Thermal Explosion Theory for Reactive Shear Localizing Solids

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Partial Review

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- Caspar, R. J., Powers, J. M., and Mason, J. J., 1998, Investigation of reactive shear localization in energetic solids, *Combustion Science and Technology*, to appear.

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Motivation

Development of insensitive solid explosives

Development of transient detonation models for solid explosives

- steady detonation relatively well-characterized,
- late-time hydrodynamic transients relatively well-characterized,
- early time ignition events poorly understood
  - thermal stimuli
  - mechanical stimuli, e.g. shear localization, also known as shear banding

Shear Localization

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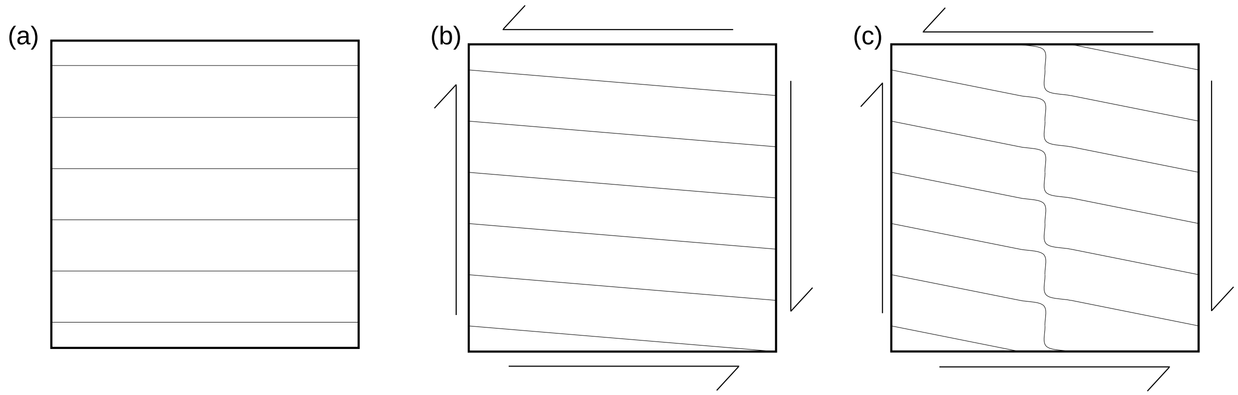

a) Initial homogeneous unstrained state,

b) Applied shear force induces uniform strain,

c) Shear localization induced by local inhomogeneity

- Shear localization occurs when thermal softening dominates over strain and strain rate hardening
- Hypothesized hot spot location for reaction initiation

Approach and Novelty

- Approach
  - Obtain data for high strain rate constitutive theory from Notre Dame torsional split-Hopkinson bar
  - Use simple model to predict
    - spatially homogeneous time-dependent solutions
    - spatially inhomogeneous time-independent solutions
- Novelty
  - Experimental stress-strain-strain rate characterization of inert simulant (Mock 900-20) of heterogeneous explosive LX-14 (95.5 % HMX, 4.5 % Estane 5703-P; $C_{1.52}H_{2.92}N_{2.59}O_{2.66}$)
  - Extension of Frey's (1981) analysis to include strain rate effects
  - new application of thermal explosion theory
  - sensitivity analysis performed

