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Validation Experiments for Modeling Slow Cook-off

Harold W. Sandusky and G. Paul Chambers
NAVSEA Indian Head Division, Maryland
&
William W. Erikson and Robert G. Schmitt
Sandia National Laboratory, New Mexico

NAVSEA INDIAN HEAD
Surface Warfare Center Division

Sandia National Laboratories

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Objective

Demonstrate estimation of time to slow cook-off and violence of reaction with DOE codes

Technical Challenges

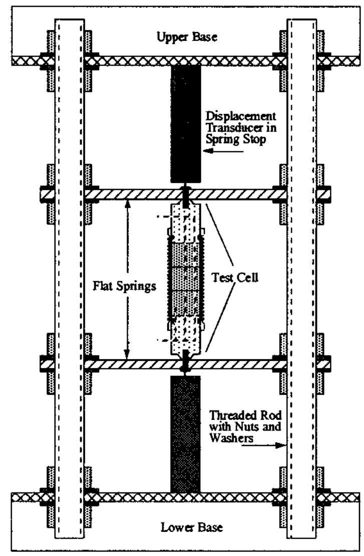
Design and implementation of well instrumented experiments against which modelers can compare their predictions

Characterization of properties and reaction of heated materials

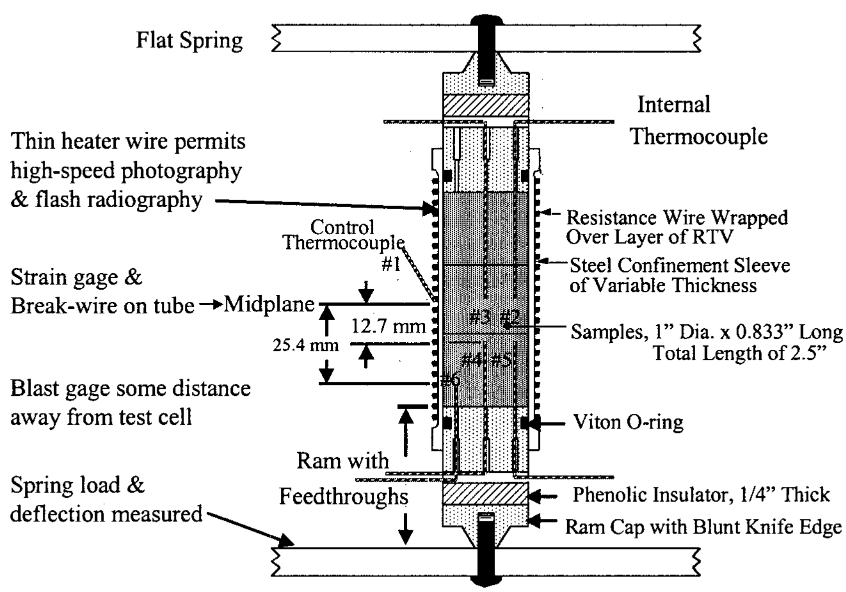
Modeling fragmentation from deflagrations & explosions

Experimental Apparatus

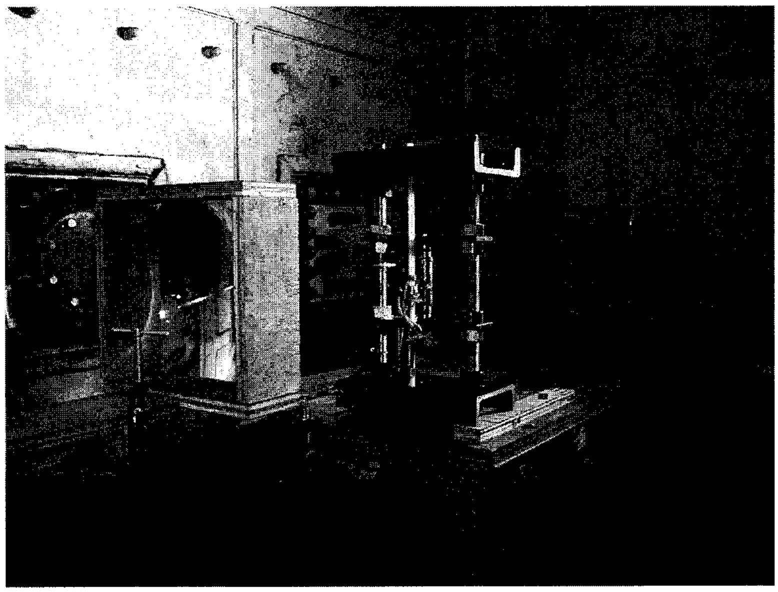
- Test cell mounted between flat springs in load cell
- Springs allow axial expansion of test cell
  - Reduces internal pressure so that seals are not breached without including ullage
  - Displacement transducer on each spring provides means of continually measuring sample expansion
- Clear field of view for test cell for high-speed photography and flash radiography



