A COMPARISON OF TECHNIQUES FOR MODELING XDT IN EXPLOSIVES AND PROPELLANTS

Edward J. O'Connor
Naval Surface Warfare Center Dahlgren Division (540) 653-4658

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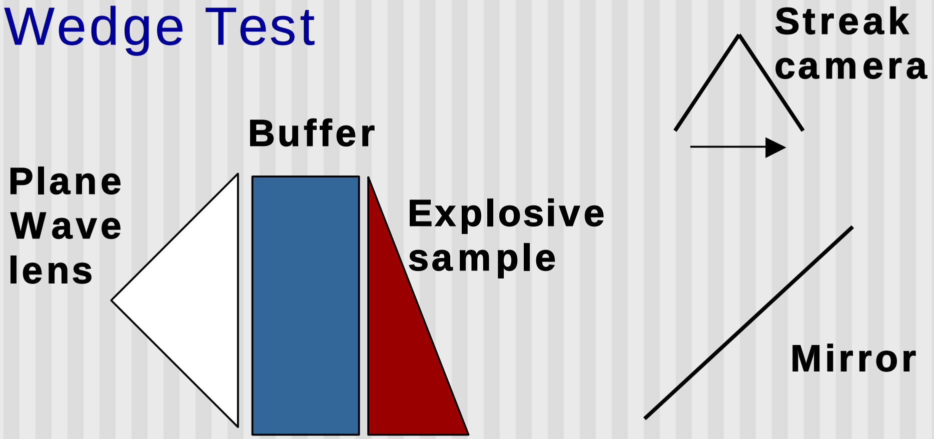
OVERVIEW

- Background – The SDT methodology
- Phenomenological & Physical aspects of XDT
- PERMS approach for modeling XDT
- CDAR approach for modeling XDT
- Final Thoughts

BACKGROUND (SDT)

- ‘Shock to Detonation Transition’
- Basis for most hydrocode reactive modeling techniques.
- Structural response primarily Hydrostatic.
- Thermo-mechanical equilibrium.

Example – Wedge Test



BACKGROUND (SDT)

- Hydrodynamic Conservation

Mass

$$\frac{d}{dt}\int_{b_t} r\,dv=0$$

Linear Momentum

$$\frac{d}{dt}\int_{b_t} r\,\mathbf{v}\,dv-\int_{\partial b_t}\mathbf{s}^{T}\hat{\mathbf{n}}\,ds=\mathbf{0}$$

Energy

$$\frac{d}{dt}\int_{b_t} r\left(\frac{1}{2}\mathbf{v}\cdot\mathbf{v}+u\right)dv-\int_{\partial b_t}\left(\mathbf{s}^{T}\mathbf{v}-\mathbf{q}\right)\cdot\hat{\mathbf{n}}\,ds-\int_{b_t} r\,z\,dv=0$$

- Chemical Kinetics

$$l' = f(l,p)$$

BACKGROUND (SDT)

- Mixed-Phase Thermodynamics

Mixture Density

$$r = j_s r_s + j_g r_g$$

Mixture Internal Energy

$$u = g_s u_s + g_g u_g$$

Dynamic Equilibrium

$$\mathbf{v} = \mathbf{v}_s = \mathbf{v}_g$$

Thermal Equilibrium

$$T = T_s = T_g$$

Structural Equilibrium

$$p = p_s = p_g$$

- Constitutive Response

Equation of State

$$p = \underline{f(r)} + \underline{g(r,u)}$$

‘cold curve’