Experimental Method

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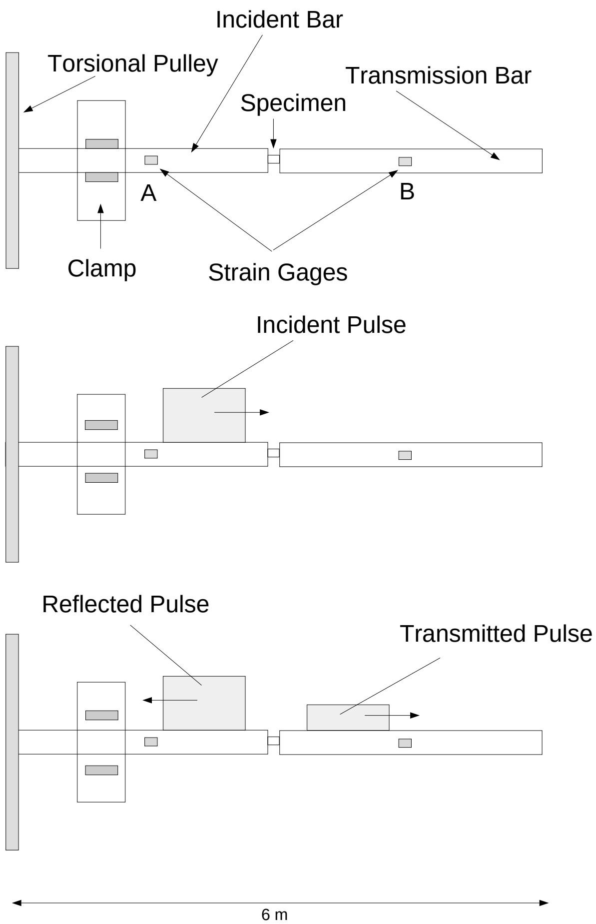
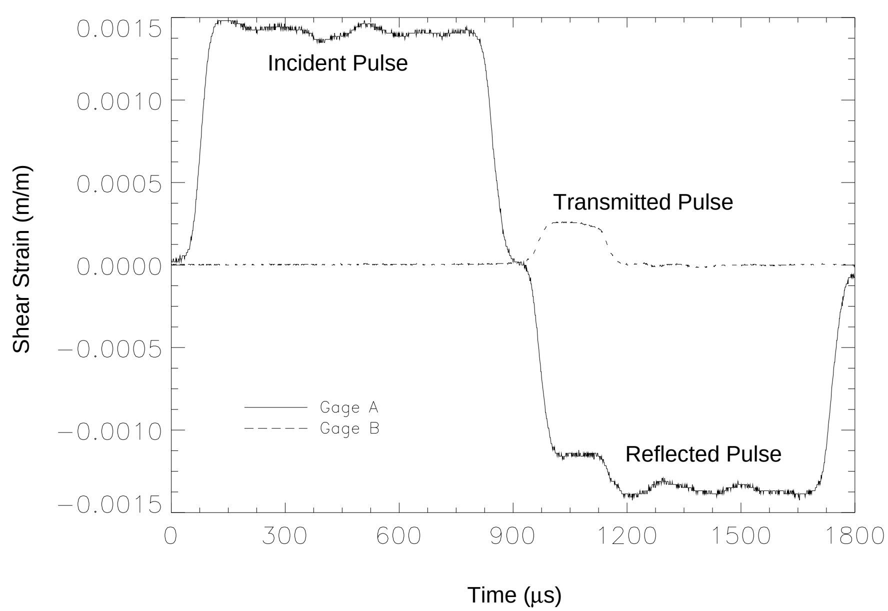
Torsional Split Hopkinson Bar-Notre Dame Solid Mechanics Laboratory





