Model Formulation and Predictions for a Pyrotechnically Actuated Pin Puller

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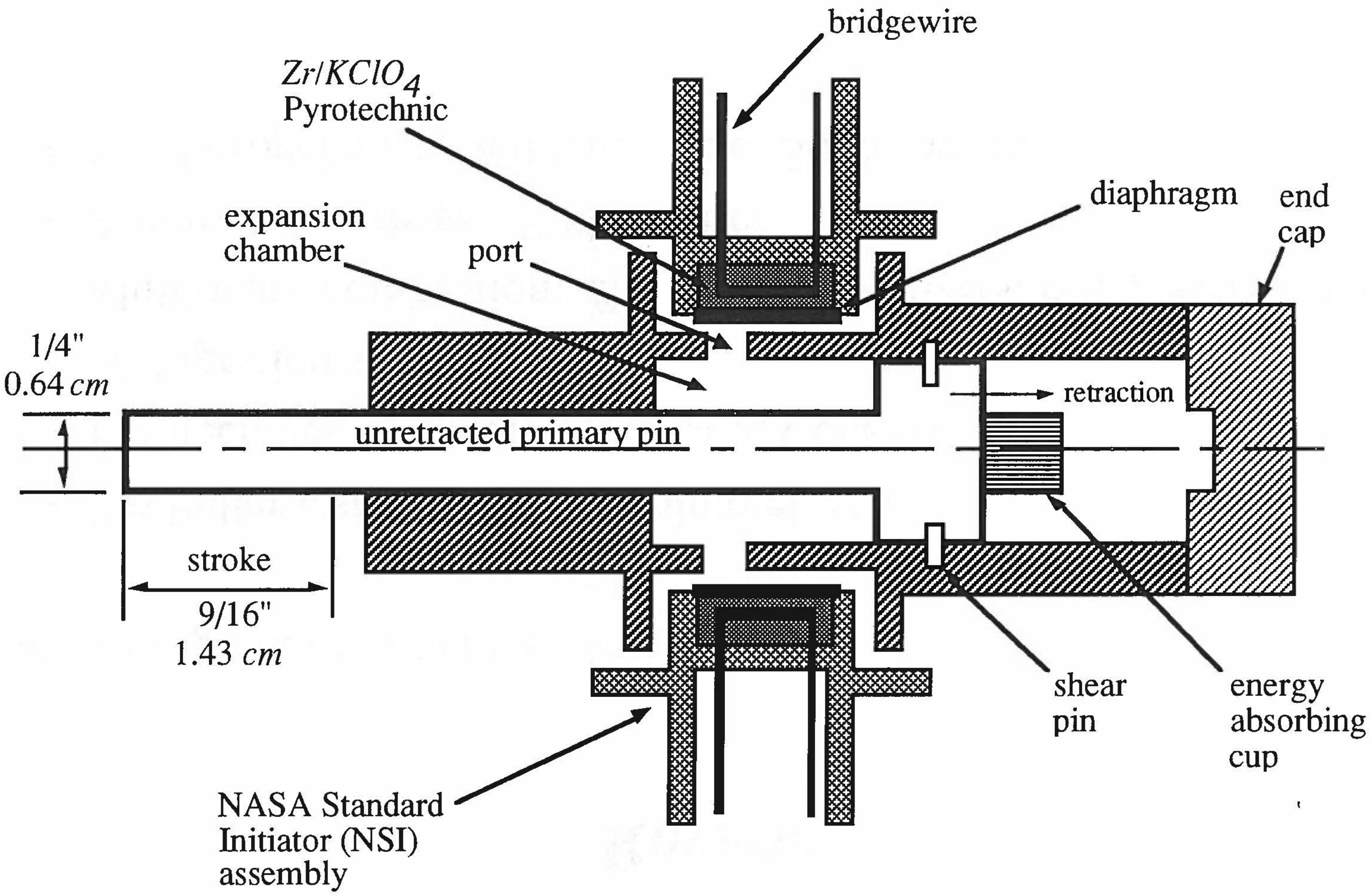
Pyrotechnically Actuated Pin Puller



Review

Sources for guidance in model development:

- Pin Puller tests: Bement, Schimmel, *et al.*
- Pyrotechnics Chemistry: McLain, Conklin
- NSI ignition study: Varghese
- Multiphase combustion: Krier, Butler, Powers, Baer, Nunziato, etc.
- Automobile airbags: Butler, Krier
- Solid Propellants: Williams, Kuo, Strehlow, etc.

Engineering Problems

- Operational failures.
- Qualification after many tests.
- Difficult to predict behavior of new formulations.
- Difficult to quantify effects of modifications:
    - diffusive processes,
    - pin puller geometry,
    - friction.

Modeling Approaches

- Full Scale Models:
  - time dependent,
  - 3-D spatial gradients,
  - multiple species,
  - fully resolved chemical kinetics,
  - compressibility,
  - turbulence,
  - real gas effects,
  - *limited kinetic data available*,
  - *more complex than justified by data.*

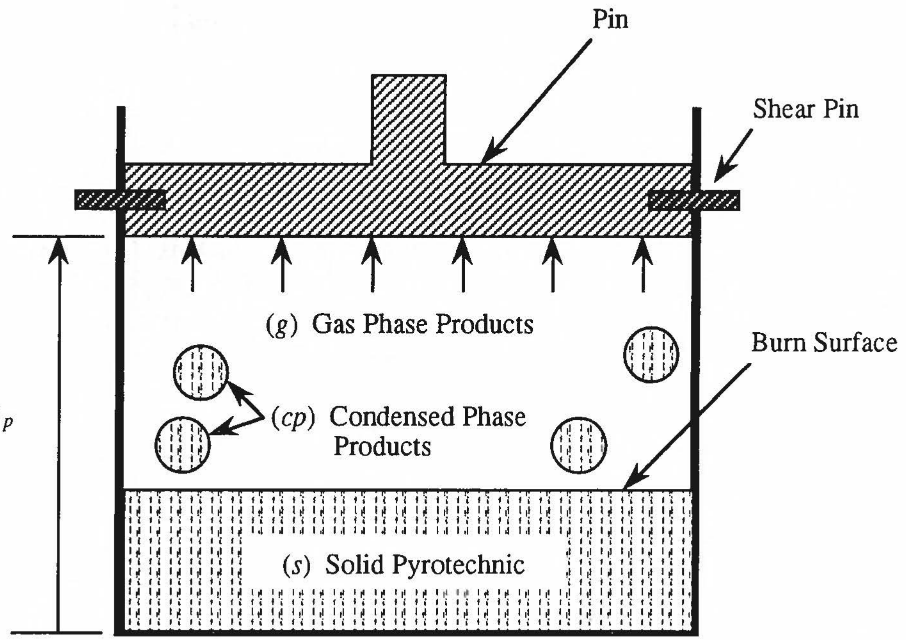
Modeling Approaches (continued)

- Empirical Models:
  - experimentally-based correlations,
  - somewhat inflexible.

