Pyrotechnic Modelling for the NSI Driven Pin Puller

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Review

Sources for guidance in model development:

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

Engineering Problems

- Occurance of operational failures.
- Qualification only after many tests.
- Difficult to predict behavior of new formulations.
- Difficult to quantify effects of modifications:
  - diffusive heat transfer,
  - molecular heat transfer,
  - pin puller geometry,
  - friction,
  - apparently random sample behavior.

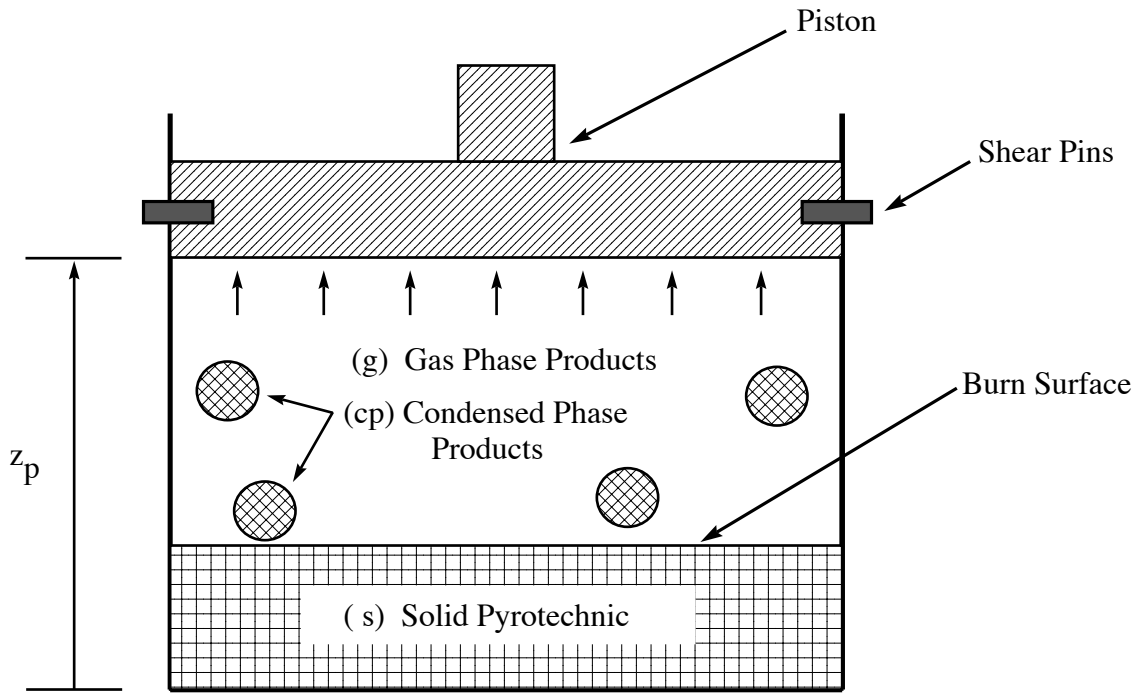
Modeling Approaches

- Full Scale Models:
  - time-dependent,
  - three-dimensional spatial gradients,
  - multiple species, multiple reactions,
  - fully resolved chemical kinetics,
  - compressibility,
  - turbulence,
  - real gas effects,
  - boundary layers,
  - *essentially no detailed kinetic data available*,
  - *more complex than justified by data.*

Modeling Approaches, cont'd.

- Empirical Models:
  - experimentally-based correlations,
  - reliable in limited ranges,
  - somewhat inflexible.
- Simple Models - *present approach*:
  - analytically tractable,
  - judgement required,
  - simplicity at expense of loss of rigor,
  - introduction of ad hoc assumptions.
- Stochastic Models:
  - estimates for uncertainty required,
  - could be coupled with simple model.

Assumptions for the Preliminary Model



- Model total system as 3 subsystems:
  - solid pyrotechnic reactants (s)
  - gas phase products (g)
  - condensed phase products (cp)
- Well stirred reactor:
  - spatial homogeneity
  - time-dependent variables
  - no mass, momentum, or energy diffusion

Assumptions cont'd.

Mass and Energy Exchange

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

Combustion Process

- Combustion products produced in ratios which minimize Gibbs free energy (CEC76 routine):
  - mass fractions frozen,
  - gas phase products described by single mixture specific heat and mixture gas constant,
  - condensed phase products characterized by a single mixture density,
- Global kinetic burn rate estimated from solid propellant data.

