# Explosion dynamics of propellants and laser ablation of metals

## Workshop on Energetics-Past and Present
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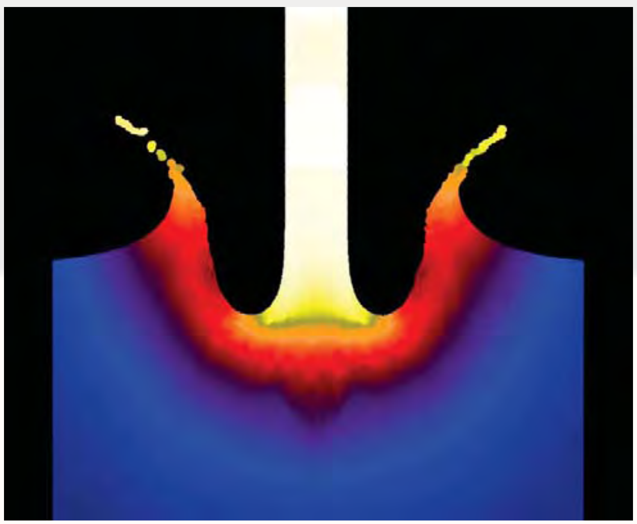
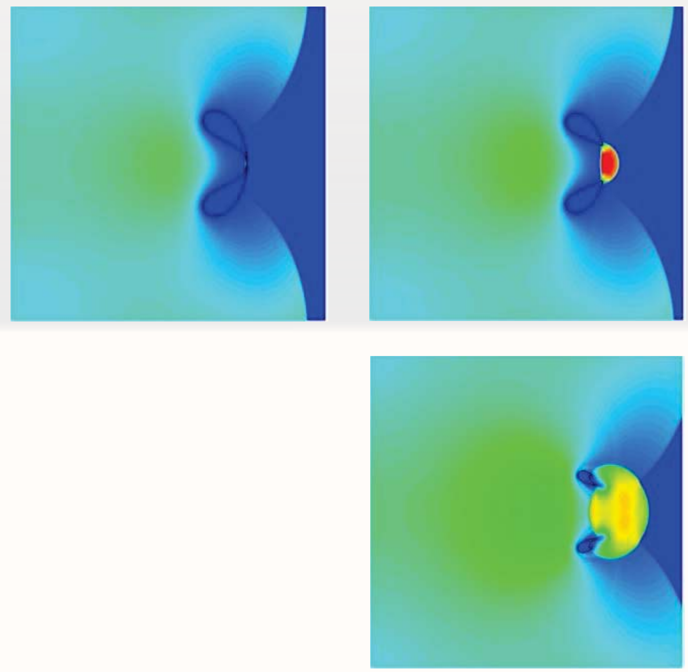
# ENERGETICS RESEARCH

- **Hydrodynamic Shock Physics code** for energetic materials
- **Laser** induced detonation of metals
- Phenomena of great interest include
  - **Deflagration and detonation** of high energy materials
  - High energy thermo-fluid simulation
  - Explosion, Impact, Jet formation

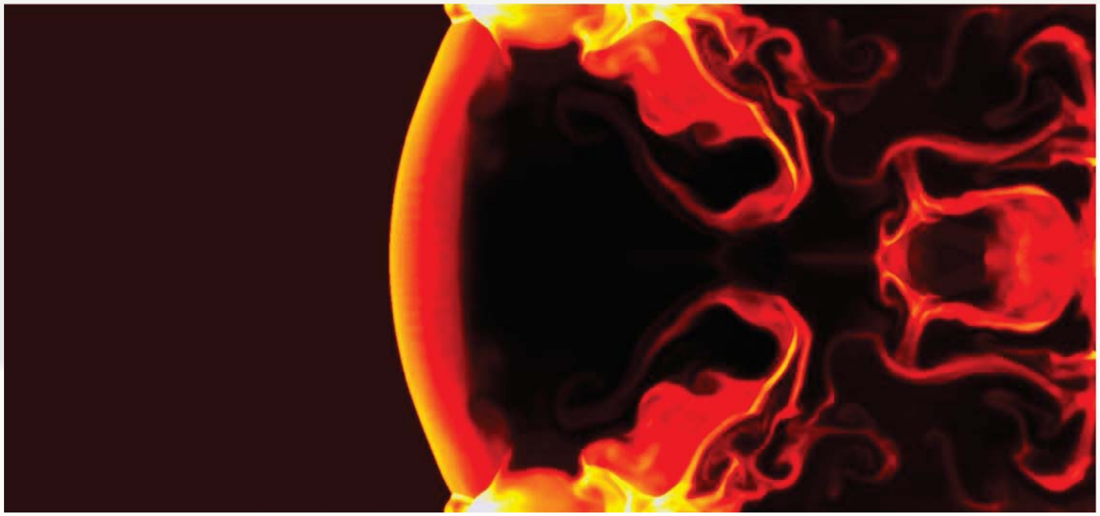




High strain rate phenomena of multi-material interactions

# Cookoff and Flame acceleration

- **Rocket propellant (Liquid and Solid) flame acceleration due to external stimuli (shock wave and thermal load - cookoff)**
  - **Deflagration and Detonation**
  - **Accidents and failures**
  - **Preventions and insensitive energetic materials**