Thermal contribution

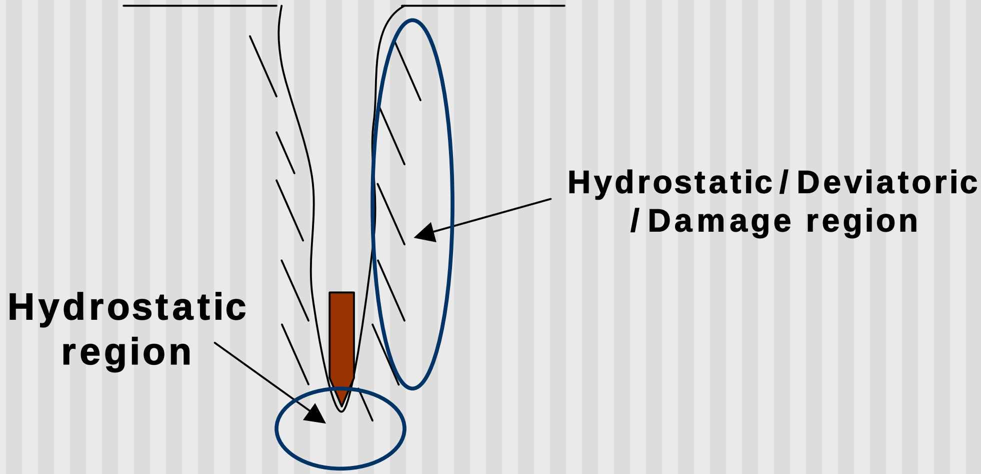
Linear Elasticity

$$s_{ij} = 2me_{ij} + l e_{kk} d_{ij}$$

XDT

- Low Amplitude/Long Duration (LALD) mechanical loading.
  - Delayed detonative or sub-detonative response.
- Phase Disequilibria (transport effects vs hydro timescale)
- Plasticity (J_1, J_2) ⇒ Thermal Dissipation.
- Damage (morphological change) ⇒ Sensitization.

Example – Low-speed bullet impact (bare explosive charge)



XDT

- Continuum Mixture Theory (Truesdell, 1969)

Mass

$$\frac{d}{dt}\int_{b_t} j_a r_a dv = \boxed{\int_{b_t} c_a^{+} dv}$$

Reaction Rate

Linear Momentum

Inter-phase drag, etc.

$$\frac{d}{dt}\int_{b_t} j_a r_a \mathbf{v}_a dv - \int_{\partial b_t} \mathbf{s}_a \cdot \hat{\mathbf{n}}\, ds = \boxed{\int_{b_t} \mathbf{m}_a^{+} dv}$$

Energy

Conduction, Convection, etc

$$\frac{d}{dt}\int_{b_t} j_a r_a \left(\frac{1}{2}\mathbf{v}_a \cdot \mathbf{v}_a + u_a\right) dv - \int_{\partial b_t} \left(\mathbf{s}_a^{T}\mathbf{v}_a - \mathbf{q}_a\right) \cdot \hat{\mathbf{n}}\, ds - \int_{b_t} j_a r_a z_a\, dv = \boxed{\int_{b_t} u_a^{+} dv}$$

XDT

- Dissipated plastic work

Total work

$$W = \int_0^t s_{ij}(t) e_{ij}(t) dt$$

Strain Decomposition

$$e_{ij}(t) = e_{ij}^{e}(t) + e_{ij}^{p}(t)$$

Cauchy stress Decomposition

$$s_{ij}(t) = s_{ij}(t) - \frac{1}{3} s_{kk}(t) d_{ij}$$

Dissipated plastic work Compaction/Distension energy

$$W = \int_0^t \left[\underline{s_{ij}(t) e_{ij}^{e}(t)} + \underline{s_{ij}(t) e_{ij}^{p}(t)} - \frac{1}{3} \underline{s_{kk}(t) e_{kk}^{e}(t)} - \frac{1}{3} \underline{s_{kk}(t) e_{kk}^{p}(t)} \right] dt$$

Elastic strain energy Elastic compression energy

XDT

- Damage / Morphological change
  - Distension ⇒ hot spot formation (hole burning)
  - Grain break up ⇒ surface area increase (grain burning)
  - Crack evolution ⇒ thermal pathways (flame spread)

XDT versus SDT

SDT	**XDT**
Initiation via Strong-Shock	Initiation via Low-Amplitude / Long Duration loading
‘Infinitely-fast’ kinetics propagated by shock	‘Slow ⇒ Fast’ kinetics propagated (initially) thermo-mechanically
Kinetics directly linked to hydrostatic (EOS) response	Kinetics linked to tensorial stress state and damage histories (CM)
Solid / Gas phases in thermo-mechanical equilibrium	Equilibrium approximation questionable

PERMS Model

- Propellant Response to Mechanical Stimuli
  - LLNL (Maienschein, Reaugh, and Lee) - 1998

- Motivation - Propellant ‘fallback’ scenario.

