\, (\rho_D)(\rho_D)$
Viton-sol. → Viton-gas	$r_{vs} = Z_{vs} \exp(-E_{vs}/RT)\, \rho_{vs}$

Chemical kinetics parameters are adjusted to fit ODTX data for LX-04 and LX-10



The deflagration propagates as a front in a burn rate model



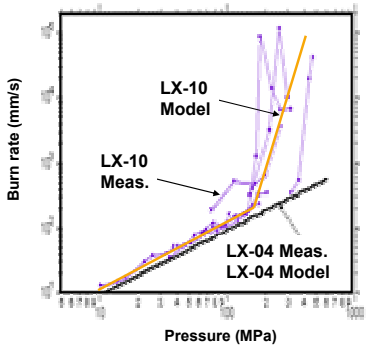
- Deflagration front propagates

$$\phi_t + V_n \bullet \nabla \phi = 0$$

- Propagation velocity (burn rate):

$$V_n = a\,(P)^n$$

- Burn rate parameters (*a, n*) are obtained from Strandburner



This model is used during the fast burn phase

Two ways of modeling dynamic gaps; mixed elements and sliding interfaces

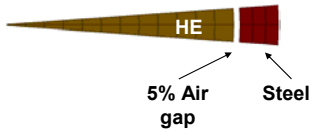
- Good models for gap behavior are needed to obtain accurate strain/pressure results at ignition
- An inadequate gap model leads to large model strains and pressures at ignition
- Accurate gap model can help predict the thermal explosion violence
- Several combinations of ALE3D approaches are developed for modeling dynamic gaps in slow processes

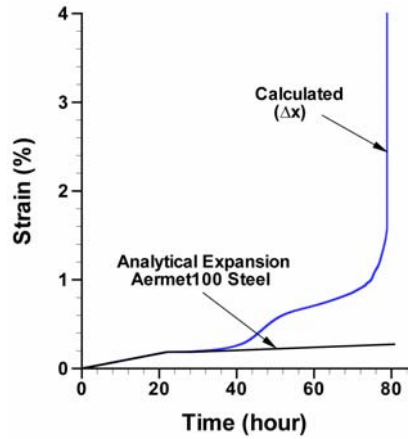
	Mixed elements (HE, Case)	Sliding interface (HE, Case)
Explicit hydro	Mass scaling Soft materials Robustness Oscillatory strain results	Mass scaling Soft materials Robustness Oscillatory strain results
Implicit hydro	No oscillation Larger Δt Work in progress – soft materials	No oscillation Larger Δt Work in progress – soft materials

1D and 2D Results

1D cylindrical test problem is used to assess the accuracy of numerical methods for STEX LX-10

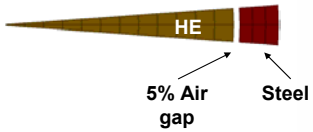
Calculated hoop strain curve is in agreement with pure thermal expansion of steel until the inner pressure starts to build up.

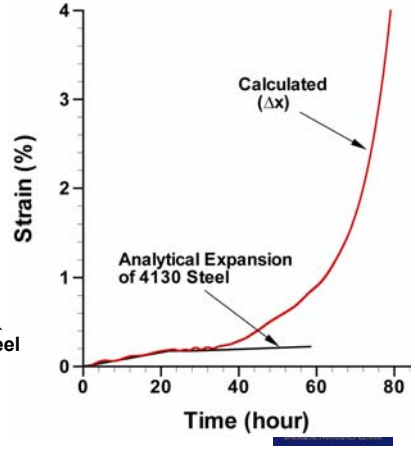




1D cylindrical test problem is used to assess the accuracy of numerical methods for STEX LX-04

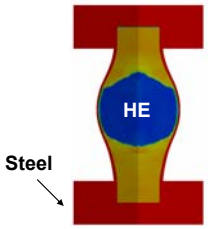
Calculated hoop strain curve is in agreement with pure thermal expansion of steel until the inner pressure starts to build up.