Experimental Results

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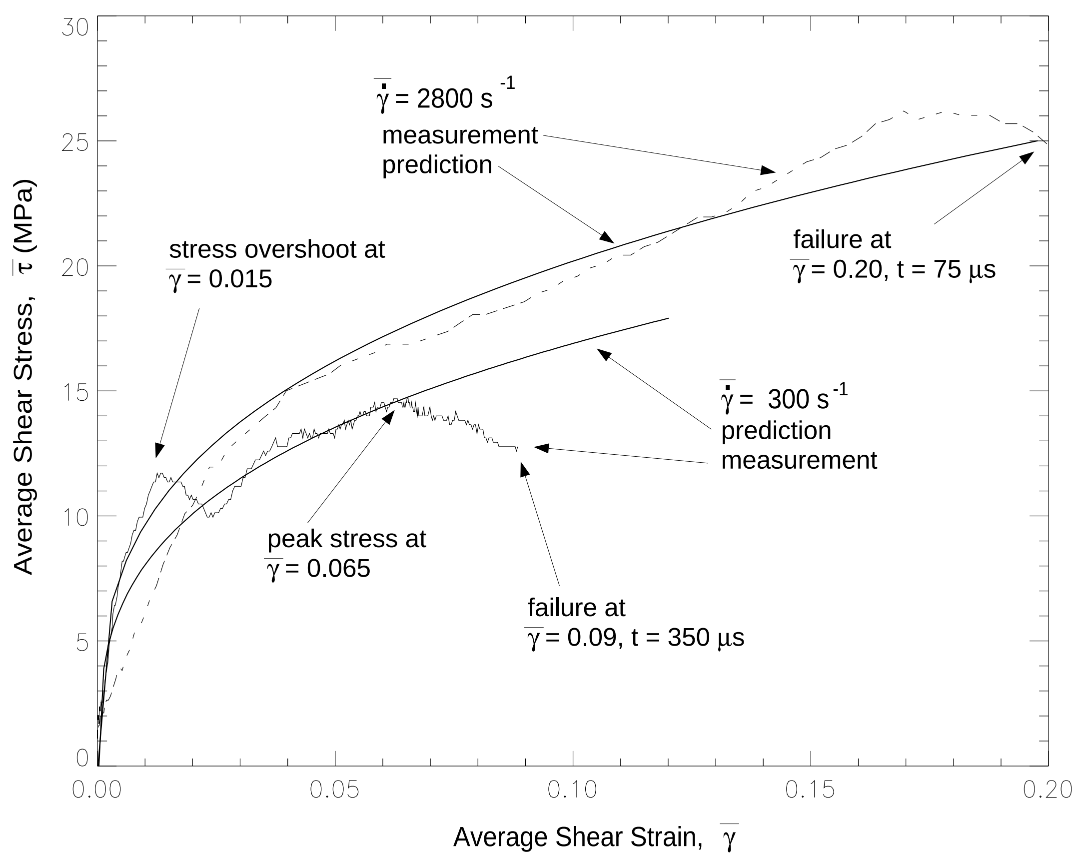
Torsional Split Hopkinson Bar Test Results for LX-14 simulant (Mock 900-20) and theoretical model predictions



where $\tau \propto \overline{\gamma}^{\,\eta} \left(\frac{\partial \overline{\gamma}}{\partial t}\right)^{\mu}$

Model Assumptions

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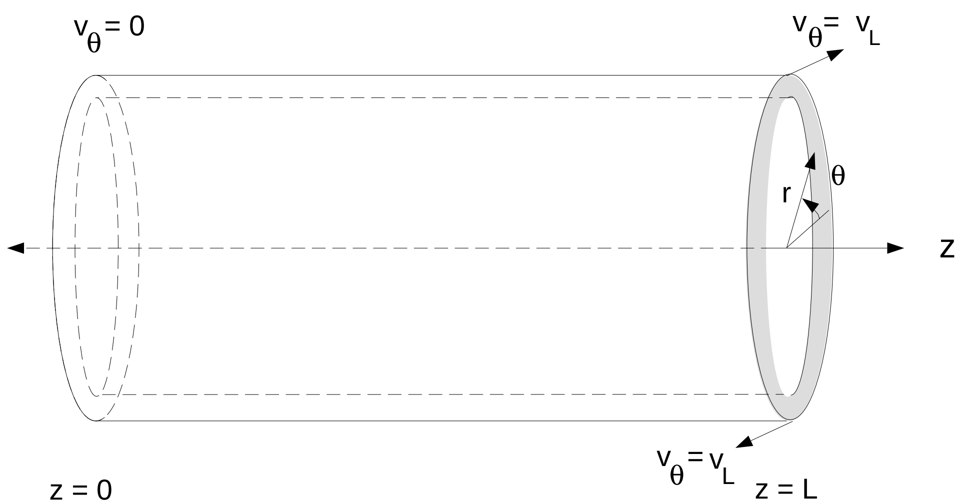