**Shock-induced Detonation Transition (Ethylene-Air)**

# Thermal decomposition of Propellant

- **AP/HTPB Reaction Model**
  - **Modified 2-step Beckstead model**
    - **AP 88%, HTPB 12%**
    - **Mixed combustion (premixed flame, primary diffusion flame, final diffusion flame)**

$R_1$ : AP (X)→decomposition product (Z)

$R_2$ : βZ + binder (Y)→final product

(β=88/12=7.33)

**2-Step Kinetics**

$$R_1 = \rho Y_X Z_1 P_0^{1.744} \exp\left(-E_{a,1}/RT\right)$$

$$R_2 = \rho Y_Y \rho Y_Z Z_2 P_0^{1.75} \exp\left(-E_{a,2}/RT\right)$$

**Reaction Rate**

$$\frac{\partial \rho Y_X}{\partial t} = r_X = -R_1 \qquad \frac{\partial \rho Y_Y}{\partial t} = r_Y = -R_2$$

$$\frac{\partial \rho Y_Z}{\partial t} = r_z = R_1 - 7.51 R_2$$

$$\rho Y_{product} = \rho - (\rho Y_X + \rho Y_Y + \rho Y_Z)$$

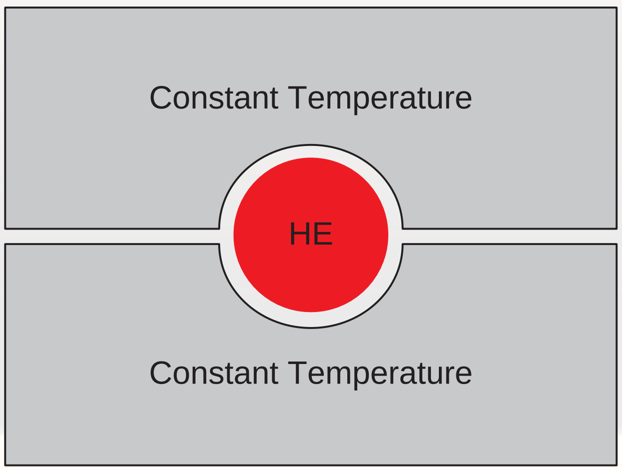
**Species evolution**

| Reaction Step | Z | E(KJ/mol) | Reaction Order | Heat of Reaction Q (kJ/kg) |
|---|---|---|---|---|
| 1 | 800 | 137.18 | 1 | -297 |
| 2 | 1100 | 178.75 | 2 | +9643.2 |

**Reaction coefficients**

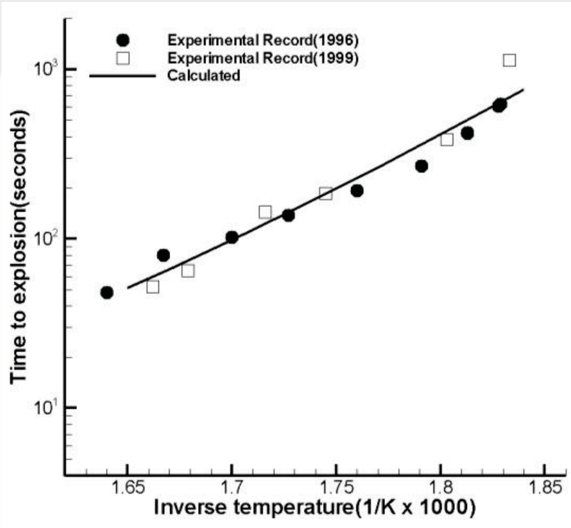
# Thermal decomposition

- **One dimensional time to explosion(ODTX)**
  - **Kinetics verification apparatus**
  - **Constant volume explosion analysis of sample of 1.27cm in diameter: time to explosion is measured (LLNL)**



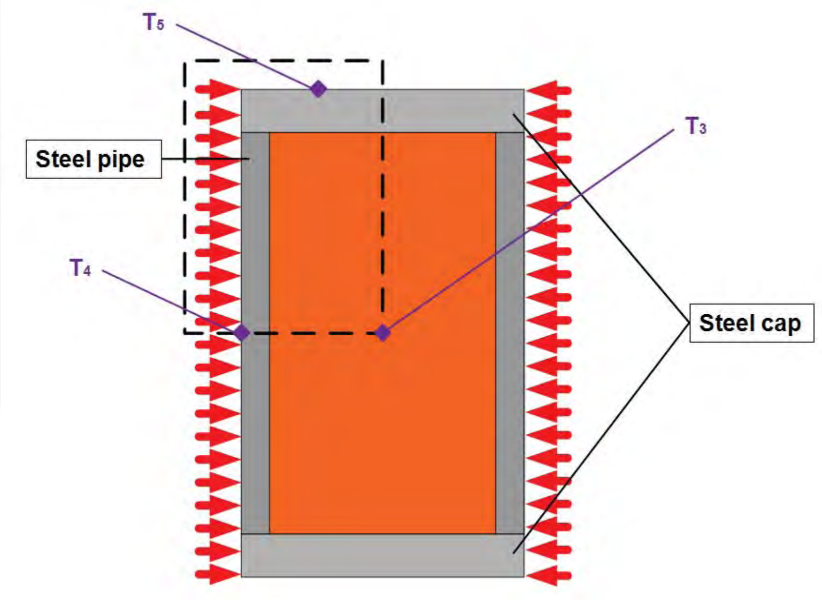

$$\rho C \frac{\partial T}{\partial t} = -\nabla \cdot \vec{q} - \sum_{j=1}^{N} R_j q_j$$