Assumptions cont'd.

Other assumptions

- Ideal gas with temperature dependent specific heat (CHEMKIN II data base and subroutines),
- Constant temperature vessel wall,
- No wall friction,
- Constant density solid pyrotechnic,
- Constant density condensed phase products,
- Kinetic energy of total system assumed negligible,
- Body forces assumed negligible.

Mass, Momentum, and Energy Principles

Mass Evolution Equations:

$$\frac{d}{dt}\left[\rho_s V_s\right] = -\rho_s A_p r,$$

$$\frac{d}{dt}\left[\rho_{cp} V_{cp}\right] = \eta_{cp}\rho_s A_p r,$$

$$\frac{d}{dt}\left[\rho_g V_g\right] = [1-\eta_{cp}]\rho_s A_p r.$$

Energy Evolution Equations:

$$\frac{d}{dt}\left[\rho_s V_s e_s\right] = -\rho_s A_p e_s r,$$

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

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

Newton's Second Law:

$$m_p \frac{d^2 z_p}{dt^2} = F_p.$$

Geometrical and Constitutive Relations

A. Geometry

Total volume:

$$V = V_s + V_{cp} + V_g.$$

Piston position:

$$z_p = \frac{V}{A_p}.$$

Geometrical and Constitutive Relations, cont'd.

B. Combustion Model

Reaction occurs in a single step:

$$\sum_{i=1}^{N_s} \nu_{s_i} X_{s_i} \longrightarrow \sum_{i=1}^{N_{cp}} \nu_{cp_i} X_{cp_i} + \sum_{i=1}^{N_g} \nu_{g_i} X_{g_i},$$

- X_{s_i}, X_{cp_i}, X_{g_i}: chemical species,
- ν_{s_i}, ν_{cp_i}, ν_{gi}: stoichiometric coefficients,
- ν_{s_i}, X_{s_i}: specified as inputs to the CEC76 code,
- Y's, η_{cp} can be determined from knowledge of ν's.

Linear pyrotechnic burn rate:

$$r = r(P_g, T_g) = a(T_g) + b(T_g) P_g^n,$$

- $a(T_g)$, $b(T_g)$, n: empirically determined.

Geometrical and Constitutive Relations, cont'd.

C. Thermal Equation of State

$$P_g = \rho_g R T_g,$$

where

$$R = \Re \sum_{i=1}^{N_g} \frac{Y_{g_i}}{M_{g_i}}, \qquad Y_{g_i} = \frac{\nu_{g_i} M_{g_i}}{\Sigma_{j=1}^{N_g} \nu_{g_j} M_{g_j}}.$$

D. Caloric Equations of State

$$e_s(T_s) = \sum_{i=1}^{N_s} Y_{s_i} e_{s_i}(T_s),$$

$$e_{cp}(T_{cp}) = \sum_{i=1}^{N_{cp}} Y_{cp_i} e_{cp_i}(T_{cp}),$$

$$e_g(T_g) = \sum_{i=1}^{N_g} Y_{g_i} e_{g_i}(T_g).$$

- Calculated using CHEMKIN II subroutines and data base.

Geometrical and Constitutive Relations, cont'd.

D. Model for $\dot{Q}_{in}$:

$$\dot{Q}_{in} = \underbrace{hA_w \left[T_w - T_g\right]}_{convection} + \underbrace{\sigma A_w \left[\alpha T_w^4 - \epsilon T_g^4\right]}_{radiation},$$

- Parameters:
  - h, convective heat transfer coefficient,
  - ϵ, emmissivity of the gas,
  - α, absorptivity of the vessel's walls,
  - T_w, temperature of the vessel's walls,
  - σ, Stefan-Boltzmann constant.

E. Model for $\dot{W}_{out}$:

$$\dot{W}_{out} = P_g \frac{dV}{dt}.$$

- Only allow for pressure volume work.

F. Model for F_p:

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

- F_{crit}, constant critical force necessary for shear pin failure.

Geometrical and Contitutive Relations, cont'd.

G. Model for $\dot{Q}_{cp,g}$:

$$\dot{Q}_{cp,g} = h_{cp,g} \left[T_{cp} - T_g \right] .$$

- $h_{cp,g}$, heat transfer parameter.