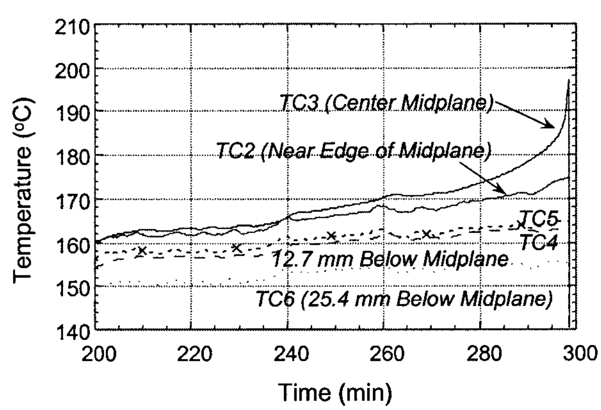
Test Cell with Insulated Rams



Firing Chamber Arrangement, Shot CV-2

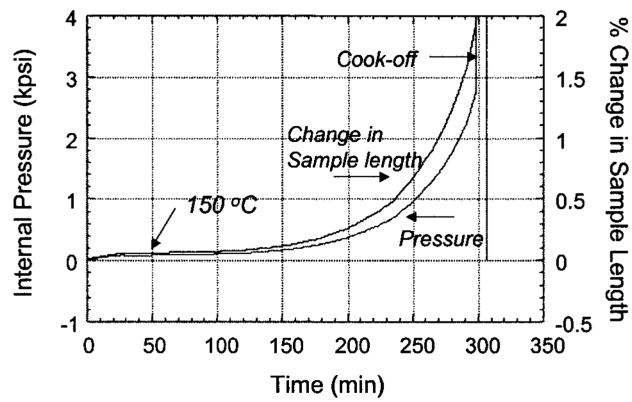


Late-Time Internal Temperatures, PBXN-109 Shot CV-2



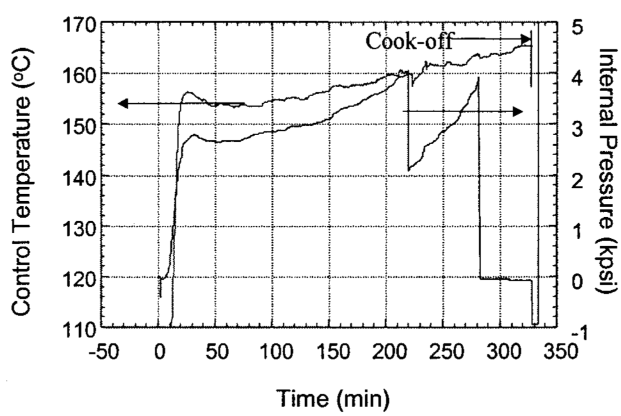
Uniform midplane temperatures until 1 hr before cook-off
Onset of thermal run-away begins between 160 and 165°C
No self-heating at off-axis on midplane nor 12.7 mm below midplane
At cook-off, on-axis midplane temperature ~25 °C higher than near edge
Thermal run-away occurs in a zone with a radius less than 10 mm

Internal Pressure and Change in Sample Length from Spring Displacement with ~3.6% Ullage, Shot CV-2



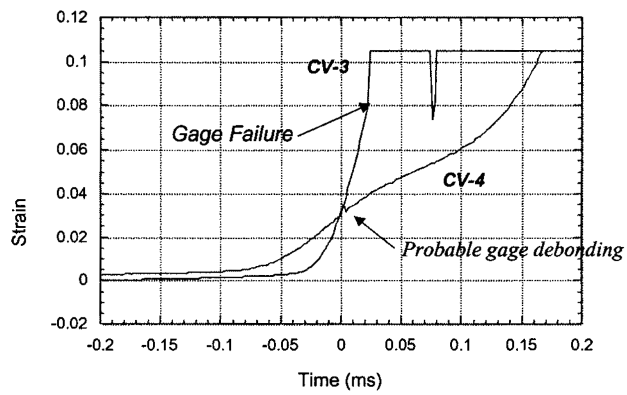
No thermal expansion beyond original ullage
Entire response from thermal damage and pyrolysis

Internal Pressure and Control Temperature with Minimal (~1%) Ullage, PBXN-109 Shot CV-3



Thermal expansion observed
Loss of sealing resulted in more violent reaction
Corrected sealing in Shot CV-4 achieved 500 MPa (7 kpsi) at cook-off and resulted in mild reaction as in Shot CV-2