$$\rho \frac{\partial Y_i}{\partial t} = r_i$$

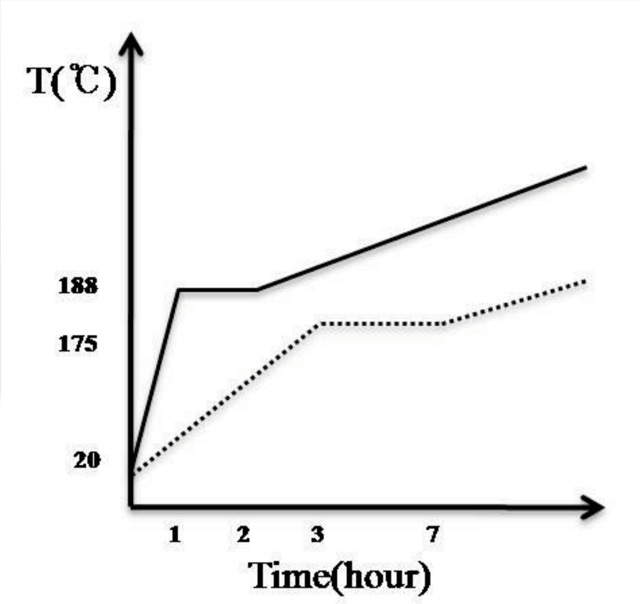


# AP/HTPB slow cookoff experiment

- **2 AP/HTPB Propellant (AP 88%, HTPB 12%) Tests**
  1. **188 ℃/hour heat, 1 hour soak, and 6 ℃/hour heat (2006)**
  2. **175 ℃/3hours, 4 hour soak, 1.8 ℃/hour (2009)**