- Simple Models - *present approach:*
  - analytically tractable,
  - introduction of *ad hoc* assumptions.

- Stochastic Models:
  - estimates for uncertainty required,
  - could be coupled with simple model.

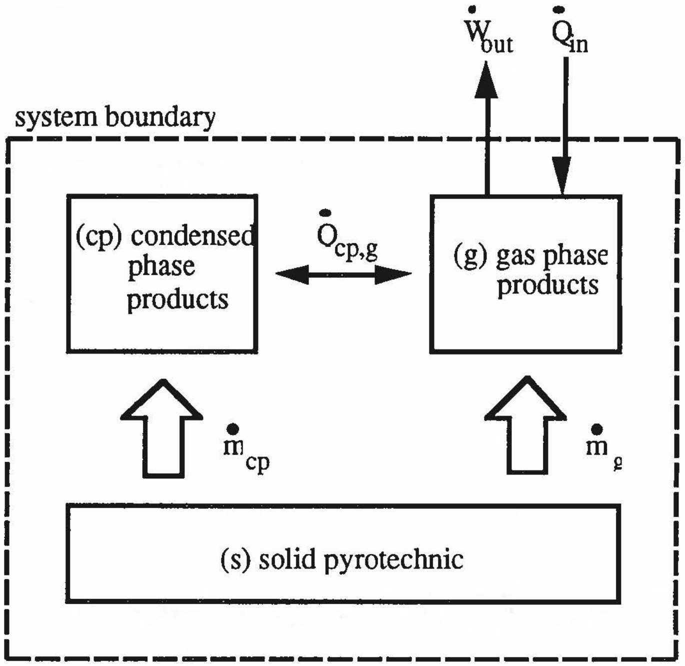
Model Assumptions



Fundamental Assumptions

- <u>Well-stirred reactor</u>:
  - no spatial variations,
  - time-dependent variables.
- <u>Total system modeled as three subsystems</u>:
  - solid pyrotechnic reactants,
  - condensed phase products,
  - gas phase products.

Model Assumptions (continued)



Mass and Heat Transfer

- No mass exchange between total system and surroundings.
- Mass exchange from reactants to products.
- Heat and work exchange between gas phase subsystem and surroundings.
- Heat exchange between product subsystems.
- No work exchange between subsystems.

Model Assumptions (continued)

Combustion Process

- Combustion products produced in ratios which <u>minimize the Gibbs free energy</u>:
  - constant mass fractions.
- Ideal gas.
- Gas has temperature dependent specific heat.

Model Assumptions (continued)

Remaining Assumptions

- Vessel's wall temperature is constant.
- Solid pyrotechnic has constant density.
- Condensed phase products have constant density.
- Total kinetic energy of system is negligible.
- Body forces are negligible .

Non-Dimensional Governing Equations

mass evolution:

$$\frac{d}{dt}\left[\rho_s V_s\right] = -\rho_s r, \qquad \frac{d}{dt}\left[\rho_g V_g\right] = \left(1-\eta_{cp}\right)\rho_s r, \qquad \frac{d}{dt}\left[\rho_{cp} V_{cp}\right] = \eta_{cp}\rho_s r,$$

energy evolution:

$$\frac{d}{dt}\left[\rho_s V_s e_s\right] = -\rho_s e_s r, \qquad \frac{d}{dt}\left[\rho_{cp} V_{cp} e_{cp}\right] = \eta_{cp}\rho_s e_s r - \dot{Q}_{cp,g},$$

$$\frac{d}{dt}\left[\rho_g V_g e_g\right] = \left(1-\eta_{cp}\right)\rho_s e_s r + \dot{Q}_{in} + \dot{Q}_{cp,g} - \dot{W}_{out}.$$

Newton's Law of Motion:

$$\frac{d^2}{dt^2}\left[z_p\right] = \left[\frac{\tilde{F}_c}{\tilde{m}_p \tilde{V}_c^{1/3} / \tilde{t}_c^{\,2}}\right] F_p.$$

Scaling used in Non-Dimensionalization

- Thermodynamic variables and time are *O(1)* quantities at completion of the combustion process.

$$\tilde{V}_c = \tilde{V}_{so}, \qquad \tilde{\rho}_c = \left(1-\eta_{cp}\right)\left(\frac{\tilde{V}_{so}}{\tilde{V}_o}\right)\tilde{\rho}_s, \qquad \tilde{T}_c = \tilde{T}_{ad},$$

$$\tilde{e}_c = \tilde{e}_{so}, \qquad \tilde{P}_c = \tilde{\rho}_c \tilde{R} \tilde{T}_c, \qquad \tilde{F}_c = \tilde{A}_p \tilde{P}_c,$$

$$\tilde{r}_c = \tilde{b}\,\tilde{P}_c^{\,n}, \qquad \tilde{t}_c = \frac{\tilde{V}_c}{\tilde{A}_p \tilde{r}_c}$$

Geometrical and Constitutive Relations

A. Geometry

- Total Volume: $V = V_s + V_{cp} + V_g$
- Pin Position: $z_p = \left(\frac{\tilde{V}_c^{2/3}}{\tilde{A}_p} \right) V$