thin-walled cylindrical geometry

initially unreacted, unstressed, and cold

$v_r = v_z = u_r = u_z = 0$

$\frac{\partial}{\partial \theta} = \frac{\partial}{\partial r} = 0$

one step Arrhenius chemistry

incompressible

constant properties

Model Equations

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$$
\begin{aligned}
\rho \frac{\partial v_\theta}{\partial t} &= \frac{\partial \tau}{\partial z} \,, && \text{momentum conservation} \\
\rho \frac{\partial e}{\partial t} &= \tau \frac{\partial v_\theta}{\partial z} - \frac{\partial q_z}{\partial z} \,, && \text{energy conservation} \\
\frac{\partial \lambda}{\partial t} &= a\,(1-\lambda)\,\exp\left(-\frac{E}{\Re T}\right), && \text{reaction kinetics} \\
\frac{\partial u_\theta}{\partial t} &= v_\theta \,, && \text{displacement definition} \\
\tau &= \alpha \left(\frac{T}{T_0}\right)^{\nu} \left(\frac{\partial u_\theta}{\partial z}\right)^{\eta} \left(\frac{\partial v_\theta}{\partial z}\frac{L}{v_L}\right)^{\mu} \,, && \text{constitutive equation for stress} \\
q_z &= -k \frac{\partial T}{\partial z} \,, && \text{Fourier's Law} \\
e &= c\,T - \lambda\,\tilde{q} \,. && \text{caloric state equation}
\end{aligned}
$$

Boundary and Initial Conditions

Boundary Conditions

specified velocity and displacement at both ends, thermally insulated

$$v_\theta(t,0) = 0, \qquad v_\theta(t,L) = v_L, \qquad u_\theta(t,0) = 0, \qquad u_\theta(t,L) = v_L t,$$

$$\frac{\partial T}{\partial z}(t,0) = 0, \qquad \frac{\partial T}{\partial z}(t,L) = 0.$$

Initial Conditions

spatially homogeneous strain rate, unstrained, unreacted, temperature perturbation near center

$$v_\theta(0,z) = v_L \frac{z}{L}, \qquad u_\theta(0,z) = 0, \qquad \lambda(0,z) = 0,$$

$$T(0,z) = \begin{cases} T_0, & z \notin \left[\frac{L}{2}(1-\hat{\epsilon}_L), \frac{L}{2}(1+\hat{\epsilon}_L)\right], \\ T_0(1+\hat{\epsilon}_T), & z \in \left[\frac{L}{2}(1-\hat{\epsilon}_L), \frac{L}{2}(1+\hat{\epsilon}_L)\right]. \end{cases}$$

Scaling

Scaled independent variables

$$z_* = \frac{z}{L}, \qquad t_* = \frac{v_L}{L} t,$$

Scaled dependent variables

$$v_* = \frac{v_\theta}{v_L}, \qquad T_* = \frac{T}{T_0}, \qquad \lambda_* = \lambda, \qquad u_* = \frac{u_\theta}{L}.$$

Dimensionless Parameters

$$\hat{\alpha} = \frac{\alpha}{\rho v_L^2}, \quad \widehat{Ec} = \frac{v_L^2}{c T_0}, \quad \widehat{Pe} = \frac{\rho c}{k} v_L L, \quad \hat{q} = \frac{\tilde{q}}{c T_0}, \quad \hat{a} = \frac{L}{v_L} a, \quad \hat{\Theta} = \frac{E}{\Re T_0}.$$

Reduced Dimensionless Equations, Initial and Boundary Conditions

$$
\begin{aligned}
\frac{\partial v_*}{\partial t_*} &= \hat{\alpha} \frac{\partial}{\partial z_*}\left(T_*^{\nu}\left(\frac{\partial u_*}{\partial z_*}\right)^{\eta}\left(\frac{\partial v_*}{\partial z_*}\right)^{\mu}\right), \\
\frac{\partial T_*}{\partial t_*} &= \hat{\alpha}\, \widehat{Ec}\, T_*^{\nu}\left(\frac{\partial u_*}{\partial z_*}\right)^{\eta}\left(\frac{\partial v_*}{\partial z_*}\right)^{\mu+1} + \frac{1}{\widehat{Pe}}\frac{\partial^2 T_*}{\partial z_*^2} + \hat{a}\,\hat{q}\,(1-\lambda_*)\exp\left(-\frac{\hat{\Theta}}{T_*}\right), \\
\frac{\partial \lambda_*}{\partial t_*} &= \hat{a}\,(1-\lambda_*)\exp\left(-\frac{\hat{\Theta}}{T_*}\right), \\
\frac{\partial u_*}{\partial t_*} &= v_*.
\end{aligned}
$$

$$
v_*(t_*,0)=0, \quad v_*(t_*,1) = 1, \quad u_*(t_*,0)=0, \quad u_*(t_*,1)=t_*,
$$

