Pyrotechnic Modeling for the NSI and Pin Puller

Joseph M. Powers[1] and Keith A. Gonthier[2]

Department of Aerospace and Mechanical Engineering

University of Notre Dame

Notre Dame, Indiana 46556-5637

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[1] Assistant Professor, 219-239-5978, powers@neumann.ame.nd.edu

[2] Graduate Assistant

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Discussions

Prof. P. Barry Butler
University of Iowa

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
  - apparantly random sample behavior

Modeling Approaches

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

- Empirical Models
  - experimentally-based correlations
  - reliable in limited ranges
  - somewhat inflexible
- Simple Models-*present approach*
  - analytically tractable
  - judgment 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 Simple Model

- no spatial variation
  - $t_{acoustic} \sim \frac{L}{c} \sim \frac{0.01m}{1000m/s} = 1 \times 10^{-5}s$
- constant density solid pyrotechnic
- constant surface area of pyrotechnic
- linear pyrotechnic burn rate known
- constant temperature wall
- simple convective heat transfer
  - $t_{conv} << t_{cond} \sim \frac{L^2}{\alpha} \sim \frac{(0.01m)^2}{0.001m^2/s} = 0.1s$
- simple radiative heat transfer
  - $t_{rad} \sim \frac{\rho_g c_{vg} L}{\sigma T^3} \sim \frac{1kg/m^3 1000J/(kgK) 0.01m}{1 \times 10^{-7} J/(sm^2K^4)(1000K)^3} = 0.1s$

- negligible heat tranfer from gas to solid
- negligible wall friction and shear pin resistance
- non-negligible pin inertia
- multicomponent ideal gas behavior
- temperature dependent specific heat
- Gibbs free energy minimization
  - determines heat of reaction
  - determines mass fractions of gas products

Conservation Principles

for background see

Powers, Stewart, and Krier, "Theory of Two-Phase Detonation–Part I: Modeling, Part II: Structure," *Combustion and Flame*, V. 80, 1990.

$$
\begin{aligned}
\frac{d}{dt}\left[\rho_g V_g\right] &= \rho_s A r \\
\frac{d}{dt}\left[\rho_s V_s\right] &= -\rho_s A r \\
\frac{d}{dt}\left[\rho_g V_g e_g\right] &= \rho_s A r e_s + hA(T_w - T_g) \\
&\quad +\sigma A(\alpha T_w^4 - \epsilon T_g^4) - P_g \frac{dV}{dt} \\
\frac{d}{dt}\left[\rho_s V_s e_s\right] &= -\rho_s A r e_s \\
m_p \frac{d^2}{dt^2}\left[\frac{V}{A}\right] &= P_g A
\end{aligned}
$$

Constitutive Relations

$$
\begin{aligned}
r &= a + bP_g^n \\
P_g &= \rho_g R T_g \sum_{i=1}^{N_g} \frac{Y_i}{M_i} \\
e_g &= \sum_{i=1}^{N_g} Y_i \left(h_{fi}^o + \int_{T^o}^{T_g} c_{pi}(\hat{T}_g) d\hat{T}_g \right) - R T_g \sum_{i=1}^{N_g} \frac{Y_i}{M_i} \\
e_s &= \sum_{i=1}^{N_s} Y_i \left(h_{fi}^o + \int_{T^o}^{T_s} c_{pi}(\hat{T}_s) d\hat{T}_s \right) \\
V &= V_g + V_s
\end{aligned}
$$

Y_i estimated from minimization of Gibbs free energy

Variables

$e_g, V_g, T_g, P_g, \rho_g,$

$e_s, V_s, T_s,$

V, Y_i, r

Constants

$\rho_s, A, h, T_w, \sigma, \alpha, \epsilon, m_p, a, b, n, R, M_i$

Piston Energy calculation

Knowledge of $P_g(t)$ and $V(t)$ allows calcuation of work done by pyrotechnic material:

$$W(t) = \int_0^t P_g(\hat{t}) \frac{dV(\hat{t})}{d\hat{t}} d\hat{t}$$

Current Solution Approach

- use NASA Lewis CEC code to estimate equilibrium products via minimization of Gibbs free energy
- solve coupled ODE–algebraic system
  - numerical integration of ODE
  - SLNL-CHEMKIN package to determine gas energy
- calculate work done by gas
- compare peak pressure and work with observations

Future

- wall friction
- shear pin effects
- spatial resolution
- grain size effects
- burn rate experiments
- detailed chemistry
- stochastic effects

Conclusions

- literature search shows little published articles on modeling of pyrotechnically driven actuators
- insufficient constitutive data for full-scale model
- simple deterministic model appears useful to better guide design
- assumptions of simple model preclude capturing of many observed phenomena
- results from simple model should be first evaluated then decisions made regarding where to make improvements