B. Combustion Model

- Irreversible reaction: $\sum_{i=1}^{N_s} \upsilon_{s_i} X_{s_i} \longrightarrow \sum_{i=1}^{N_{cp}} \upsilon_{cp_i} X_{cp_i} + \sum_{i=1}^{N_g} \upsilon_{g_i} X_{g_i}$
- Pyrotechnic burn rate: $r = r(P_g) = P_g^n$

Geometrical and Constitutive Relations (continued)

C. Thermal Equation of State: $P_g = \rho_g T_g$

D. Caloric Equations of State:

$$e_s(T_s) = \sum_{i=1}^{N_s} Y_{s_i} e_{s_i}(T_s), \quad e_{cp}(T_{cp}) = \sum_{i=1}^{N_{cp}} Y_{cp_i} e_{cp_i}(T_{cp}), \quad e_g(T_g) = \sum_{i=1}^{N_g} Y_{g_i} e_{g_i}(T_g)$$

E. Constant Volume Specific Heats:

$$c_{v_s}(T_s) = \sum_{i=1}^{N_s} Y_{s_i} \frac{d}{dT_s}\left[e_{s_i}(T_s)\right], \qquad c_{v_{cp}}(T_{cp}) = \sum_{i=1}^{N_{cp}} Y_{cp_i} \frac{d}{dT_{cp}}\left[e_{cp_i}(T_{cp})\right],$$

$$c_{v_g}(T_g) = \sum_{i=1}^{N_g} Y_{g_i} \frac{d}{dT_g}\left[e_{g_i}(T_g)\right]$$

Geometrical and Constitutive Relations (continued)

F. <u>Heat Transfer Models</u>

- Gas phase products - Condensed phase products:

$$\dot{Q}_{cp,g} = \dot{Q}_{cp}\left(T_{cp}, T_{g}\right) = \left[\frac{\tilde{h}_{cp,g}\tilde{T}_{c}}{\tilde{\rho}_{c}\tilde{A}_{p}\tilde{r}_{c}\tilde{e}_{c}}\right]\left(T_{cp} - T_{g}\right)$$

- Gas phase products - surroundings:

$$\dot{Q}_{in} = \dot{Q}_{in}\left(T_{g}\right) = \left[\frac{\tilde{h}\tilde{V}_{c}^{2/3}\tilde{T}_{c}}{\tilde{\rho}_{c}\tilde{A}_{p}\tilde{r}_{c}\tilde{e}_{c}}\right]A_{w}\left(T_{w} - T_{g}\right) + \left[\frac{\tilde{\sigma}\tilde{V}_{c}^{2/3}\tilde{T}_{c}^{4}}{\tilde{\rho}_{c}\tilde{A}_{p}\tilde{r}_{c}\tilde{e}_{c}}\right]A_{w}\left(\alpha T_{w}^{4} - \varepsilon T_{g}^{4}\right)$$

Geometrical and Constitutive Relations (continued)

G. Rate of work done by gas phase products in moving pin:

$$\dot{W}_{out} = \left[\frac{\tilde{P}_c}{\tilde{\rho}_c \tilde{e}_c}\right] P_g \frac{dV}{dt}$$

F. Force acting on the pin:

$$F_p = \begin{cases} 0 \text{ if } P_g < F_{crit} \\ P_g \text{ if } P_g \geq F_{crit} \end{cases}$$

- F_{crit}, critical force necessary for shear pin failure,
- work done in shearing the pin is not accounted for.

Final Form of Model Equations

$$\frac{dV}{dt}=\left[\frac{\tilde{P}_c\,\tilde{V}_c}{\tilde{m}_p\,\tilde{r}_c^2}\right]\dot{V},$$

$$\frac{dV_s}{dt}=-r\left(V,V_s,V_{cp},T_g\right),$$

$$\frac{dV_{cp}}{dt}=\eta_{cp}\left(\frac{\rho_s}{\rho_{cp}}\right)r\left(V,V_s,V_{cp},T_g\right),$$

$$\frac{dT_{cp}}{dt}=\frac{\eta_{cp}\,\rho_s\,r\left(V,V_s,V_{cp},T_g\right)\left(e_{so}-e_{cp}\left(T_{cp}\right)\right)-\dot{Q}_{cp,g}\left(T_{cp},T_g\right)}{\rho_{cp}\,V_{cp}\,c_{v_{cp}}\left(T_{cp}\right)},$$

$$\frac{dT_g}{dt}=\frac{(1-\eta_{cp})\rho_s\,r\left(V,V_s,V_{cp},T_g\right)\left(e_{so}-e_g\left(T_g\right)\right)+\dot{Q}_{cp,g}\left(T_{cp},T_g\right)+\dot{Q}_{in}\left(T_g\right)-\kappa P_g\left(V,V_s,V_{cp},T_g\right)\dot{V}}{\rho_g(V,V_s,V_{cp})\left(V-V_s-V_{cp}\right)c_{v_g}\left(T_g\right)},$$

$$\frac{d\dot{V}}{dt}=F_p\left(V,V_s,V_{cp},T_g\right).$$

Initial Conditions:

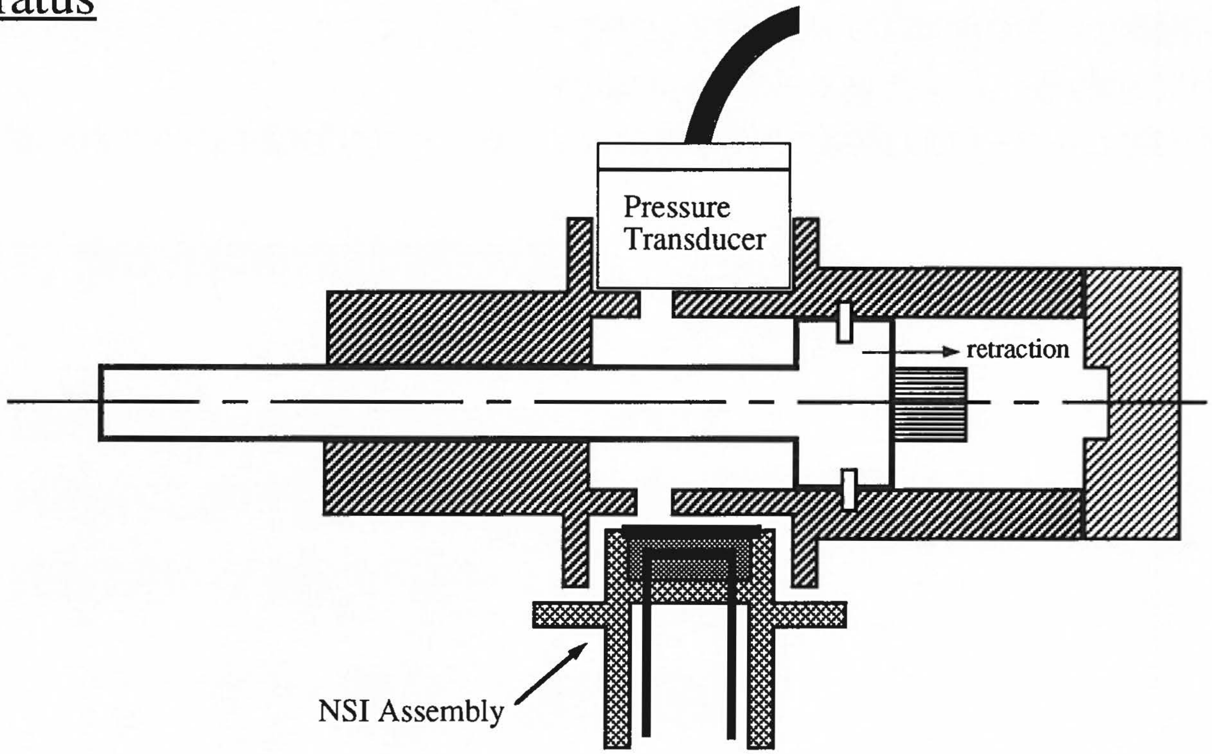
$$V(t=0)=V_o,\quad V_s(t=0)=V_{so},\quad V_{cp}(t=0)=V_{cpo},$$

$$T_{cp}(t=0)=T_o,\quad T_g(t=0)=T_o,\quad \dot{V}(t=0)=0.$$

Experimental

- Tests conducted by Mr. Laurence J. Bement
- NASA Langley Research Center, Hampton, Virginia, USA

Apparatus



Results

- NSI Driven Pin Puller
- 10 cm^3 Closed Bomb Combustion of NSI
- NSI Driven Dynamic Test Device

Balanced Stoichiometric Equation:

$$\begin{aligned} 3.7735\,Zr(s) + 2.6917\,KClO_4(s) \longrightarrow\ & 3.1563\,Zr(cp) + 1.9246\,O(g) + 1.7031\,KCl(g) \\ & + 0.9715\,Cl(g) + 0.8590\,K(g) + 0.6309\,O_2(g) \\ & + 0.5178\,ZrO_2(g) + 0.1220\,KO(g) + 0.0993\,ZrO(g) \\ & + 0.0106\,ClO(g) + 0.0022\,K_2Cl_2(g) + 0.0016\,K_2(g) \\ & + 0.0011\,Cl_2(g) + 0.0001\,Zr(g) \end{aligned}$$

NSI Pyrotechnic Composition:

- 114 *mg* of a $Zr/KClO_4$ mixture:
  - 53.6 *mg* of $Zr\ (s)$,
  - 60.4 *mg* of $KClO_4\ (s)$

Parameters used in pyrotechnic combustion simulations.

parameter	*value*
$\tilde{A}_p$	$0.64^a, 2.0^b, 5.07^c\ cm^2$
$\tilde{\rho}_s$	$3.0\ g/cm^3$
$\tilde{T}_s$	$288.0\ K$
$\tilde{\rho}_{cp}$	$1.5\ g/cm$
$\tilde{h}$	$1.25 \times 10^6\ g/s^3/K$
ε	0.60
α	0.60
$\tilde{h}_{cp,g}$	$3.2 \times 10^{10}\ g\ cm^2/s^3/K$
$\tilde{F}_{crit}$	3.56×10^7 *dyne* (80 *lbf*)
$\tilde{b}$	$0.004\ dyne^{-0.69} cm/s$
n	0.69

(a - pin puller, b - closed bomb, c - Dynamic Test Device)

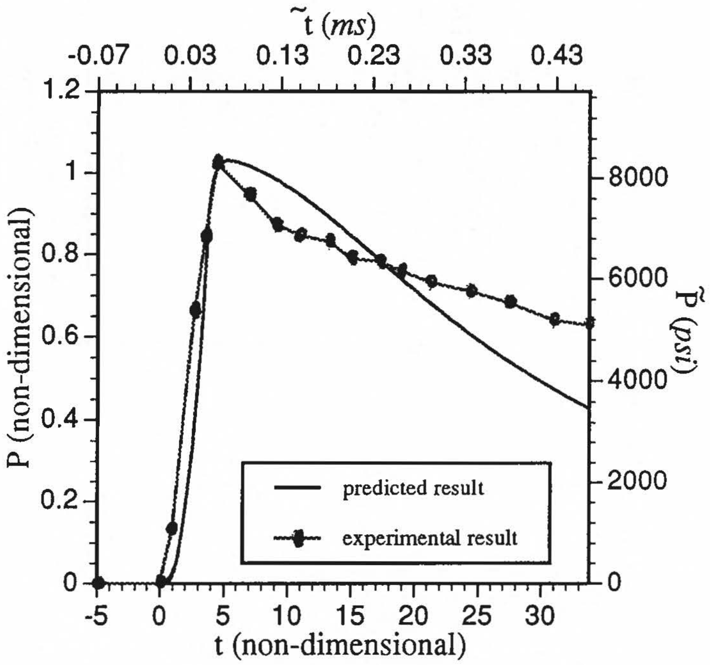
Initial conditions used in pyrotechnic combustion simulations.

initial condition	*value*
V_o	$21.69^a, 263.15^b, 32.59^c$
V_{so}	1.0
V_{cpo}	8.56×10^{-5}
T_o	5.66×10^{-2}
$\dot{V}_o$	0.0