Mathematical Reductions

Goal:

- To perform intermediate operations leading to a refined final model:
  - six O.D.E.'s for V, V_s, V_{cp}, T_{cp}, T_g, and $\dot{V}$
  - all other variables expressed as a function of these six variables.
- Final model suitable for numerical integration.

Step I. Determination of ρ_g.

- Add together *mass evolution equations*:

$$\frac{d}{dt}\left[\rho_s V_s + \rho_{cp} V_{cp} + \rho_g V_g\right] = 0.$$

- Integrate, apply intital conditions, and solve for ρ_g:

$$\rho_g(V, V_s, V_{cp}) = \frac{\rho_s V_{so} + \rho_{cp} V_{cpo} + \rho_{go} V_{go} - \rho_s V_s - \rho_{cp} V_{cp}}{V - V_s - V_{cp}}.$$

Mathematical Reductions, cont'd.

Step II. Expression for mixture energy evolution.

- Add together *energy evolution equations*:

$$\frac{d}{dt}\left[\rho_s V_s e_s + \rho_{cp} V_{cp} e_{cp} + \rho_g V_g e_g\right] = \dot{Q}_{in} - \dot{W}_{out}.$$

  - Note: this expression is *not* explicitly used in the analysis.
  - For special case $\dot{Q}_{in} = \dot{W}_{out} = 0$, can integrate:

$$\rho_s V_s e_s + \rho_{cp} V_{cp} e_{cp} + \rho_g V_g e_g = \rho_s V_{so} e_{so} + \rho_{cp} V_{cpo} e_{cpo} + \rho_{go} V_{go} e_{go}.$$

  - Can use algebraic relation to evaluate code performance.

Step III. Determination of P_g.

- Use ρ_g from Step I and *thermal equation of state* to obtain:

$$P_g(V, V_s, V_{cp}, T_g) = \rho_g(V, V_s, V_{cp}) R T_g.$$

Mathematical Reductions, cont'd.

Step IV. Determination of r and F_p.

- Using P_g from Step III, can obtain:

$$r = r(V, V_s, V_{cp}, T_g) = a(T_g) + b(T_g)P_g^n(V, V_s, V_{cp}, T_g),$$

$$F_p = F_p(V, V_s, V_{cp}, T_g).$$

Step V. Simplify remaining differential mass equations.

- Since ρ_s and ρ_{cp} are constants:

$$\frac{dV_s}{dt} = -A_p r(V, V_s, V_{cp}, T_g), \tag{1}$$

$$\frac{dV_{cp}}{dt} = \eta_{cp}\left[\frac{\rho_s}{\rho_{cp}}\right] A_p r(V, V_s, V_{cp}, T_g). \tag{2}$$

Mathematical Reduction, cont'd.

Step VI. Simplification of energy equations.

- Consider energy evolution equation for *solid pyrotechnic*:

$$\frac{d}{dt}\left[\rho_s V_s e_s\right] = -\rho_s A_p e_s r,$$

  – subtract the following from this equation:

$$\left[\frac{d}{dt}\left[\rho_s V_s\right] = -\rho_s A_p r\right] e_s,$$

  – obtain:

$$\frac{de_s}{dt} = 0, \qquad \Longrightarrow \qquad e_s = e_{so}.$$

- Consider energy evolution equation for *condensed phase products*:

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

  – subtract the following:

$$\left[\frac{d}{dt}\left[\rho_{cp} V_{cp}\right] = \eta_{cp}\rho_s A_p r\right] e_{cp},$$

  – obtain:

$$\rho_{cp} V_{cp}\frac{de_{cp}}{dt} = \eta_{cp}\rho_s A_p r(V, V_s, V_{cp}, T_g)[e_{so} - e_{cp}(T_{cp})] - \dot{Q}_{cp,g}(T_{cp}, T_g),$$

Mathematical Reductions, cont'd.

– using caloric equation of state $e_{cp}(T_{cp})$:

$$\frac{dT_{cp}}{dt} = \frac{\eta_{cp}\rho_s A_p r(V, V_s, V_{cp}, T_g)[e_{so} - e_{cp}] - \dot{Q}_{cp,g}(T_{cp}, T_g)}{\rho_{cp} c_{cp}(T_{cp}) V_{cp}}. \quad (3)$$

- Consider energy evolution equation for *gas phase products*:

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

– subtract the following:

$$\left[\frac{d}{dt}\left[\rho_g V_g\right] = [1 - \eta_{cp}]\rho_s A_p r\right] e_g,$$

– obtain:

$$\rho_g V_g \frac{de_g}{dt} = [1 - \eta_{cp}]\rho_s A_p r[e_{so} - e_g] + \dot{Q}_{in} - \dot{W}_{out},$$

– using caloric equation of state $e_g(T_g)$:

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

$$+ \quad \frac{\dot{Q}_{in}(T_g) - P_g(V, V_s, V_{cp}, T_g)\dot{V}}{\rho_g(V, V_s, V_{cp}) c_{vg}(T_g)[V - V_s - V_{cp}]}, \quad (4)$$

Mathematical Reductions, cont'd.