$$
\frac{\partial T_*}{\partial z_*}(t_*,0)=0, \quad \frac{\partial T_*}{\partial z_*}(t_*,1) = 0, \quad v_*(0,z_*)=z_*, \quad u_*(0,z_*)=0, \quad \lambda_*(0,z_*)=0,
$$

$$
T(0,z_*) = \begin{cases} 1, & z_* \notin \left[\frac{1}{2}(1-\hat{\epsilon}_L), \frac{1}{2}(1+\hat{\epsilon}_L)\right], \\ 1+\hat{\epsilon}_T, & z_* \in \left[\frac{1}{2}(1-\hat{\epsilon}_L), \frac{1}{2}(1+\hat{\epsilon}_L)\right]. \end{cases}
$$

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Thermal Explosion Theory

- Unsteady solutions indicate early time behavior is largely spatially homogeneous
- Formally examine such behavior by assuming
  - negligibly small temperature perturbation ϵ_T
  - $T_* = T_*(t_*)$ (requires $\widehat{Pe} >> 1$)
  - $\lambda_* = \lambda_*(t_*)$
  - $v_* = z_*$
  - $u_* = z_* t_*$

Result is two non-autonomous ordinary differential equations in T_* and λ_*:

$$\frac{dT_*}{dt_*} = \hat{\alpha}\ \widehat{Ec}\ T_*^{\nu} t_*^{\eta} + \hat{a}\ \hat{q}\ (1 - \lambda_*) \exp\left(-\frac{\hat{\Theta}}{T_*}\right), \qquad T_*(0) = 1,$$

$$\frac{d\lambda_*}{dt_*} = \hat{a}\ (1 - \lambda_*) \exp\left(-\frac{\hat{\Theta}}{T_*}\right), \qquad \lambda_*(0) = 0.$$

Approximate Solution

Neglect reaction in favor of plastic work at early time

$$\frac{dT_*}{dt_*} = \hat{\alpha}\ \widehat{Ec}\ T_*^{\nu}\ t_*^{\eta}, \qquad t_* < t_{*i}, \qquad T_*(0) = 1.$$

Exact solution available:

$$T_*(t_*) = \left(\frac{1-\nu}{1+\eta} \hat{\alpha}\ \widehat{Ec}\ t_*^{\eta+1} + 1 \right)^{\frac{1}{1-\nu}}, \qquad t_* < t_{*i}.$$

Determine time when reaction balances plastic work:

$$\hat{\alpha}\ \widehat{Ec}\ \left(\frac{1-\nu}{1+\eta} \hat{\alpha}\ \widehat{Ec}\ t_{*i}^{\eta+1} + 1 \right)^{\frac{\nu}{1-\nu}} t_{*i}^{\eta} = \hat{a}\ \hat{q}\ \exp\left[-\hat{\Theta} \left(\frac{1-\nu}{1+\eta} \hat{\alpha}\ \widehat{Ec}\ t_{*i}^{\eta+1} + 1 \right)^{-\frac{1}{1-\nu}} \right].$$

Asymptotic Solution

Consider high activation energy limit

$$T_* = 1 + \frac{1}{\widehat{\Theta}} T_{*1} + \cdots, \qquad \lambda_* = \frac{1}{\widehat{\Theta}} \lambda_{*1} + \cdots,$$

Energy equation reduces to

$$\frac{dT_{*1}}{dt_*} = \widehat{\beta}_1 \left(t_*^{\eta} + \widehat{\beta}_2 e^{T_{*1}} \right), \qquad T_{*1}(0) = 0, \qquad \widehat{\beta}_1 = \widehat{\Theta}\ \widehat{\alpha}\ \widehat{Ec}, \qquad \widehat{\beta}_2 = \frac{\widehat{a}\ \widehat{q}}{\widehat{\alpha}\widehat{Ec}\ e^{\widehat{\Theta}}}.$$

For $\eta = 0$, induction time is

$$t_{*i0} = \frac{1}{\widehat{\Theta}\ \widehat{\alpha}\ \widehat{Ec}} \ln \left(\frac{\widehat{\alpha}\ \widehat{Ec}\ e^{\widehat{\Theta}}}{\widehat{a}\ \widehat{q}} \right), \qquad (\eta = 0).$$