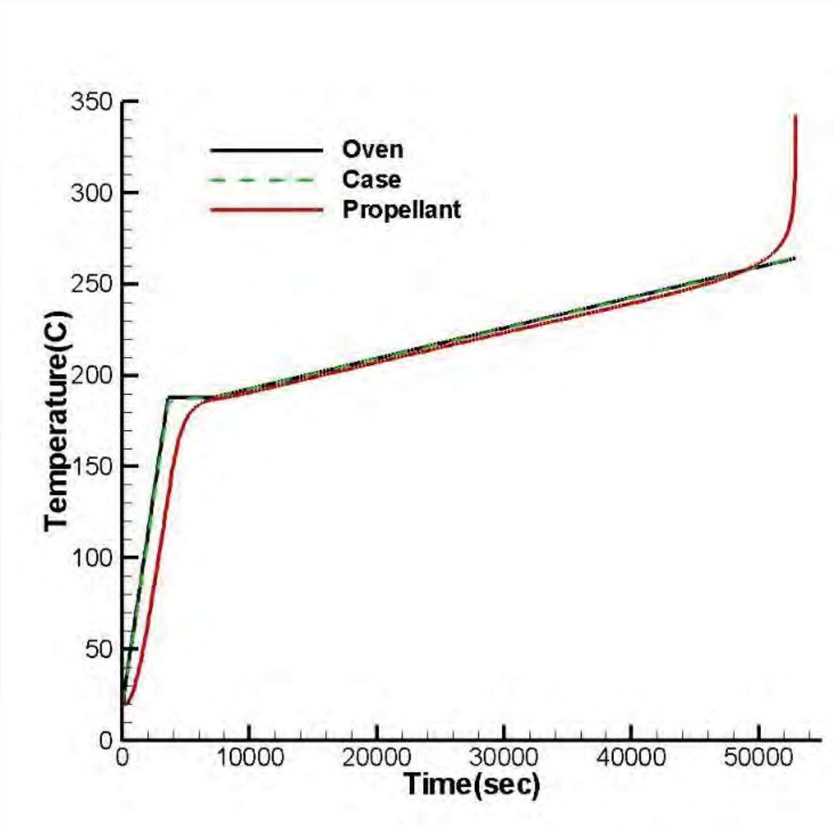

**Modeling schematics**

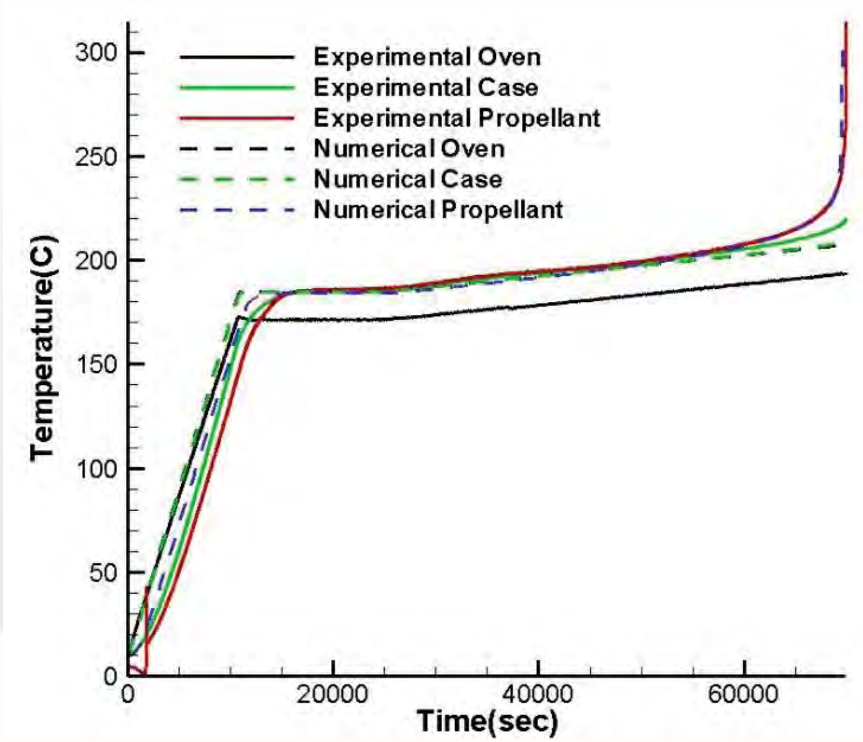



**Control TC comparisons of two experiments**

# AP/HTPB cookoff results

- **Time and Temperature of explosion predictions**




**TEST 1 (2006)**

**Experiment ~ 15 hours**

**Calculation ~ 14.7 hours**

**TEST 2 (2009)**

**Experiment ~ 19.4 hours**

**Calculation ~ 19.4 hours**

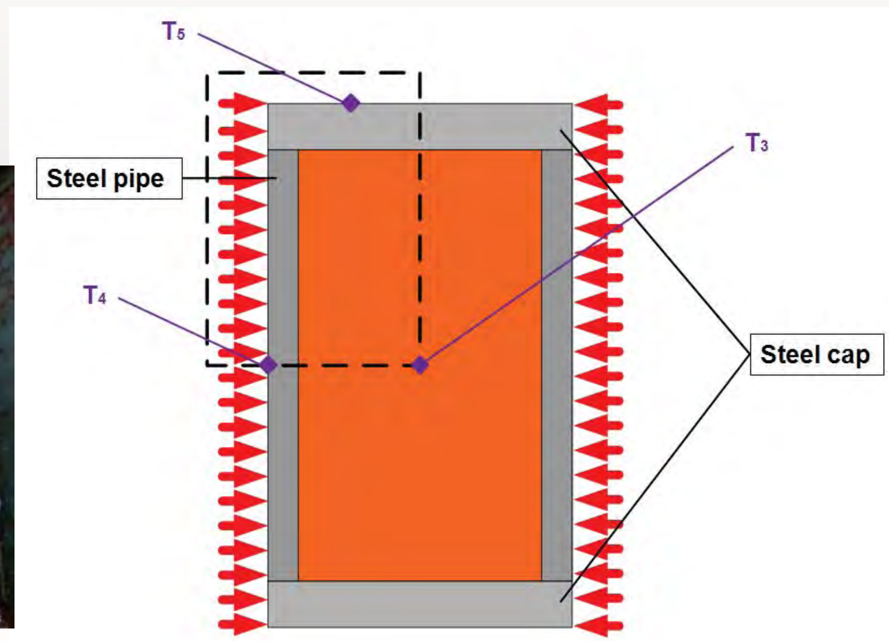
# AP/HTPE Insensitive Propellant

- **AP-AN/BuNENA-HTPE**
  - AP/HTPB's lower decomposition temperature
    - AP/HTPB decomposes at 250℃ while AP/HTPE decomposes at 150℃
    - AP/HTPE meets safety requirement
  - AP/HTPE's thermal properties
    - Modified AP/HTPB meets preliminary AP/HTPE model

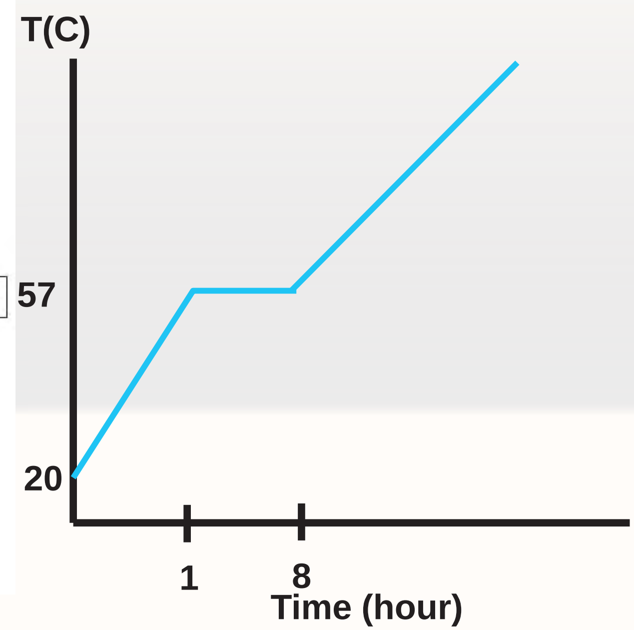
# AP/HTPE slow cookoff test

- **AP/HTPE Propellant**
  - **AP 88%, HTPE 12%**
  - **Heat 57 ℃/3 hours, soak for 7 hours, 3.3 ℃/1 hour heat**

