SHOCK-INITIATION AND DETONATION EXTINCTION
IN HOMOGENEOUS OR HETEROGENEOUS EXPLOSIVES:
SOME EXPERIMENTS AND MODELS

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Prepared for:
High-Speed Combustion in Gaseous and Condensed-Phase Energetic Materials,
Institute for Mathematics and its Applications,
The University of Minnesota,
November 8-12, 1999
THIS TALK

CRITICAL PHENOMENA IN DETONATION PHYSICS

competitions between productions and losses

• shock-to-detonation transition in homogeneous explosives

Attempts to understand and model a broader variety of impact problems than previously considered, i.e., incompressible or compressible, planar or curved, constant-speed or accelerated pistons

• first stage of the initiation process in homogeneous explosives
• critical piston dynamics for initiation

• critical diameter for steady-detonation propagation in heterogeneous explosives

Attempts to understand and synthesize a large amount of experimental data, i.e., to relate the explosive microstructure to the detonation macroscopic (critical) behavior

• diameter effect
• critical diameter, shock-sensitivity reversal effect
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1. CRITICAL DYNAMICS FOR SHOCK-INDUCED ADIABATIC EXPLOSIONS

1.1. SDT state-of-the-art from experiments in liquids and gases

<table>
<thead>
<tr>
<th>Liquids: planar impact experiments in NM: flyer plate ~ piston</th>
</tr>
</thead>
<tbody>
<tr>
<td>t&lt;0 piston → u_p NM</td>
</tr>
<tr>
<td>t=0+ D(u_p) + ...</td>
</tr>
</tbody>
</table>

--- previous work ---

Chaiken (1957)  
Campbell et al. (1961)  
Travis (1965)  
Presles (1979)  
Hardesty (1976)  
Sheffield (1989)  
Leal-Crouzet (1998)

--- overall picture ---

An adiabatic explosion takes place at the Piston-Explosive interface at time $\tau$. A super-(CJ?) detonation then builds up in the vicinity of the PE interface, overtakes the shock and eventually decays to the normal CJ regime. Details of the explosion process (multi-step chemistry?) and of the super-detonation build-up (how and where?) remain controversial.
shock-induced ignition of gases (Meyer & Oppenheim, XIII\textsuperscript{th} Symp. Comb.)
As for liquid NM, recent optical pyrometric (nonintrusive) measurements by Leal-Crouzet (1998) would support the strong-ignition scenario (#2), at pressure loadings above 80 kbar (8 GPa).

Given a reactive mixture, both scenarios are indeed possible (e.g., shock-tube Schlieren observations in gases by Meyer and Oppenheim 1970). Their occurrence depends on the detailed kinetic mechanism of the chemical decomposition process and on the loading amplitude.

**Conclusion from experiments:**

*Mild ignition is more likely to occur for weaker loadings (shock-temperature), presumably due to the relatively larger influence of such heterogeneities as turbulence, bubbles, piston roughness, wall-effects, (“hot-spots”), i.e., not strictly one-dimensional phenomena.*

How to get a simple, yet consistent, estimate of the time $\tau$ for adiabatic explosion under more general piston conditions than previously considered?
1.2. *shock initiation as an initial value (Cauchy) problem*

A Lagrangian approach

___ previous related works ___
Kailasanath & Oran (1983)
Jackson & Kapila (1985)
Clarke & Cant (1985)
Jackson, Kapila & S.Stewart (1985)
Kapila & Dold (1985)
Blythe & Crighton (1989)
Short & Dold (1996)
Bauwens (1999)

_______________ this work _______________

We tried to bypass the difficult problem of the coupled determination of the flow field and of the shock motion that is usually addressed by means of perturbation methods.