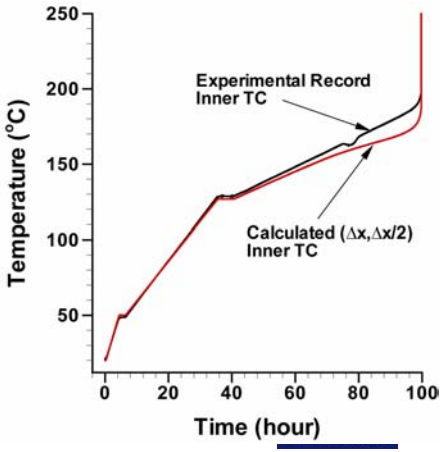




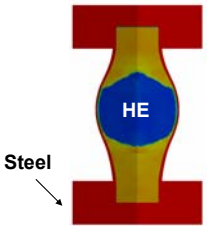
2D STEX simulation is compared against the LX-04 measurements (TE-029, 2001)

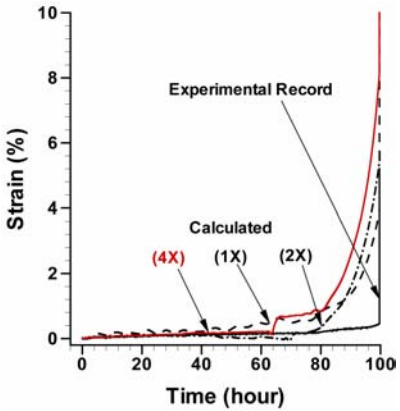
As shown in the internal TC comparison, the time-to-explosion is accurately calculated.





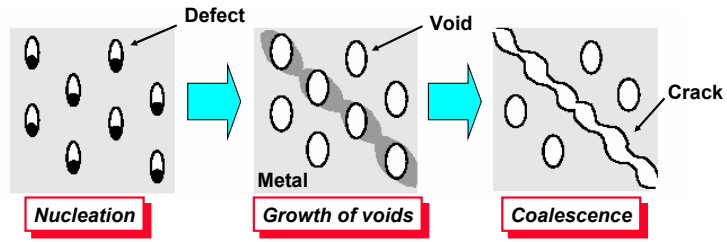
Calculated 2D strain curves are plotted against STEX hoop strain (slowscan) data for LX-04





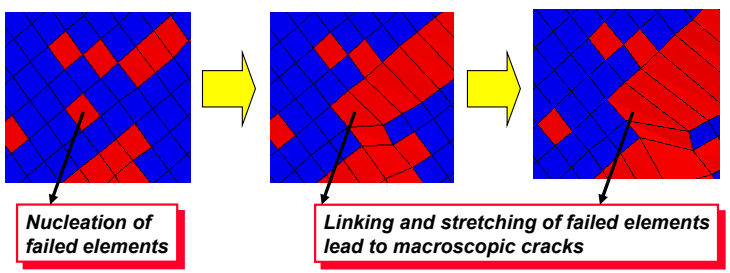
3D Thermal explosion violence and fragmentation simulation

Microscopic event leads to macroscopic crack or fracture formation in metals



- Voids are formed around inclusions, defects, or impurities in metals
- Voids' radius increases due to tensile stress and plastic strain
- Voids linking occurs and ultimately forms macroscopic cracks (*See Anderson 1995*)

Mechanism of metal fracture based on the computational failure model of Johnson and Cook (1985)



$$D = \Sigma \frac{\Delta\varepsilon}{\Delta\varepsilon_f}$$ Accumulated damage to an element

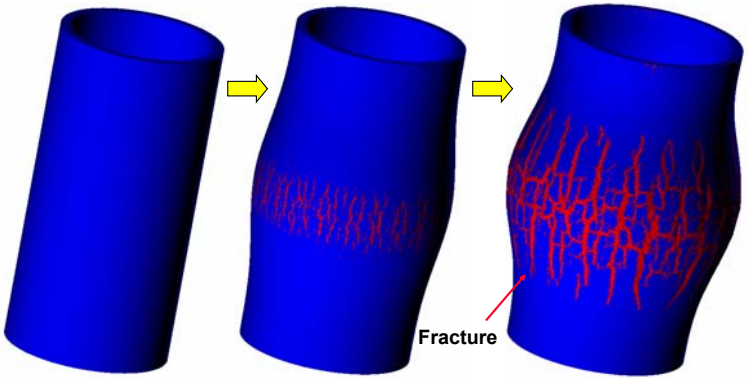
$$\varepsilon_f = D_1 + D_2 \exp D_3 \left(\frac{-p}{\sigma_v}\right)$$ Empirical rule proposed by Hancock & McKenzie (1976), modified by Springer, Becker, Couch (2002)