Step VII. Newton's second law governing piston motion.

- Split 2^{nd} order O.D.E. into two 1^{st} order O.D.E.'s:

$$\frac{dV}{dt} = \dot{V}, \tag{5}$$

$$\frac{d\dot{V}}{dt} = \frac{F_p(V, V_s, V_{cp}, T_g)A_p}{m_p}. \tag{6}$$

Final Form of Preliminary Model

Governing O.D.E.'s:

$$\frac{dV}{dt} = \dot{V},$$

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

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

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

$$\frac{dT_g}{dt} = \frac{[1-\eta_{cp}]\rho_s A_p r(V, V_s, V_{cp}, T_g)\,[e_{so} - e_g(T_g)] + \dot{Q}_{cp,g}(T_{cp}, T_g)}{\rho_g(V, V_s, V_{cp}) c_{vg}(T_g)[V - V_s - V_{cp}]}$$
$$+ \quad \frac{\dot{Q}_{in}(T_g) - P_g(V, V_s, V_{cp}, T_g)\dot{V}}{\rho_g(V, V_s, V_{cp}) c_{vg}(T_g)[V - V_s - V_{cp}]},$$

$$\frac{d\dot{V}}{dt} = \frac{F_p(V, V_s, V_{cp}, T_g) A_p}{m_p},$$

Initial Conditions:

$$V(t=0) = V_o, \qquad V_s(t=0) = V_{so}, \qquad V_{cp}(t=0) = V_{cpo},$$
$$T_{cp}(t=0) = T_{cpo}, \qquad T_g(t=0) = T_{go}, \qquad \dot{V}(t=0) = 0.$$

Initial Results

The following results are presented:

- pressure-time predictions for a 10 cm^3 closed bomb combustion of 114 mg of $Zr/KClO_4$,
- pressure-time predictions and piston energy calculations for typical operation of NSI driven pin puller.

Balanced Stoichiometric Equation:

$$\begin{aligned} 3.6162Zr(s) + 2.6849KClO_4(s) \longrightarrow\ & 3.2354Zr(l) + 1.9712O(g) \\ & +1.6988KCl(g) + 0.9766Cl(g) \\ & +0.9041K(g) + 0.7454O_2(g) \\ & +0.3407ZrO_2(g) + 0.0790KO(g) \\ & +0.0401ZrO(g) + 0.0065ClO(g) \\ & +0.0009K_2ClO_2(g) + 0.0006Cl_2(g) \\ & +0.0006K_2(g). \end{aligned}$$

NSI Pyrotechnic Composition:

- 114 mg of a $Zr/KClo_4$ mixture:
  - 53.6 mg of $Zr(s)$,
  - 60.4 mg of $KClO_4$.

Closed Bomb Combustion (10 cm^3)

- NASA specifications: firing an NSI containing 114 mg of $Zr/KClo_4$ mixture into a 10 cm^3 volume shall produce a peak pressure of 650±125 psi within 5 ms.

- Initial Conditions:

intial condition	*value*
V_o	10.0 cm^3
V_{so}	0.038 cm^3
V_{cpo}	5.10×10^{-7} cm^3
T_{cpo}	288.0 K
T_{go}	288.0 K
$\dot{V}$	0.0 cm^3/s