Our approach essentially features a 1st order expansion, from the shock along the piston material path. The (initial) shock dynamics is determined afterwards from the piston dynamics at the time of impact.
1.2. shock initiation as an initial-value (Cauchy) problem

\[ y \]

\[ \tau \]

\[ x \]

\[ t \]

\[ \tau \]

\[ \text{initial induction state, (e.g., shocked state)} \]
\[ f(t = 0) = f_0 \]
\[ y(t = 0) = y_0 = 0 \]
\[ \frac{dy}{dt} = w : \text{reaction rate} \]
\[ w = t_c^{-1}F(1 - y)^b\exp(-Ta/T) : \text{Arrhenius rate} \]
\[ T_a, T : \text{activation temperature and temperature} \]
\[ \frac{df}{dt} = \frac{\partial f}{\partial t} + u\cdot \text{grad } f : \text{material derivative} \]
\[ u : \text{material speed} \]

\[ f(t) = f_0 + t \left( \frac{df}{dt} \right)_0 \cdots, \quad y(t) = t \left( \frac{dy}{dt} \right)_0, \]
\[ f(y) = f_0 + y \left( \frac{df}{dt} / w \right)_0 \cdots, \quad t = y/w_0, \]

\[ f \leftrightarrow -Ta/T \Rightarrow \frac{dy}{dt} = w_0 \exp(y/\tau w_0), \]
\[ y(t), \quad f(t) = f_0 + \tau \left( \frac{df}{dt} \right)_0 \ln \left( \frac{1}{1 - t/\tau} \right), \]

\[ \tau = \frac{1}{\frac{\partial}{\partial t} \left( -\frac{Ta}{T} \right)_0} = \frac{T_0}{T_a} / \left( \frac{1}{T \frac{dT}{dt}} \right)_0, \]
\[ \tau \equiv \frac{1}{\left( \frac{d \ln w}{dt} \right)_0}, \text{for any rate law sufficiently convex during induction.} \]

\[ \Rightarrow \text{INDUCTION TIME } \tau : \text{RECIPROCAL OF THE INITIAL RATE OF REACTION RATE} \]
1.2. shock initiation as an initial-value (Cauchy) problem

Induction time: \( \tau = 1/ \frac{d}{dt} \left( \frac{-T_a}{T} \right)_0 = \frac{T_0}{T_a} / \left( \frac{1}{T} \frac{dT}{dt} \right)_0 \) : a function of initial state and initial derivatives.

- **Step 1**: at the shock, get as many equations as unknowns, e.g. 1D problems:

<table>
<thead>
<tr>
<th>equations</th>
<th>unknowns</th>
<th>parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 balance equations (jump) (+ eq. of state)</td>
<td>3 initial variables ( f_0 ) (mat. speed ( u_{n0} ), pressure ( p_0 ), volume ( v_0 ))</td>
<td>normal shock velocity ( D_n ) (+ state ahead of the shock) ( \infty )</td>
</tr>
<tr>
<td>3 balance equations (Euler) 3 compatibility equations ( \left( \frac{\partial f}{\partial t} \right)_0 + D_n \left( \frac{\partial f}{\partial n} \right)_0 = \frac{\delta f_0}{\delta t} ) (+ eq. of state &amp; chem. rates)</td>
<td>6 initial derivatives ( z = t, n ), ( \frac{\partial}{\partial z} \left( \begin{array}{c} u_n \ p \ v \end{array} \right)_0 )</td>
<td>normal shock velocity ( D_n ) normal shock acceleration ( \frac{\delta D_n}{\delta t} ) total shock curvature ( C ) (+ state ahead of the shock) ( \infty )</td>
</tr>
</tbody>
</table>

\[ \iff f_0 = f_0 (D_n), \ \frac{\delta f}{\delta t} = \frac{df_0}{dD_n} \frac{\delta D_n}{\delta t}, \left\{ \left( \frac{df}{dt} \right)_0, \tau \right\} = \left\{ \left( \frac{df}{dt} \right)_0, \tau \right\} \left( D_n, \frac{\delta D_n}{\delta t}, C \right) \]

- **Step 2**: get the shock-dynamics parameters \( D_n, \frac{\delta D_n}{\delta t}, C \) from the rear-boundary (piston) dynamics:

The simplest case is that of an incompressible piston: the rear-boundary dynamics, i.e. the piston (material) initial speed, acceleration and curvature are data of the problem (§ 1.3 application #1)

A more complicated one is that of a compressible piston (§ 1.4 application #2).

\[ \iff f_0, D_n, \frac{\delta D_n}{\delta t}, C, \left( \frac{df}{dt} \right)_0, \tau = \text{functions of the user’s parameters} \]
1.2. shock initiation as an initial-value (Cauchy) problem

\[
\begin{align*}
\frac{v_\infty}{D_n} \frac{dp}{dt} & = -v \sigma w - S_1, & \frac{1}{v} \frac{dv}{dt} & = -\frac{\sigma w - M^2 S_1}{1-M^2}, \\
\frac{1}{D_n} \frac{dn}{dt} & = -v \sigma w - S_2, & \frac{1}{T} \frac{dT}{dt} & = g \frac{1-\theta M^2 \sigma w + \theta - 1}{\theta - 1} \frac{\theta - 1}{1-\theta M^2} S_1, \\
S_1 & = \left( \frac{v}{v_\infty} - 1 \right) \left( \frac{v}{v_\infty} D_n C + \frac{3+\Omega}{1-\Omega} \frac{\delta D_n}{\delta t} \right), \Omega \neq M_\infty^2 \equiv \left( \frac{c_\infty}{D_n} \right)^2, \\
S_2 & = \left( \frac{v}{v_\infty} - 1 \right) \left( \frac{v}{v_\infty} D_n C + \frac{1+2M^2+\Omega \delta D_n}{1-\Omega} \frac{\delta t}{\delta t} \right).
\end{align*}
\]

\[
\begin{align*}
\tau & = \left( 1 - \frac{\Delta}{\Delta_{cr}} \right)^{-1} \quad \text{(st : 1D steady-state)} \\
\tau_s & = \frac{1-\theta M^2}{1-\theta M^2}, \quad \ell_s = (D_n - u_n) \tau_s, \\
\Delta & = \frac{\tau_s}{D_n} \frac{\delta D_n}{\delta t} + \frac{1-\Delta}{3+\Omega} \ell_s C, \\
\Delta_{cr} & = \frac{-T_0}{3+\Omega} \frac{1-\theta M^2}{\theta - 1}.
\end{align*}
\]

\[
\tau \to \infty \quad \text{when} \quad \Delta \to \Delta_{cr}
\]

**first principle**

\[
\frac{1}{T} \frac{dT}{dt} = \frac{Q_v T}{C_v T} w - \frac{g}{v} \frac{dv}{dt} \equiv g \left( \frac{\theta}{\theta - 1} w - \frac{1}{v} \frac{dv}{dt} \right) \equiv g \left( \frac{\sigma}{\theta - 1} w + \frac{v}{c_s^2} \frac{dp}{dt} \right)
\]

isochoric transformation: \( \tau_v = \frac{T_0 C_v T}{T_0 Q_v T} \exp \left( \frac{T_0}{T} \right) \equiv \frac{T}{T_0} \frac{\theta - 1}{g \theta \sigma w}, \) (isobaric: \( \tau_p = \theta \tau_v, \quad \theta \neq \gamma \)),

**initiation principle** : predominance of heat production over heat loss

**initiation criterion** : initial heat-production rate \( \geq \) initial volumetric expansion rate (# Dremin 1970 ?)

\[
\text{in temperature-sensitive material: isothermal process } \frac{dT}{dt} \to 0 \Rightarrow \tau \to \infty
\]

**critical expansion** : \( \left( \frac{1}{v} \frac{dv}{dt} \right)_{cr} = (g Z \tau_v)^{-1}, \)

\( \approx O(\tau_v)^{-1}, \) with \( g \neq \gamma - 1 \approx O(10)^{-1} \) and \( Z = \frac{T_0}{T} \approx O(10) \)