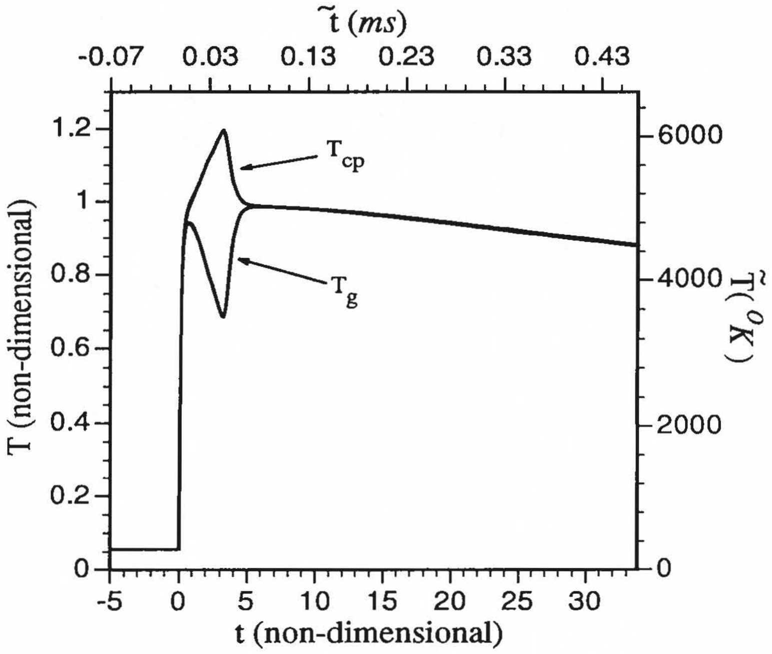
(a - pin puller, b - closed bomb, c - Dynamic Test Device)

Pin Puller Simulation

Pressure Prediction



Temperature Prediction



- Model *correctly* predicts time scales and pressure magnitudes.

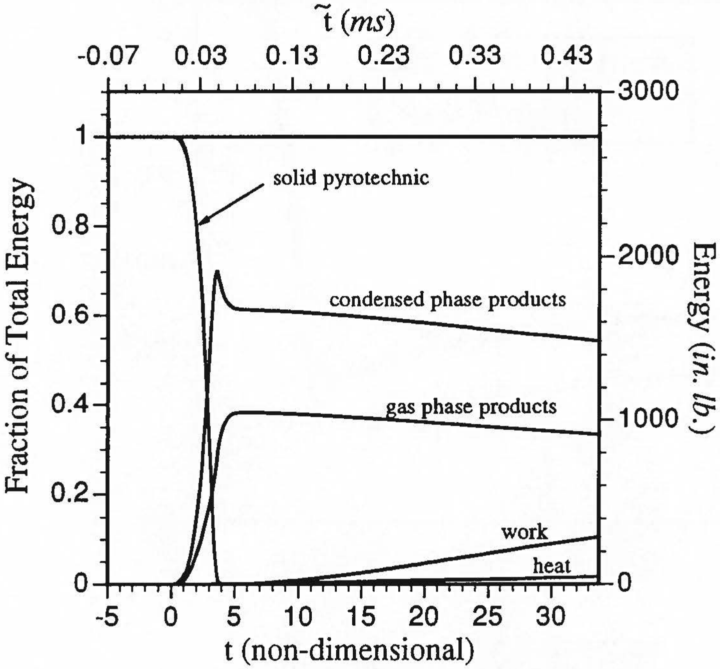
Pin Puller Simulation (continued)

Kinetic Energy of Pin at completion of stroke:

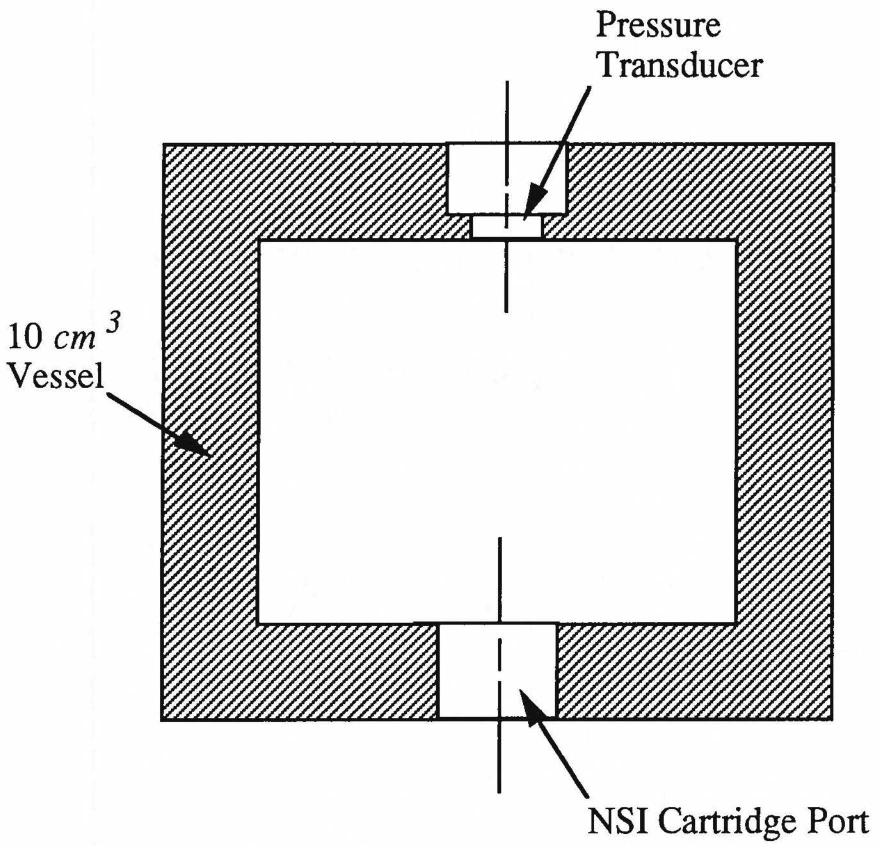
Predicted: 240 *in-lb* [27 *J*]

Experimental: 200 *in-lb* [22.6 *J*]