Experiment (2009)



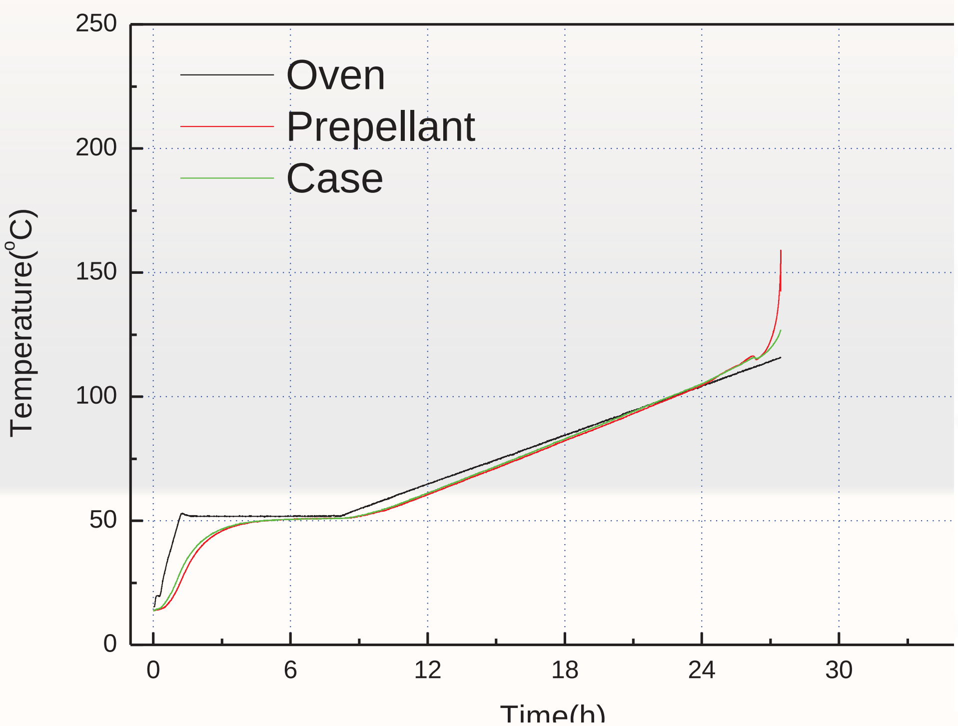

Simulation setup



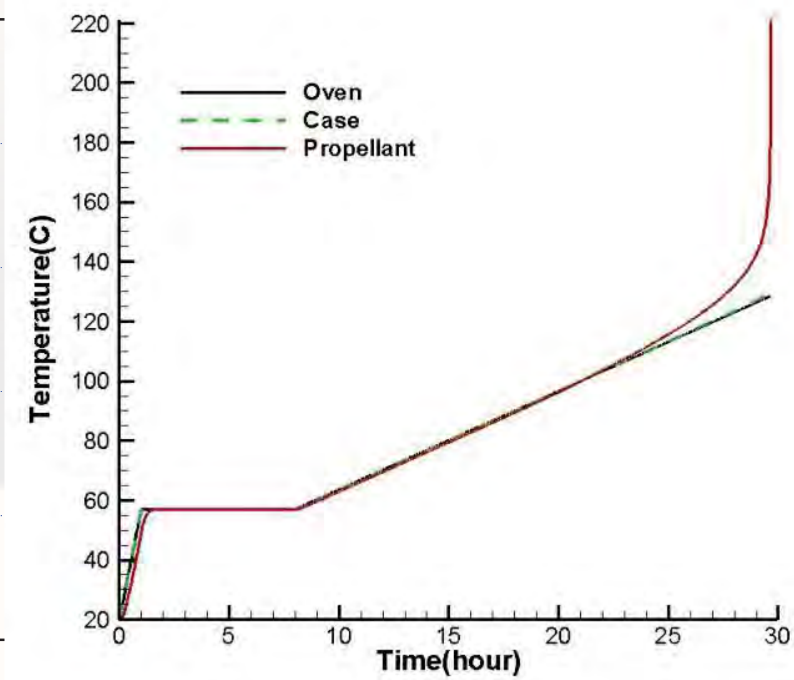

Control TC

# AP/HTPE slow cookoff calculated

- **Thermal explosion time-temperature comparison**
  - **Measured : ~ 27.5 hours**
  - **Calculated : ~ 28.5 hours**