Numerical Solution Method

- ODE's from thermal explosion theory solved with NDSolve in Mathematica 3.0 to 16 digits of accuracy; solution time less than one minute on Sun UltraSparc1 workstation.
- PDE's from full equations solved with method of lines marching technique embodied in Fortran 77 code on Sun UltraSparc1 workstation
  - forty-nine spatial nodes
  - second order centered spatial finite difference technique
  - implicit time integration of ODE's which result from discretization using DLSODE package
  - convergence of error norms consistent with order of numerical method
  - solution time ten minutes
  - extremely stiff near shear localization events

Thermal Explosion Theory Predictions

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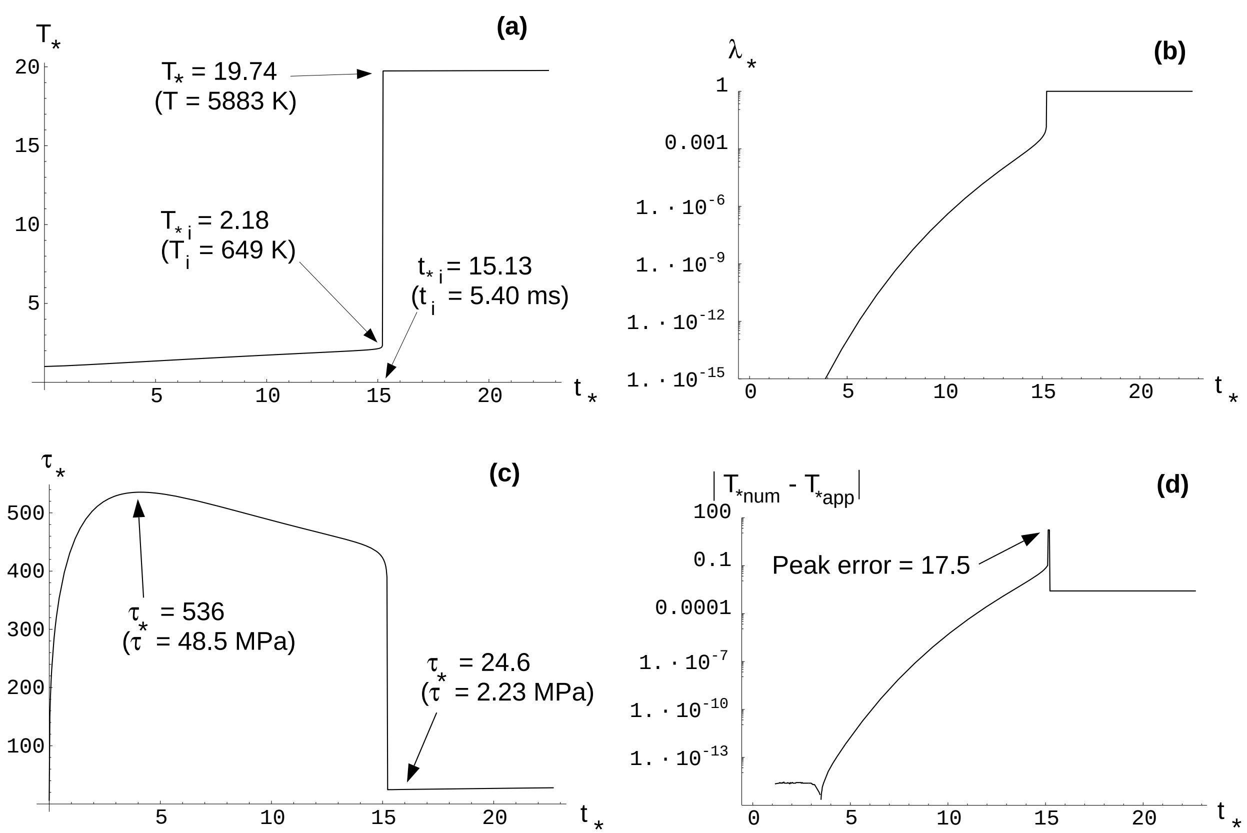
Results from numerical solution of spatially homogeneous ordinary differential equations away from asymptotic limits