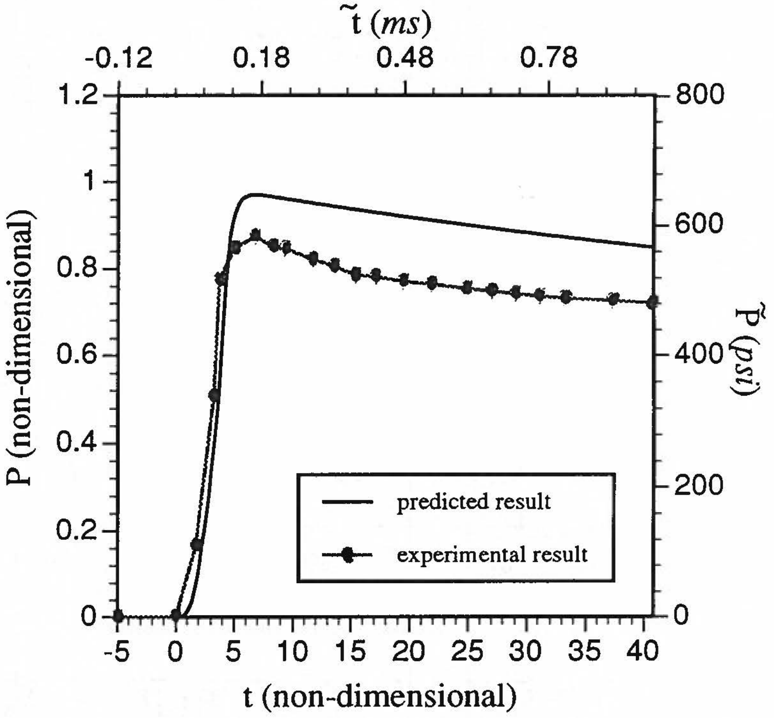
Predicted Energy Distribution



10 cm^3 Closed Bomb Simulation



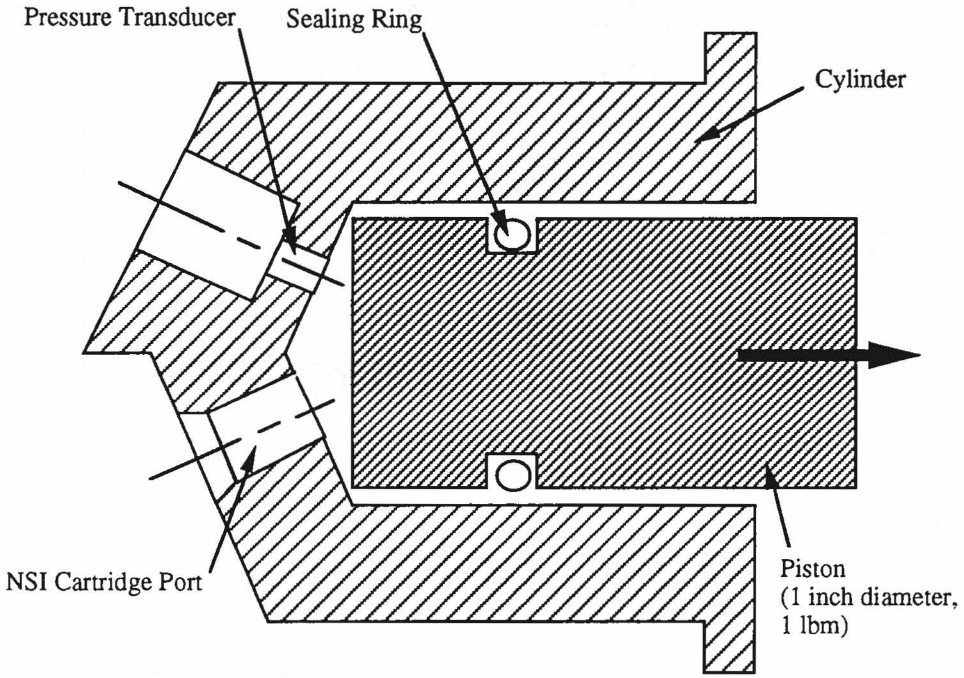
Pressure Prediction

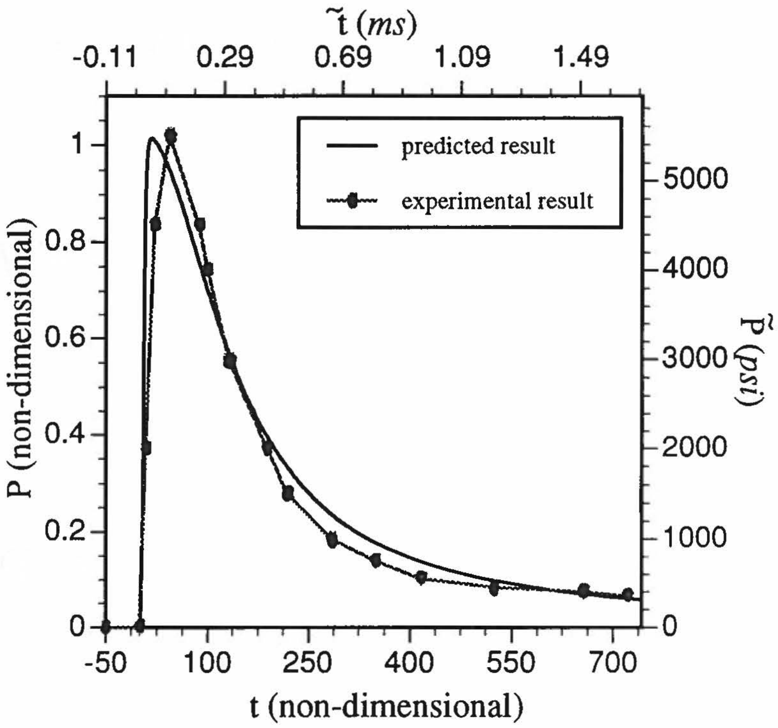


NASA Specification:

- firing of an NSI into a 10 cm^3 bomb shall produce a peak pressure of 650 ± 125 *psi* [4.48 ± 0.86 *MPa*] within 5 *ms*.