Material coefficients for steel in our Johnson-Cook (JC) Failure Strain Model

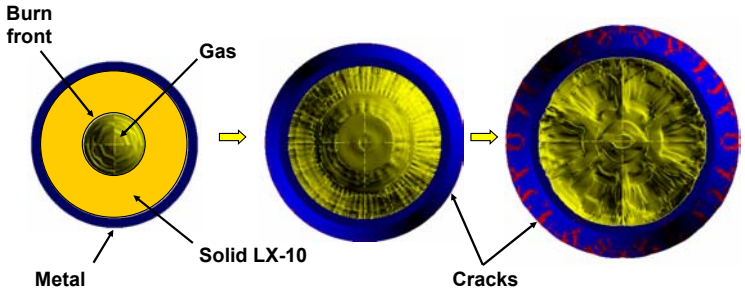
	AerMet® 100 Steel JC Failure Coefficients
D_1	0.1 with 20% standard deviation (see Springer, Becker, Couch, *2003)*
D_2	0.156 (Chhabildas *et al. 2001)*
D_3	0.296 (Chhabildas *et al. 2001)*

Center loaded spherical deflagration exerts tensile stress on outer layer causing the pipe to fracture (1 million zones, $\Delta x = 250\ \mu m$)

AerMet 100 steel tube: 3 mm thick X 2 in. OD X 4 in. L

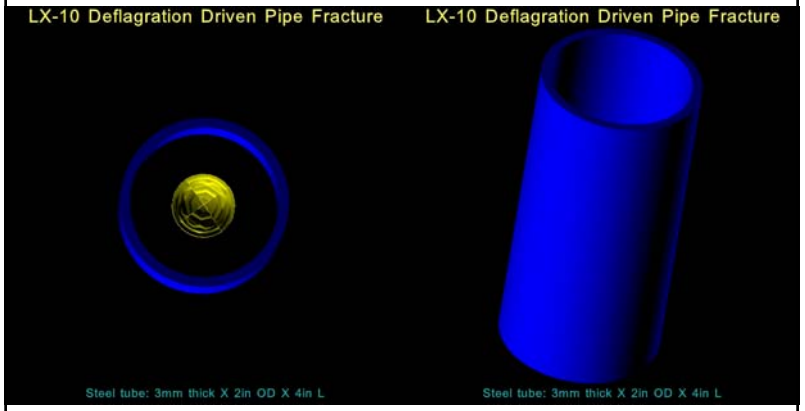


Center loaded spherical deflagration exerts tensile stress on outer layer causing the pipe to fracture (1 million zones, $\Delta x = 250\ \mu m$)



Top down view shows deflagration spread

3D animations of deflagrating LX-10 show fracturing steel pipe during explosion (1 million zones, $\Delta x = 250\ \mu m$)



Summary – towards a predictive thermal explosion model for energetic materials

- I have talked about...
  - ✓ multi-physics nature of HE thermal explosion
  - ✓ needs for building capability to assess munitions sensitivity (subject to a thermal insult such as fires)
  - ✓ modeling and simulation methodology for HE thermal explosion of HMX-based explosives (LX-10, LX-04)
  - ✓ STEX experiment is in progress to measure fragmentation of AerMet100 steel tube containing LX-10

Summary – continued

Here are some forthcoming articles in the open literature:

J. J. Yoh, M. A. McClelland, J. L. Maienschein, and J. F. Wardell,
"Towards a predictive thermal explosion model for energetic materials," Journal of Computer-Aided Materials Design, June 2004

J. J. Yoh, M. A. McClelland, and C. M. Tarver,
"Simulating thermal explosion of RDX-based explosives: Model validation and comparison with experiment," submitted to Journal of Applied Physics, September 2004

J. J. Yoh, M. A. McClelland, J. L. Maienschein, H. K. Springer, and R. C. Becker,
"Computer modeling and measurement of metal fragmentation in thermal explosion experiment," in preparation, November 2004