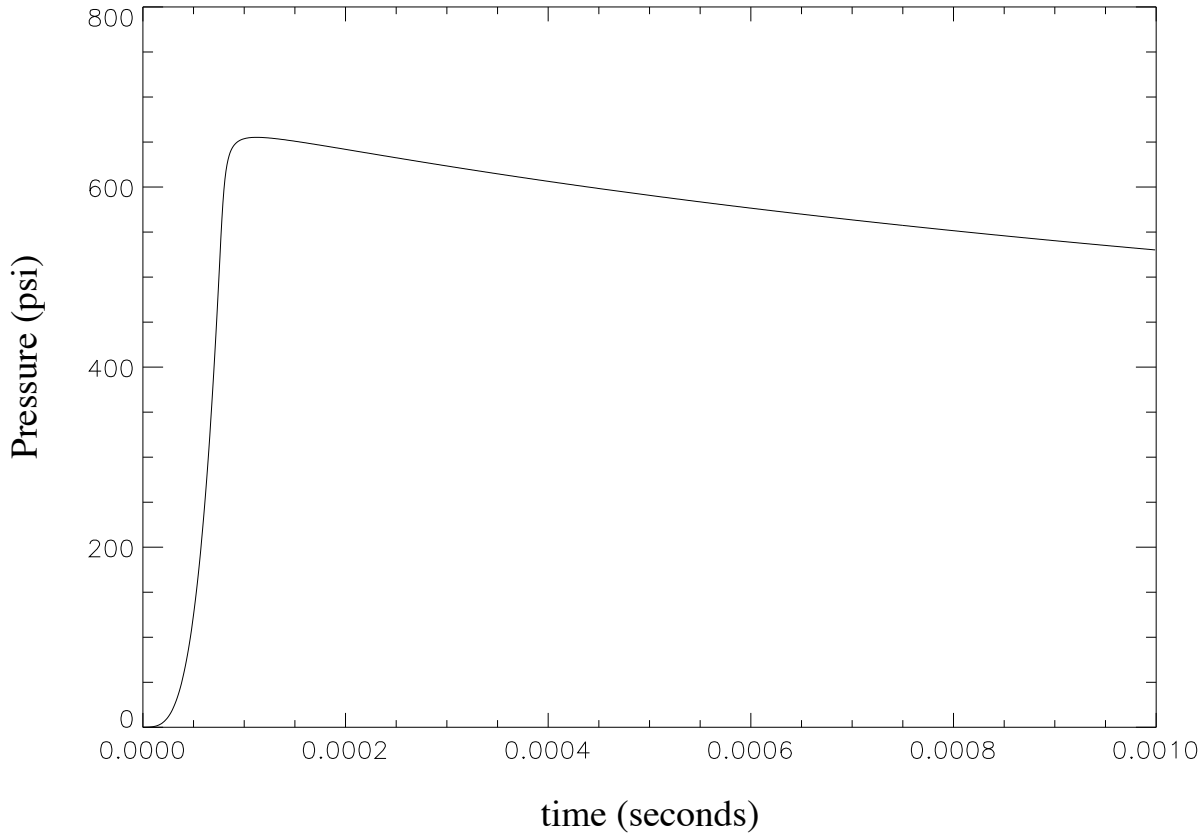
- Parameters:

parameter	*value*
burn area, A_p	2.0 cm^2
pyrotechnic density, ρ_s	3.0 g/cm^3
temperature of pyrotechnic, T_s	288.0 K
condensed phase density, ρ_{cp}	1.51 gm/cm^3
convective heat transfer coefficient, h	1.25×10^5 $g/sec^3/K$
emissivity of the gas, ϵ	0.80
absorptivity of the vessel's walls, α	0.80
heat transfer parameter, $h_{cp,g}$	12.0×10^9 $gcm^2/sec^3/K$

- Pyrotechnic Burn Rate:

$$r = 0.004 P_g^{0.69}.$$

Closed Bomb Combustion, cont'd.



NSI Driven Pinpuller Results

- Initial Conditions:

intial condition	*value*
V_o	0.824 cm^3
V_{so}	0.038 cm^3
V_{cpo}	3.40×10^{-6} cm^3
T_{cpo}	288.0 K
T_{go}	288.0 K
$\dot{V}$	0.0 cm^3/s

- Parameters:

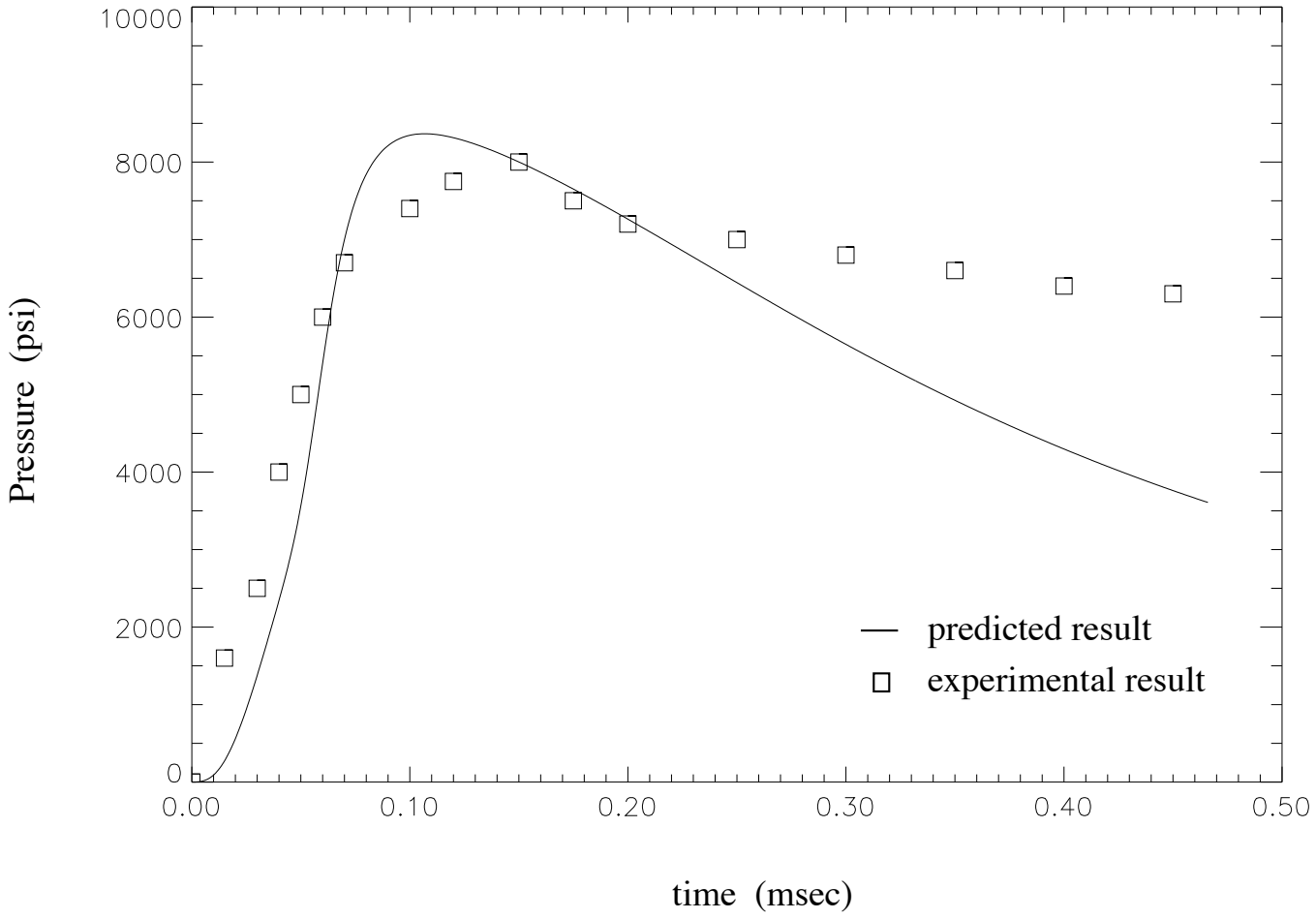
parameter	*value*
burn area, A_p	0.634 cm^2
pyrotechnic density, ρ_s	3.0 g/cm^3
pyrotechnic temperature, T_s	288.0 K
condensed phase density, ρ_{cp}	1.51 gm/cm^3
convective heat transfer coefficient, h	1.25×10^5 $g/sec^3/K$
emissivity of the gas, ϵ	0.60
absorptivity of the vessel's walls, α	0.60
heat transfer parameter, $h_{cp,g}$	12.0×10^9 $gcm^2/sec^3/K$
critical shearing force, F_{crit}	3.56×10^7 *dynes* (80 *lb*)

- Pyrotechnic Burn Rate:

$$r = 0.004P_g^{0.69}.$$

NSI Driven Pinpuller Results, cont'd.

- Pressure – time prediction:



Outline of Future Directions

- Study solution near equilibrium states,
- examine simplest possible case – constant volume, no heat transfer, constant specific heats,
- better justify heat transfer coefficients,
- study wall surface effects on heat transfer,
- continue search for accurate burn rate data,
- perform sensitivity analysis,
- include grain size effects,
- study spatially resolved field,
- include more detailed chemistry.