- Hydrodynamic Conservation
  - Single Phase

- Chemical Kinetics
  - Dual Reaction progress variables (I&G form)

$$l_1' = G_0(1-l_1)^{s_0}(h-a_0)^{y_0} + G_1(1-l_1)^{s_1} l_1^{q_1} r'(p) + \left(\frac{S}{V}\right)_0 (1-l_1)^{s_2} r'(p)$$

$$l_2' = G_2(1-l_2)^{s_2}(R l_1 - l_2)^{q_2} p^{y_2}$$

PERMS Model

- Mixed-Phase Thermodynamics
  - Thermo-mechanical equilibrium

- Constitutive Response.

$$s_y = \left[s_y^0 + a \ln\left(e'_{eps}\right)\right]\left(1 + b e_{eps}\right)^n$$

Mises Viscoplastic Flow Rule

$$\left(\frac{S}{V}\right)_0 = A\left(e_{eps} - e_0\right)\left\langle e' \right\rangle$$

Sensitization factor
(modifies primary I&G rate)

CDAR Model

- Coupled Damage And Distension
    - Lockheed, SNL (Matheson, Drumheller, and Baer) - 1999

- Motivation - Propellant / Explosive XDT.

- Hydrodynamic Conservation
    - Two Phase

- Chemical Kinetics

$$c_s^+ = -\frac{r_s\left(j_s - j_s^0\right)}{t_H} - r_s\left\langle\frac{S}{V}\right\rangle a p_g^n H\left(T_i - T^*\right)$$

Pressure dependence
w/ thermal induction

$$\left\langle\frac{S}{V}\right\rangle = \frac{6j_s}{d_p}\left(\frac{j_s^0}{j_s}\right)^{\frac{1}{3}}\left(\frac{1-j_s}{1-j_s^0}\right)^{\frac{2}{3}}$$

Sensitization factor
(Solid volume fraction dependence)

CDAR Model

- Mixed-phase thermodynamics
  - Distinct pressures, temperatures, velocities between phases

- Constitutive Response

$$e'^{vp}_{eff} = A\left(N_0 + M e^{vp}_{eff}\right) exp\left(-\frac{s^{Dr} + H\left(e^{vp}_{eff}\right)^{n_2}}{s_{eff}}\right)^{n_1}$$

Viscoelastic / Viscoplastic Model

$$e'^{p}_{d} = -D_{eff}\left(\frac{p_s}{\left|p_s\right|}\right)\left[\begin{array}{l} S_1 l_1 \left|1 - \frac{e^{d}_{eff}}{e_{\max}}\right| \left|\nabla \cdot \mathbf{v}_s\right| \\ + S_2 l_2 \left(\frac{\left|b_s\right|}{b^{0}_{s}}\right)^{n} \end{array}\right]$$

Tensile Damage & Distension

$$\frac{j'_s}{j_s} = \frac{c^{+}_{s}}{r_s} - e'_d$$

Compaction / distension law

PERMS versus CDAR

- Included Physics

Physics	**PERMS**	**CDAR**
Equilibrium Approach	Thermo-mechanical	Non-equilibrium
Inter-phase transport	No	Yes
Constitutive Approach	J2 (viscoplastic / isotropic hardening)	J2 (viscoelastic / viscoplastic)
Plastic Work	No	Step Function
Shear Damage Coupling	Yes	Yes
Tensile Damage Coupling	No	Yes
Flame Spread	No	No

Final Thoughts

- PERMS Model
  - Straightforward approach
  - Few material coefficients
    - Material characterization test costs minimized
  - May not include necessary physics for XDT modeling
    - J1, J2 plasticity
    - Dissipated plastic work
    - Volumetric damage process
    - Flame Spread
- CDAR Model
  - Highly (overly?) complex approach
  - Many (~130) material coefficients
    - Material characterization test costs quite high
  - Includes most, but not all, required physics
    - J1, J2 plasticity
    - Dissipated plastic work
    - Flame Spread