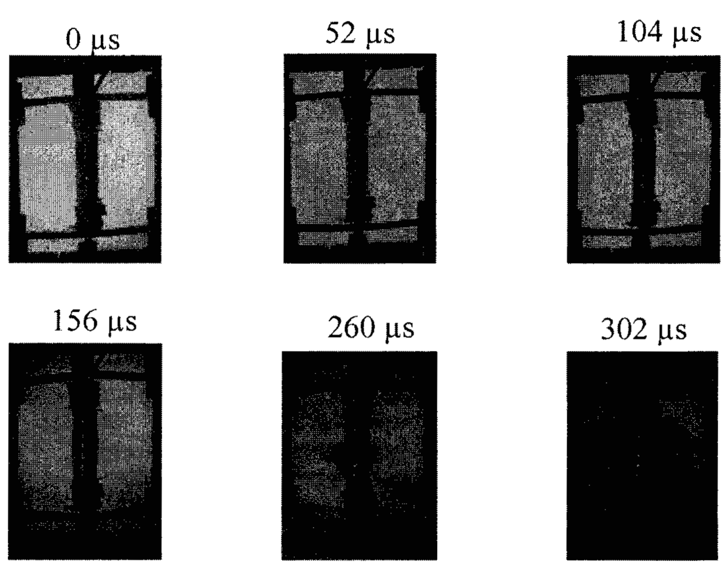
Mid-Plane Tube Strain During Cook-off in PBXN-109 (Shot CV-3 with loss of sealing versus Shot CV-4)



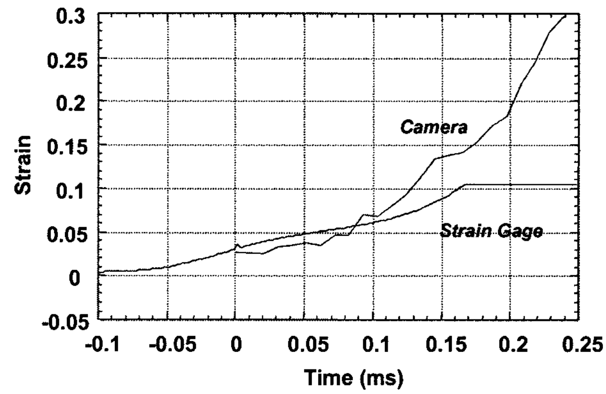
High-elongation strain gages achieved up to 10% strain

Strain rate, which is related to fragmentation, was the basis of comparison for reaction violence in the model

Shot CV-4 Camera Images During Cook-off

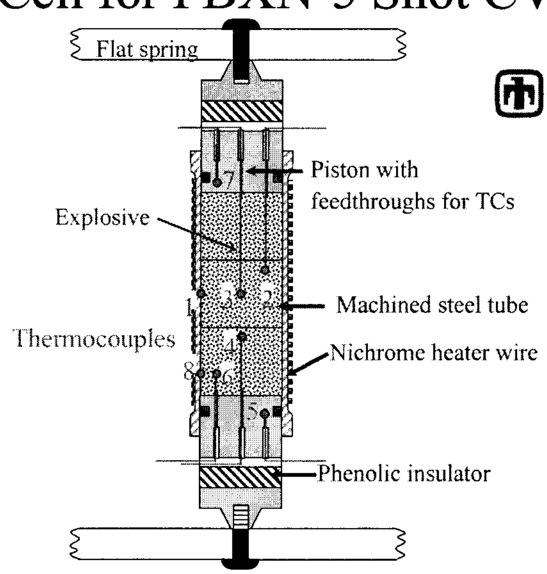


Shot CV-4 Tube Strain During Cook-off
Camera versus Strain Gage



Camera viewed tube expansion to 30%, which was the time of rupture, with no gas leakage from ends

Test Cell for PBXN-5 Shot CV-5



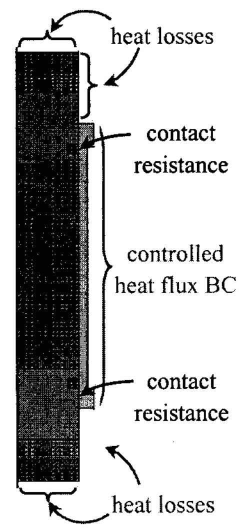
Finite Element Model of NSWC Apparatus

Geometry & BC's

- 2D-axisymmetric representation, top-to-bottom symmetry not imposed
- controlled flux boundary
- losses at ends
- piston-sleeve contact resistance
- adjusted losses & contact resistances to match measured external temperatures

Energetic Material Model

- PBXN-5 is similar to LX-10 (nominally 95% HMX, 5% Viton)
- LX-10 (Tarver-McGuire) chemistry model and properties was used.



Reaction Mechanism for PBXN-5

PBXN-5 has nominally same composition as LX-10 (95% HMX, 5% Viton)

The McGuire-Tarver (7th Det. Symposium) 3-step decomposition mechanism (fit to LX-10 data) was applied to PBXN-5 as well.