\( \Rightarrow \text{CRITICAL DYNAMICS (} \Delta_{cr} \text{), AND CRITICAL PISTON DYNAMICS} \)
1.3. Application #1: Noncompressible Impacts Including Check Against DNS

- **Initial Piston-Dynamics** $\Rightarrow$ **Initial Shock-Dynamics** (Continuity in the Material Speed and Acceleration)

\[
\begin{align*}
\frac{du_p}{dt} & = \left(\frac{du_n}{dt}\right)_0 \left( D_n, \frac{\delta D_n}{\delta t}, C \right) \Rightarrow \delta D_n = \delta D_n \left( u_p, \frac{du_p}{dt}, C \right) \\
\end{align*}
\]

\[
\Rightarrow \quad \tau \left( D_n, \frac{\delta D_n}{\delta t}, C \right) = \tau \left( u_p, \frac{du_p}{dt}, C \right)
\]

- **Initial Shock-Dynamic** $\Rightarrow$ **Induction Time**

\[
\begin{align*}
D_n & = \frac{M}{c_\infty} = \frac{\gamma + 1}{4} \left( 1 + \sqrt{1 + \left( \frac{\gamma + 1}{4} \frac{u_p}{c_\infty} \right)^{-2}} \right) \\
\frac{1}{D_n} \frac{\delta D_n}{\delta t} & = \frac{1 - \Omega}{1 + 2M^2 + \Omega} \left( \frac{\sigma w - u_p C}{u_p} + \frac{1 - M^2}{u_p} \frac{du_p}{dt} \right) \\
\end{align*}
\]

\[
\Rightarrow \quad \frac{\tau_\pi}{\tau_0} = (1 - \frac{\Delta_{\pi}}{\Delta_{\pi,cr}})^{-1}, \quad (\pi^0 : \text{planar, constant-speed})
\]

\[
\frac{\tau_0}{\tau_v} = 1 + \left( \theta - 1 \right) \left( 1 + \frac{2M^2}{1 + \Omega} \right)^{-1}
\]

- **Piston-Dynamics** $\Rightarrow$ **Critical Piston Dynamics**

\[
\Delta_{\pi} = \frac{\tau_0}{\pi_0} \frac{du_p}{u_p} - \frac{2\ell_{\pi_0} C}{3 + \Omega} > \Delta_{\pi,cr} = \frac{T}{T_a} g M^2 \left( \frac{v}{v_\infty} - 1 \right) (3 + \Omega), \quad M = \frac{D_n - u_p}{c_0} = \left( \frac{\gamma - 1 + \frac{2M^2}{1 + \Omega}}{2\gamma} \right)^{\frac{1}{2}}
\]

- **Planar, Constant-Speed Impact: Results & Comparisons**

\[
\frac{\tau_0}{\tau_v} = 1 + \gamma \left( 1 + \frac{1 + \frac{2M^2}{1 + \Omega}}{1 + \frac{M^2}{1 + \Omega}} \right)^{-1}
\]

Bl. & Cr.: Newtonian limit: $\gamma = 1^+$ (dashed lines)

\[
\frac{\tau_0}{\tau_v} \bigg|_{BC} = 1 + \gamma \left( \frac{1}{1 - M} - \frac{1}{1 + \frac{2M^2}{1 + \Omega}} \right) F(M_{\infty}^{-2}),
\]

\[
= 1 + O \left( \gamma - 1 \right)
\]

\[
= \frac{\tau_0}{\tau_v} - O \left( \gamma - 1 \right)^2
\]

\[
F(M_{\infty}^{-2}) = \frac{M}{1 - M^2} \left( \frac{1}{2} \left( 1 + \frac{2M^2}{1 - M^2} \right) + \sum_{n=0}^{\infty} a_n(n, M_{\infty}^{-2}) \right)
\]
1.3. application #1: noncompressible impacts including check against DNS