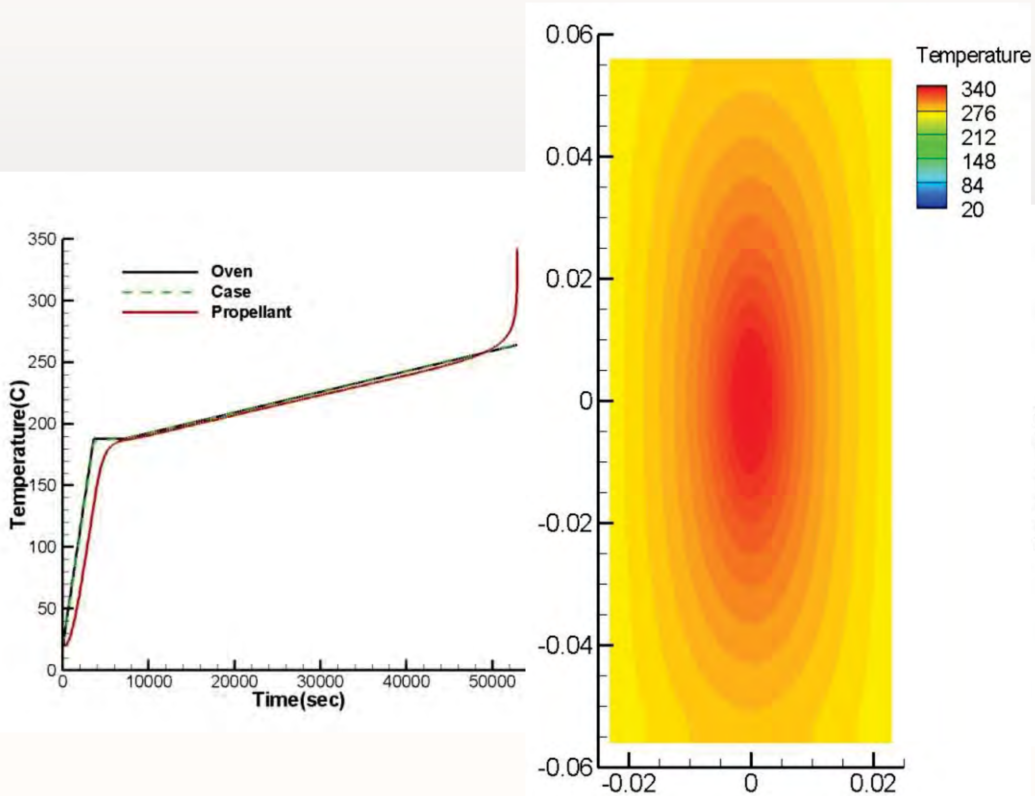

**Experiment (2009)**



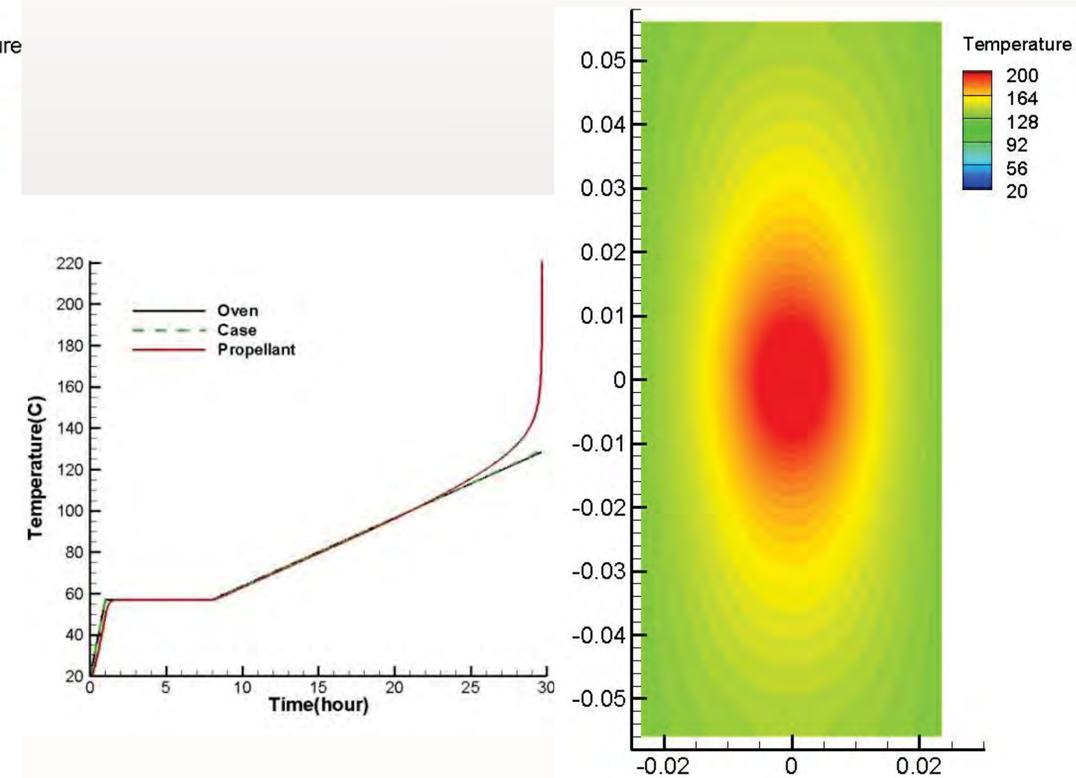

**Calculated**

# Thermal decomposition of AP propellants

- **AP/HTPB, AP/HTPE**
  - **Runaway for AP/HTPB is at 250**
  - **Runaway for AP/HTPE is at 150℃**
  - 