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C \xrightarrow{k_3} D$$

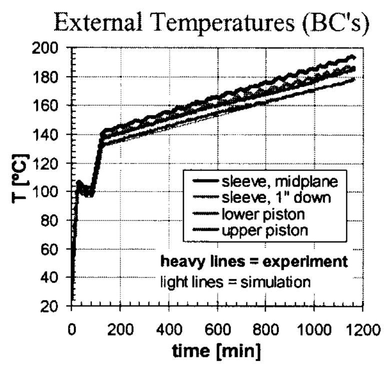
Reaction Parameters

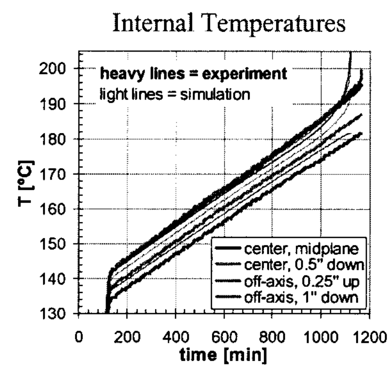
reaction step	heat release (cal/g)	ln A (1/s)	Ea (kcal/mol)
A→B	-100 (endo)	48.7	52.7
B→C	300 (exo)	37.5	44.1
C→D*	1200 (exo)	28.1	34.2

* second order in 'C'

NSWC Test CV-5

PBXN-5 Explosive





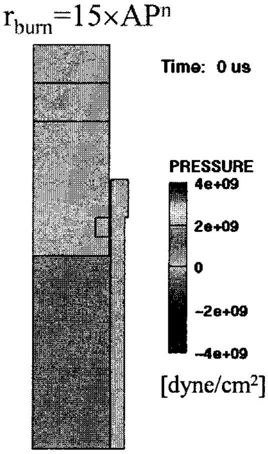
- Time to event: Experiment: 1164.3 min Simulation: 1122.7 min
- Predicted ignition location at centerline at 0.19" above midplane
- No endotherm evident in temperature traces.

Post-Ignition Burn Simulations

NSWC CV-4 Test

- 2-D simulation, *Alegra* code
- flame sheet combustion model (enhanced AP^n burn law)
- used same models as simulations of NAWC tests with PBXN-109 (elastic-plastic, Mie Gruniesen models for unreacted PBXN-109, Noble-Abel Gas EOS for reaction products)
- mild steel tube (not attached to piston)
- elastic-plastic model for steel
- spring compliance modeled by replacing part of piston with low modulus material

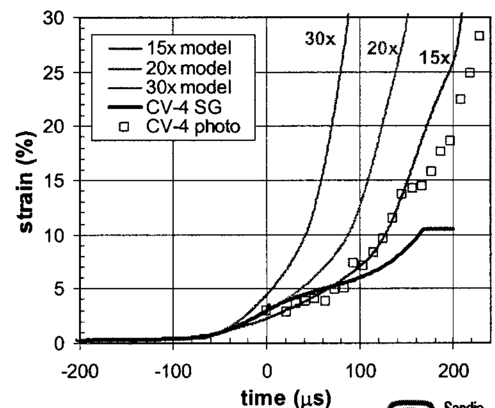
$r_{burn}=15\times AP^n$



Post-Ignition Burn Simulations
PBXN-109 Shot CV-4

- strain gages & high speed photography used for strain measurements
- strain gage debonds during test (t ≈ 80μs)
- gas first observed at about 30% wall strain
- ~15× AP^n enhancement factor fit wall strain data best to high strains (c.f. 30× best fit for NAWC to 1.5% strain)

Wall Strain During Cook-off



Summary

- Simultaneous mechanical and thermal measurements and calculations during slow cook-off
- PBXN-109:
  - Cook-off violence similar to that in other small- and full-scale tests & insensitive to conditions
  - Significant pressure from thermal expansion when ullage is essentially eliminated
  - Onset of pressure buildup from thermal damage and pyrolysis starts ~3 hr before cook-off at ~150°C
  - Self-heating on-axis in a small, <10 mm zone, starting ~1 hr before cook-off at 160 to 165°C
  - Reaction rate declines beyond zone of thermal run-away as front propagates into cooler explosive with less thermal damage

Summary, Continued

- PBXN-5:
  - Cook-off violence similar to larger experiments on nearly identical composition, LX-10, but dissimilar to VCCT
  - Sample expansion dominated by phase change
  - Little pressure buildup and self-heating before cook-off
  - Onset of reaction not at midplane, possibly influenced by holes for thermocouples
- Fragmentation proportional to strain rate, which is related to cook-off reaction rate