**Critical piston dynamics**

\[
\Delta \pi = \frac{\pi_0}{u_p} \frac{du_p}{dt} - \frac{2\ell \pi_0 C}{3+\Omega} > \Delta_{\pi cr}
\]
\[
\Delta_{\pi cr} = -\frac{T}{T_0} \frac{g M^2}{(\frac{v_\infty}{c}) - 1}(3+\Omega)
\]

\[\gamma = 1.4, \frac{T_e}{T_\infty} = 80, \frac{Q}{r_T} = 30 / \gamma = 1.2, \frac{T_e}{T_\infty} = 40, \frac{Q}{r_T} = 50\]
1.4. application #2: compressible impacts

- **Shock-tube problems**: inert high-pressure chamber (HPC) and reactive low-pressure chamber (LPC)
- **Aim**: condition for initiation of the LPC gas as function of the initial conditions, the material properties and the characteristic size of the device.

Initially constant-state HPC \( \Rightarrow \) homentropic flow

\[
J_\pm = u_n \pm \varphi (c), \quad d\varphi = \frac{\varphi}{c} dp, \quad (c = c(p), \quad \varphi = \frac{2c}{\gamma - 1}),
\]

\[
\pm \frac{dJ_\pm}{dt} = \pm \alpha \frac{u_n c}{r} \quad \text{on} \quad r^\pm (a, t) : \frac{\partial r^\pm}{\partial t} = u_n \pm c,
\]

\[
\pm \frac{d}{dt} = \frac{\partial}{\partial t} \pm (u_n \pm c) \frac{\partial}{\partial r}, \quad \frac{d}{dt} = \frac{\partial}{\partial t} + u_n \frac{\partial}{\partial r}.
\]

State and derivatives at \( t = 0^+ \), at \( r^* \), on \( (I) : (2) \)
- matching of pressure and material-speed values,
- matching of pressure and material-speed derivatives

\[
\begin{align*}
T_i / T_\infty &= 6 \\
\gamma_i &= 1.2 \\
\gamma_\infty &= 1.4
\end{align*}
\]

\[
\begin{array}{ll}
\begin{array}{l}
\Rightarrow \quad \begin{array}{c}
(u_n, p)_2 = (u_n, p)_0 (D_n) \\
\Rightarrow \quad \begin{array}{c}
D_n \\
\text{states (0) and (2)}
\end{array}
\end{array}
\end{array}
\end{array}
\]

\[
\begin{array}{l}
f (r, t) = f (z) + \ldots, \text{ with } z = \frac{r^* - r}{t},
\end{array}
\]

\[
\begin{array}{l}
\frac{d}{dt} + \frac{v}{c} \frac{dp}{dt} = -\frac{1}{2} \alpha V^2 (c)
\end{array}
\]

\[
\begin{array}{l}
\frac{d}{dt} - \frac{d(u_n, p)}{dt} = \frac{d(u_n, p)}{dt} \left( D_n \frac{\delta D_n}{\delta t} + \frac{\alpha}{r^*} \right)
\end{array}
\]

\[
\Rightarrow \quad \begin{array}{c}
\delta D_n \\
\text{derivatives (perturbative approach)}
\end{array}
\]

\[
\Rightarrow \quad \text{CRITICAL RADIUS OF THE HPC}
\]
1.5. *discussion*

- **validity of the initial-value approach:**
  - the piston dynamics must not deviate from its initial value on a faster time scale than the induction time calculated from this initial value.
  - for example, if the piston is stopped before ignition, the bounded-delay criterion must be replaced by the condition that the delay calculated from the initial value of the piston dynamics is smaller than the time when the piston is stopped.