Dynamic Test Device Simulation




Pressure Prediction

Average Kinetic Energy of the Piston during the stroke:

- <u>Predicted</u>: 391 *in. lbf* [44.2 *J*]
- <u>Experimental</u>: 258 *in. lbf* [29.2 *J*]

Preliminary Sensitivity Analysis
(Earlier Work)

Objective:

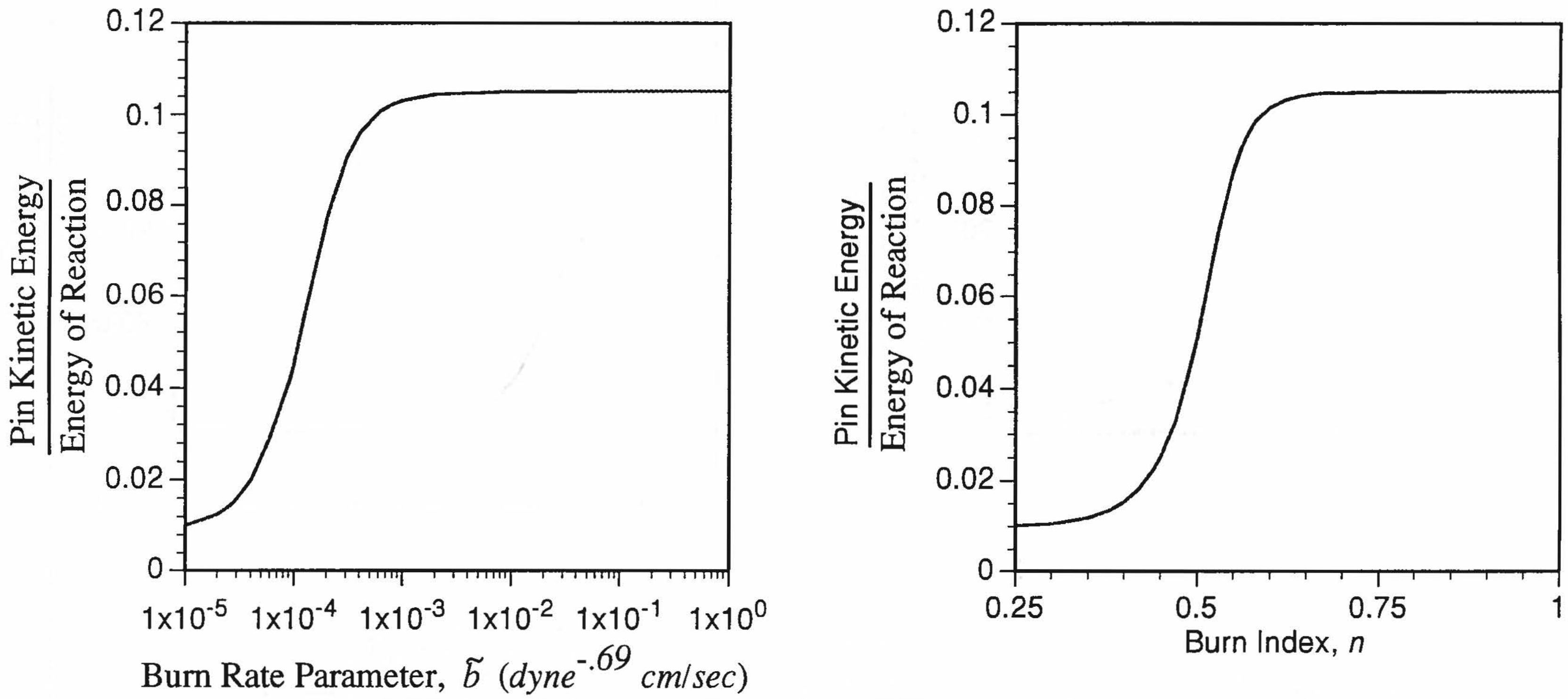
- Study sensitivity of the model to changes in model parameters.

Methodology:

- Model prediction for pin puller - *base solution.*
- Independently change parameters and note the change in the predicted *kinetic energy of pin* at completion of stroke.