**AP/HTPB**

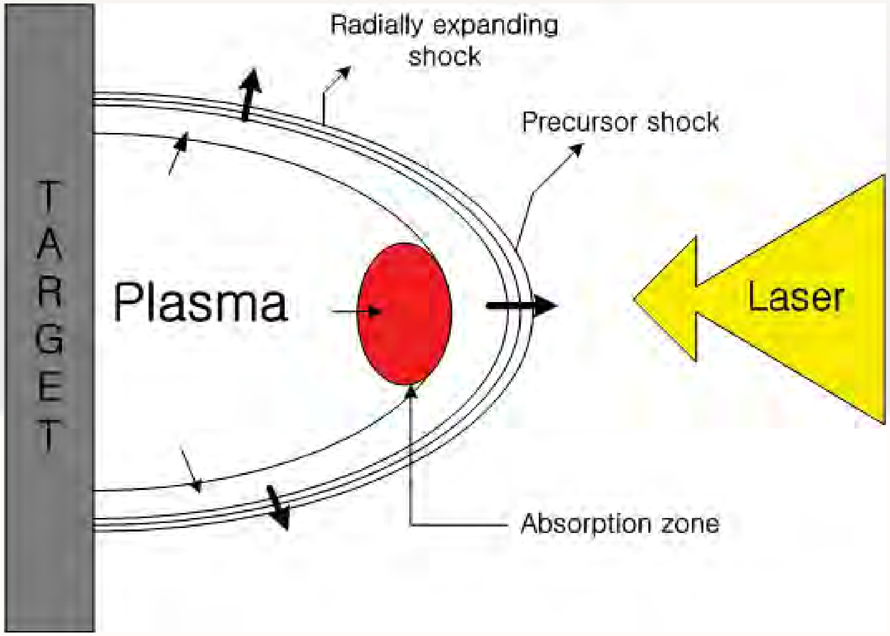



**AP/HTPE**

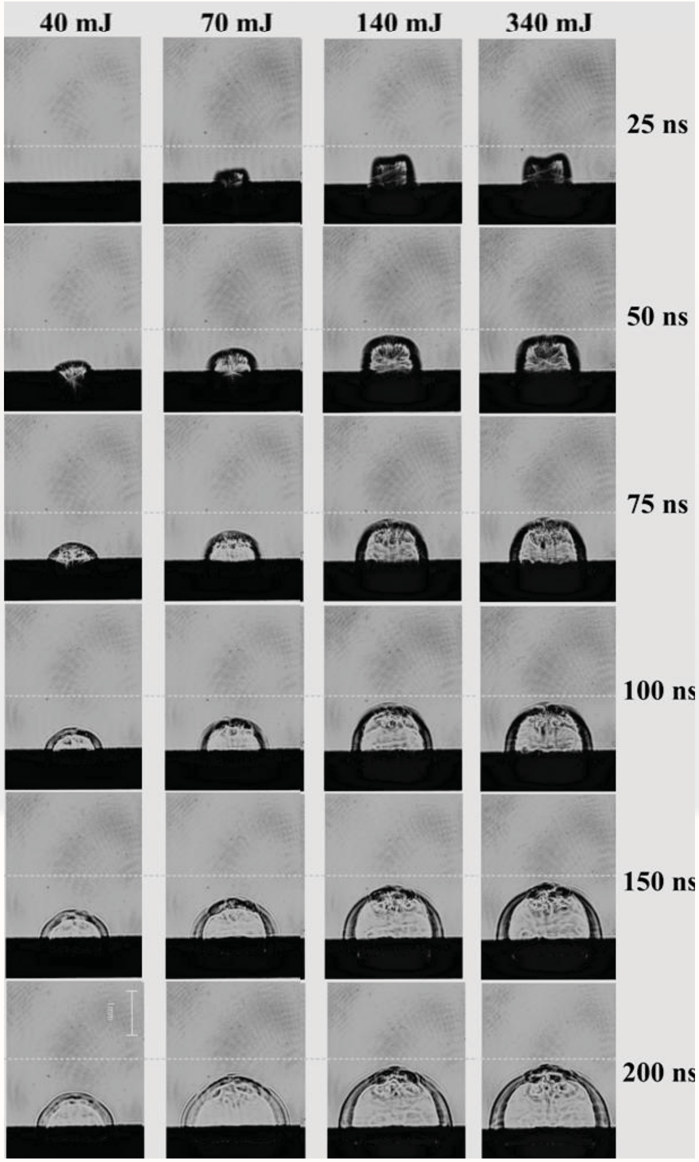
# Laser supported detonation

- **Laser ablation**
  - **Laser induced surface reaction by the beamed energy**
  - **Plasma generation followed by shock wave propagation**