- **other shock-tube problems:**
  - homentropic, self-similar HPC
  - isentropic HPC

- **applicability to nonlocal problems:** an open question

- **representativeness of the simple Arrhenius rate:** another question
2. CRITICAL DIAMETERS FOR MODEL HETEROGENEOUS EXPLOSIVES

2.1. *correlation critical diameter-reciprocal of specific surface*

- **three kinds of critical diameters** $\Phi_{CR}$
  1. unsuccessful transition from a (too) small-diameter tube to a larger-diameter one
  2. quenching in slowly-converging tube
  3. nonrealization of steady-state detonation after strong, but transient, initiation

<table>
<thead>
<tr>
<th>experimental set-up</th>
<th>typical go and no-go observations</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="tube (~ confinement)" /></td>
<td><img src="image" alt="GO" /> <img src="image" alt="NO-GO" /></td>
</tr>
<tr>
<td><img src="image" alt="explosive" /> <img src="image" alt="detonation shock" /> <img src="image" alt="plane wave generator" /></td>
<td></td>
</tr>
</tbody>
</table>
2.1. correlation critical diameter-reciprocal of specific surface

- **analysis and processing of experiments**
  - specific surface \( A_s = \) total hot-spot surface per unit volume (“ignition potential”):
    \[
    A_s = \frac{6X}{d}
    \]
  - the critical diameter \( \Phi_{CR} \) is a linear function of the reciprocal of the specific surface \( A_s \)
    \[
    \Phi_{CR} = \alpha_1 + \alpha_2 A_s^{-1}
    \]

  - \( \Phi_{CR} = \alpha_1 + \alpha_2 A_s^{-1} \)
    - better for liquid explosives sensitized by glass microballoons, air bubbles and solid particles
  - \( \Phi_{CR}^{-1} = \beta_1 + \beta_2 A_s \)
    - better for porous, low-density, solid explosives and plastic-bonded explosives (PBX)
  - lack of experimental data for high-density, pressed explosives and heterogeneous explosives with very fine particles (# very large specific surface)

- **shock-sensitivity assessment**
  - 1. run-distance to detonation (RDD) : 1D unsteady experiments (planar impact, cf. 1st part)
  - 2. critical diameter (CRD) : 2D steady-state experiments

More shock-sensitive explosives have smaller RDD or CRD because they have faster energy-release rates. Thus, rear (1, RDD) or lateral expansions (2, CRD) are less efficient at slowing down the heat release process.
2.1. correlation critical diameter-reciprocal of specific surface

- shock-sensitivity reversal effect: a property of heterogeneous explosives

<table>
<thead>
<tr>
<th>shock-pressure</th>
</tr>
</thead>
<tbody>
<tr>
<td>larger grains</td>
</tr>
<tr>
<td>smaller grains</td>
</tr>
</tbody>
</table>

run-distance to detonation

non-monotonic dependence of RDD or CRD on the grain size

impact experiments by Moulard (ISL)
(VIIIth and IXth Symposium on Detonation, 1985, 1989)

Smaller hot spots are less efficient at promoting ignition at lower shock pressure

▶ critical hot-spot size ◀

this work is an illustration of the shock-sensitivity reversal effect by means of simple modelling based on preliminary numerical analysis of experiments on detonation critical diameters of model compositions of heterogeneous explosives.
2.2. nitromethane (NM)-glass microballoons (GMB) compositions

- GMBs: a special case of hot spot
  1. only one physical mechanism to be considered for accounting for the local-temperature increases:
     → visco-plastic collapse under shock-loading
  2. model heterogeneous explosives: 1% mass fraction of GMB in NM in our experiments
     → monomodal compositions: \( d_0 = 47 \mu m \) or \( d_0 = 102 \mu m \)
     → bimodal compositions: \( d_0 = 47 \mu m \) and \( d_0 = 102 \mu m \) (0.5% and 0.5%)

- our experiments: a data base for modelling
  - 1. critical diameters
  - 2. detonation velocity vs charge diameter in STEEL or PVC tubes
  - 3. detonation shock curvature vs detonation velocity

- two dependencies on the diameter
  1. homogeneous explosive: weak dependence
  2. heterogeneous explosives: strong dependence