Burn Rate Parameters

$$r = P_g^n$$

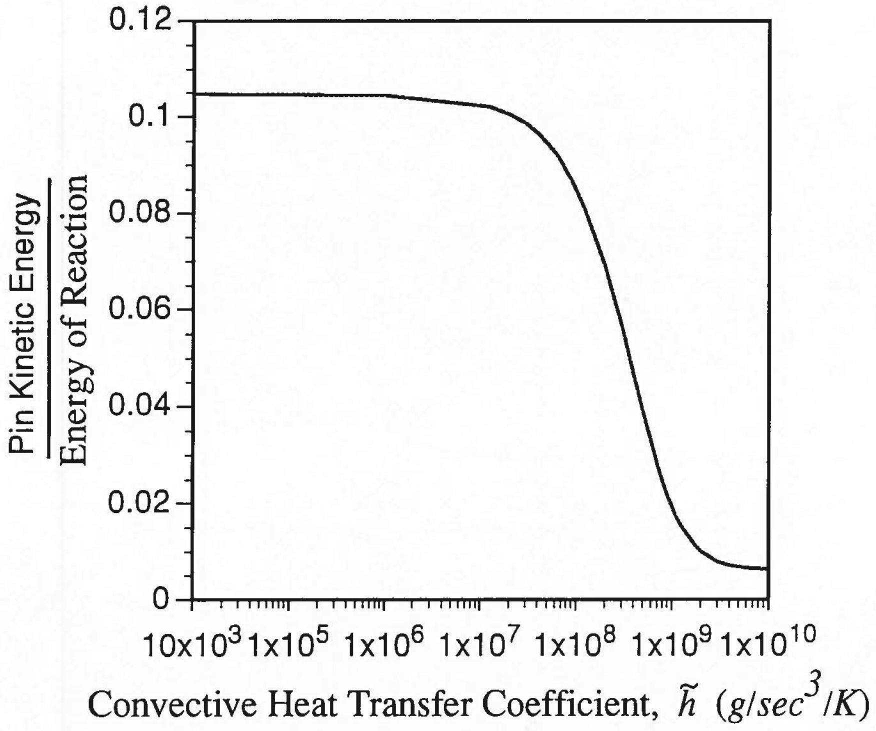


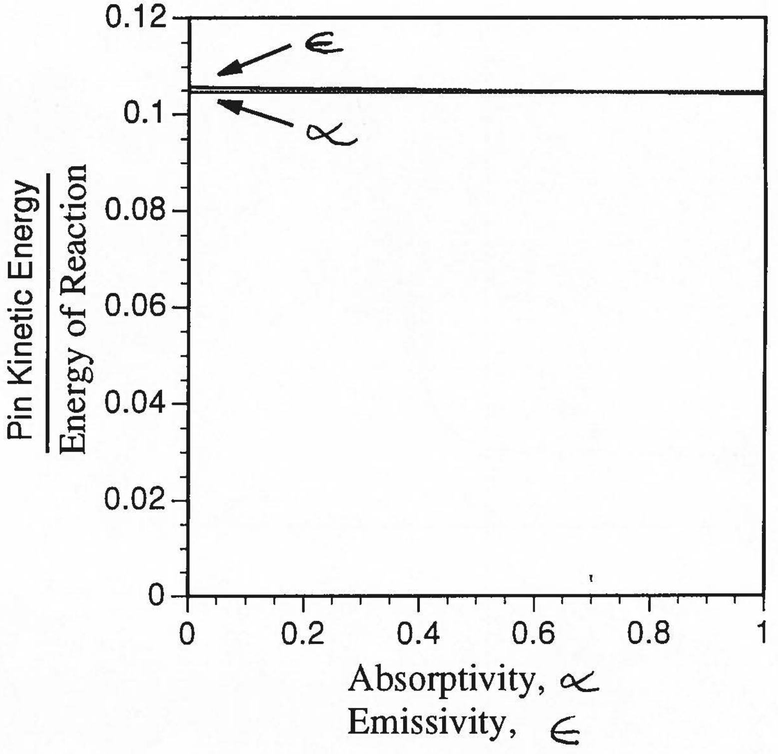
Two distinct regions are identified:

- *slow burning* (burn rate ~ heat transfer to surroundings)
- *fast burning* (burn rate > heat transfer to surroundings)

Heat Transfer Parameters

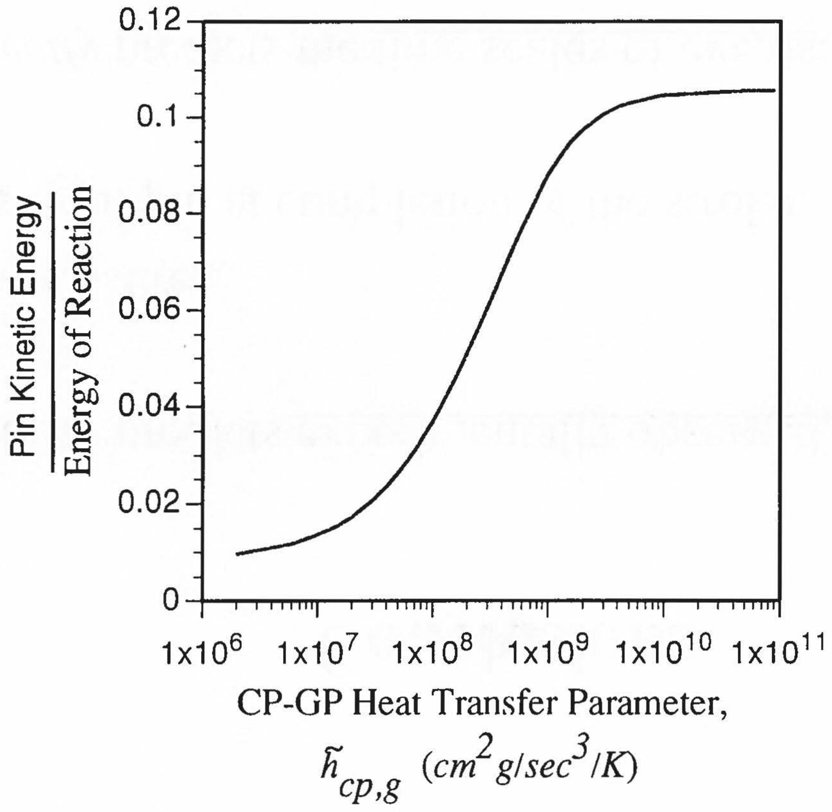
$$\dot{Q}_{in} = \left[\frac{\tilde{h}\,\tilde{V}_c^{2/3}\,\tilde{T}_c}{\tilde{\rho}_c\,\tilde{A}_p\,\tilde{r}_c\,\tilde{e}_c}\right]A_w\left(T_w - T_g\right) + \left[\frac{\tilde{\sigma}\,\tilde{V}_c^{2/3}\,\tilde{T}_c^4}{\tilde{\rho}_c\,\tilde{A}_p\,\tilde{r}_c\,\tilde{e}_c}\right]A_w\left(\alpha T_w^4 - \varepsilon T_g^4\right)$$





Heat Transfer Parameters (continued)

$$\dot{Q}_{cp,g} = \left[\frac{\tilde{h}_{cp,g}\,\tilde{T}_{c}}{\tilde{\rho}_{c}\,\tilde{A}_{p}\,\tilde{r}_{c}\,\tilde{e}_{c}}\right]\left(T_{cp} - T_{g}\right)$$



Conclusions

Model *correctly* predicts experimentally observed features:

- peak pressures,
- velocity of pin at completion of the stroke.

Model *correctly* predicts the time scales of events:

- time to peak pressure,
- time to complete the stroke.

Conclusions
(Sensitivity Study)

Sensitivity analysis suggests <u>increased model potential</u>:

- may not need *detailed* empirical data,
- predicted solution is insensitive to variations in burn rate for *fast burning rates.*

For <u>peak performance</u>:

- fast burning rate,
- low convective heat transfer rate,
- high heat rate from *condensed phase* to *gas phase* products.

Future Work

- Perform analytical studies:
  - examine *simplest possible case* (constant volume, adiabatic, constant specific heats, etc.)
  - study predicted solution near equilibrium states.
- Better justify choice of model parameters:
  - burn rate,
  - heat transfer.
- Continue sensitivity studies:
  - model parameters,
  - initial conditions.
- Include frictional effects.
- Include grain size effects.
- Study other pyrotechnic formulations.
- Study other geometries.