Comparison with Spatially Inhomogeneous Solutions

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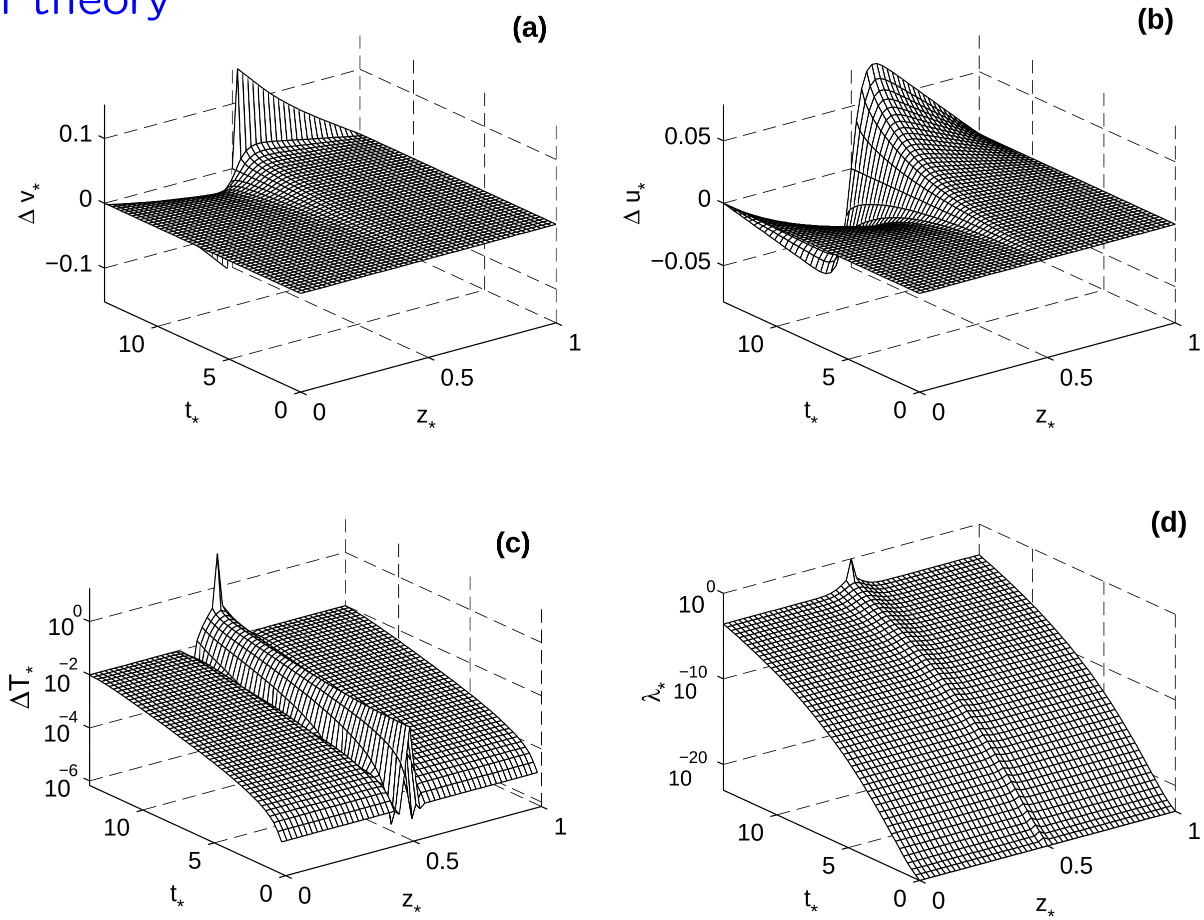
induction/localization time predicted well by spatially homogeneous thermal explosion theory



Conclusions

- Spatially homogeneous thermal explosion theory predicts ignition time accurately, even in presence of shear-localization-inducing inhomogeneities.
- While strong experimental evidence exists detailing the importance of localized hot spots in accelerating ignition in high explosives, the present theory, confined to the shear initiation mechanism, indicates the shear localization is a consequence, and not a cause, of an already imminent reaction.
- Sensitivity analysis indicates ignition time is generally more sensitive to changes in mechanical properties relative to changes in thermal properties.