- related difficult problems
  1. “low-velocity” detonation (homogeneous & heterogeneous)
  2. non-ideal explosives \( \Delta D_{fail.}/D_{CJ} > 0.1 \)
2.3. modeling assumptions

- **objectives**: from the microstructure of the explosive to the macroscopic behavior of the detonation
- **assumptions**: the simplest choices for hydrodynamics, thermodynamics and chemical kinetics

1. **quasi-onedimensional steady reaction zone**:
   *e.g. Bdzil & Stewart, 1988*
   * The 3D unsteady partial-derivative balance equations reduce to a Q1D ordinary system of equations.
   * Integration from the shock \( D_n \) to the sonic locus

2. **eigenvalue evolution law**:
   * shock normal velocity \( D_n \) - shock total curvature \( C \) relationship
   \[ D_n = D_n(C), \quad D_{CJ} = D_n(0), \quad C < C_{CR} \]
   * Self-sustained waves too strongly curved can’t exist (competition between heat-release and lateral expansion (~curvature))

3. **geometry + \( D_n(C) \) relationship**:
   * differential equation for the 2D-steady-shock shape \((z, \varphi) (r, D)\)
   * Boundary condition \( \varphi (\Phi, D) = \varphi_{edge}(D) \to D (\Phi) \)
   * Critical diameter \( \Phi_{CR} = \Phi(D), \quad D \) such that \( C_{edge} (D_n) = C_{CR} \)
2.3. modeling assumptions

- **reaction zone**: multi-phase Q1D-ST equations: \( GMBs + \text{unreacted NM} + \text{reacted NM} \)

  initiation of shocked NM: nonadiabatic explosion \( \subset \) \{inductive chemistry + conductive heat-transfer\}

  Arrhenius + viscoplastic collapse of the GMBs

  combustion of the NM: surface reaction, first expanding then converging (after coalescence of flame fronts)

- **chemical kinetics**: principle: elementary cell

  \[
  \frac{dy}{dt} = S_f V, \\
  S_f \# A_{s}^{\text{ign}}, \quad V \sim p \exp(\beta \Delta T), \\
\]

  \[
  \beta = \frac{1}{2} \frac{E_a}{RT_{\text{ign}}^p}, \\
  \Delta T = T_{NM} - T_0 \\
\]

  small collapse speed (#50 m/s) of GMB compared to particle velocity (#4000 m/s)

  \[
  \Rightarrow A_{s}^{\text{ign}} \# A_{s}^{0},
\]

- **equations of state**

  shocked NM: Mie-Gruneisen // reacted NM: Abel-type
2.4. results for nitromethane (NM)-glass microballoons (GMB) compositions

- Detonation velocity vs reciprocal of charge diameter

\[ \text{detonation velocity (mm/µs)} \]

\[ \text{reciprocal of charge diameter (1/mm)} \]

→ Given the strength of the confinement, the smaller the diameter, the smaller the detonation velocity \((D)\).

→ Given the diameter, the weaker the confinement, the smaller \(D\).

→ All curves have the downward concavity that characterizes most heterogeneous explosives.

→ The concavity is stronger in PVC tubes than in STEEL tubes.

→ Given a tube diameter, larger detonation velocities correspond to compositions with smaller GMBs because, at constant mass fraction, the GMB volumetric fraction is smaller when the GMBs diameter is smaller, so that there is more explosive (NM, energy) per unit volume.
- **critical diameters**

<table>
<thead>
<tr>
<th>$d_0$ (µm)</th>
<th>Monomodal (47 µm)</th>
<th>Monomodal (102 µm)</th>
<th>Bimodal (47 &amp; 102 µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_0$ (g/cm³)</td>
<td>1.09</td>
<td>1.04</td>
<td>1.064</td>
</tr>
<tr>
<td>X (% vol. fract.)</td>
<td>4.2</td>
<td>8.5</td>
<td>6.4</td>
</tr>
<tr>
<td>$D_{CJ}$ (mm/µs)</td>
<td>5.914</td>
<td>5.686</td>
<td>5.829</td>
</tr>
<tr>
<td>$\Phi_{CR}$ (mm) in PVC tube</td>
<td>exp/num : 8.5/10.8</td>
<td>exp/num : 9.2/13.9</td>
<td>exp/num : 8.5/13.3</td>
</tr>
<tr>
<td>$\Phi_{CR}$ (mm) in STEEL tube</td>
<td>exp/num : 2.7/2.5</td>
<td>exp/num : 3.0/3.2</td>
<td>exp/num : 2.6/2.7</td>
</tr>
</tbody>
</table>

→ the stronger the confinement, the smaller the critical diameter
→ all compositions have same specific surface, and, given the confinement, same critical diameter (approx.)

- **correlation** Critical diameter–Reciprocal of specific surface (PVC)

<table>
<thead>
<tr>
<th>critical diameter (mm)</th>
<th>reciprocal of specific surface (mm⁻¹)</th>
<th>origin : $\Phi_{CR} \sim u/(dy/dt)$, $dy/dt \sim A_S \Rightarrow \Phi_{CR} \sim 1/A_S$</th>
</tr>
</thead>
</table>
| $d_0 = 5$ µm | $0, 0.1, 0.2, 0.3, 0.4$ | considering the approximations
→ acceptable agreement between numerics and experiments for monomodal or bimodal compositions 47 µm & 102 µm.  
**but**

→ numerical predictions for monomodal compositions with smaller GMBs (5 µm) far from experimental expectations.

→ For too small GMBs, the NM induction delay is comparable to the travel time from the shock to the sonic locus
● shock-sensitivity reversal effect

▶ monomodal compositions

\[ \Phi_{CR} \sim 1/A_S \text{ for the active GMBs in the composition.} \]

⇒ nonmonotonic dependence of detonation critical diameter on GMB diameter

\[ \text{for given specific surface,} \]

small hot spots are many but not sufficiently active
(small delay for the 47 & 102 µm, much larger one for the 5 µm),

whereas

large ones are sufficiently active but, obviously, not enough of them.

▶ bimodal compositions

\[ \text{specific surface} \]

<table>
<thead>
<tr>
<th></th>
<th>monomodal composition</th>
<th>bimodal composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>critical diameter</td>
<td>( d_0 = 102 \mu m )</td>
<td>( d_0 = 102 \mu m )</td>
</tr>
<tr>
<td></td>
<td>( Y = 0.5% )</td>
<td>( d_0 = 5 \mu m )</td>
</tr>
<tr>
<td>( \sim 20 \text{ mm in PVC} )</td>
<td>( 2.6 \text{ mm}^{-1} )</td>
<td>( 6.5 \text{ mm}^{-1} )</td>
</tr>
</tbody>
</table>

at small detonation-velocity deficits, (e.g., shock pressure) the induction delay is small for both sizes of GMBs, but, for larger deficits, it increases faster around smaller GMBs.
2.5. *discussion*

- **problems**
  - questionable use of the Q1D steady-assumption
  - representativeness of simple rate law and equation of state for large detonation-velocity deficits

- **future experimental works**
  - identification of the actual collapse mechanism and effects of initial GMB diameter and input pressure
  - critical-diameter and impact experiments for bimodal compositions with small GMBs

- **future numerical works**
  - 1D unsteady calculations
  - as for any heterogeneous medium: cooperative phenomena at mass fractions larger than considered in this work
3. CONCLUSION

Critical phenomena in detonation physics

- a central and difficult set of problems
  - safety-related issues
  - compressible fluids, nonlinearities, 3D instabilities, turbulence

- condensed-phase materials: additional difficulties
  - constitutive relationships
  - local thermodynamical equilibrium

- the Euler (inviscid) equation paradigm
  - homogeneous gases and liquids: acceptable in most cases close to detonation conditions
  - heterogeneous materials: transfer phenomena at the scale of the heterogeneities