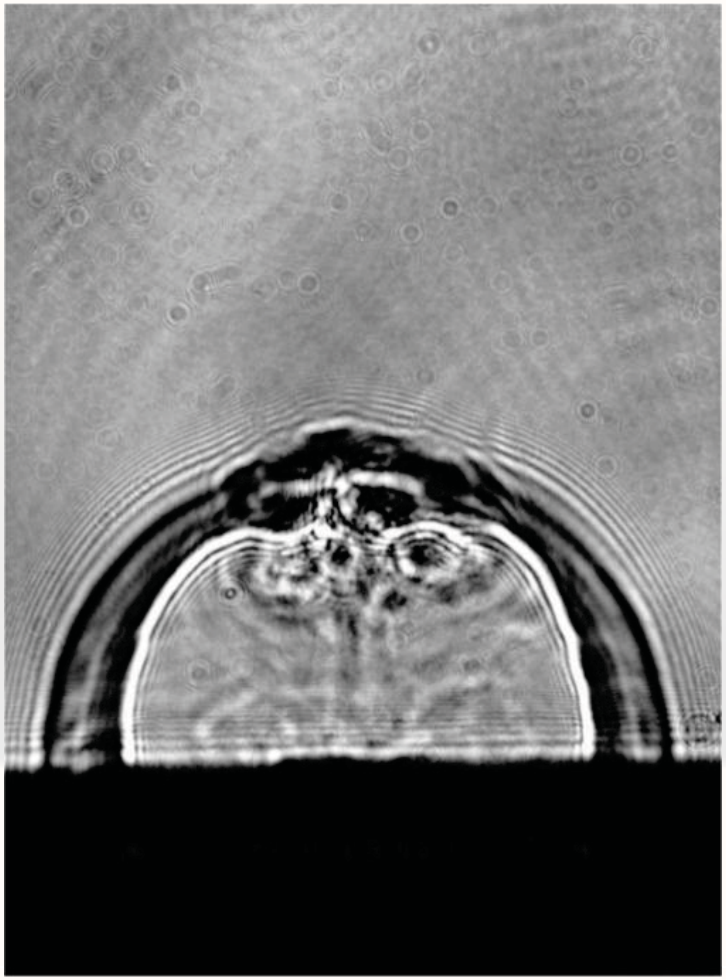
  - **Applications**
    - **Chemical analysis**
    - **Material Processing**
    - **Laser propulsion, etc**



# Shadowgraph (40–340 mJ)

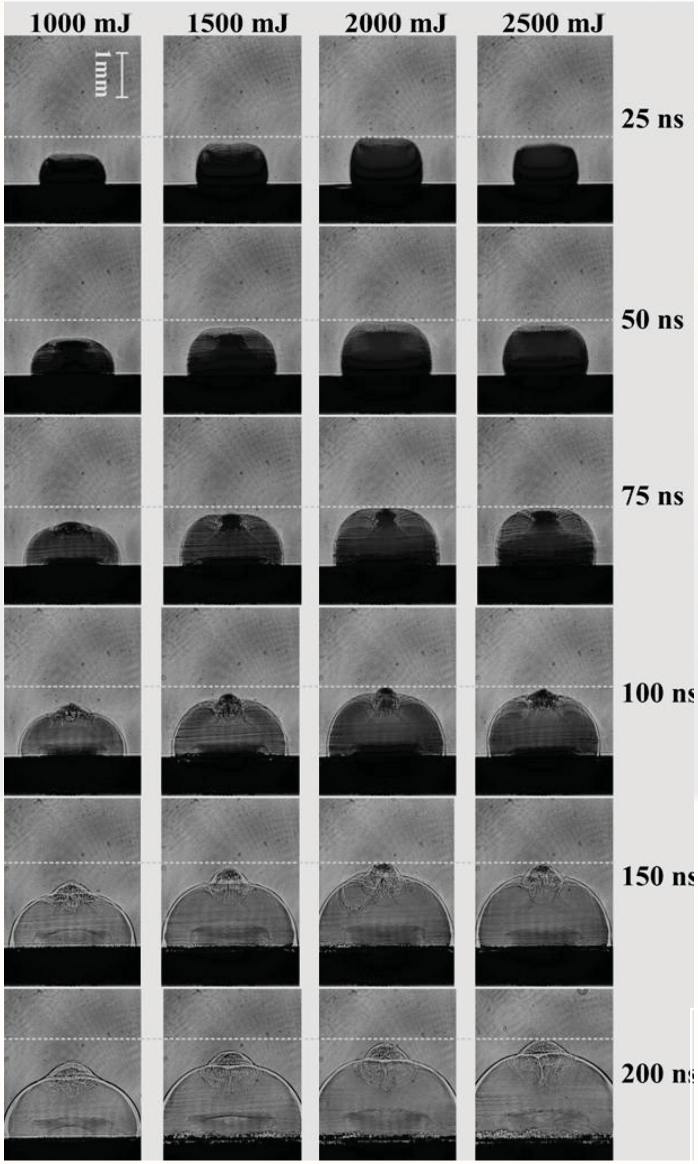



<Increasing delay times in 1 atm over an Al target>

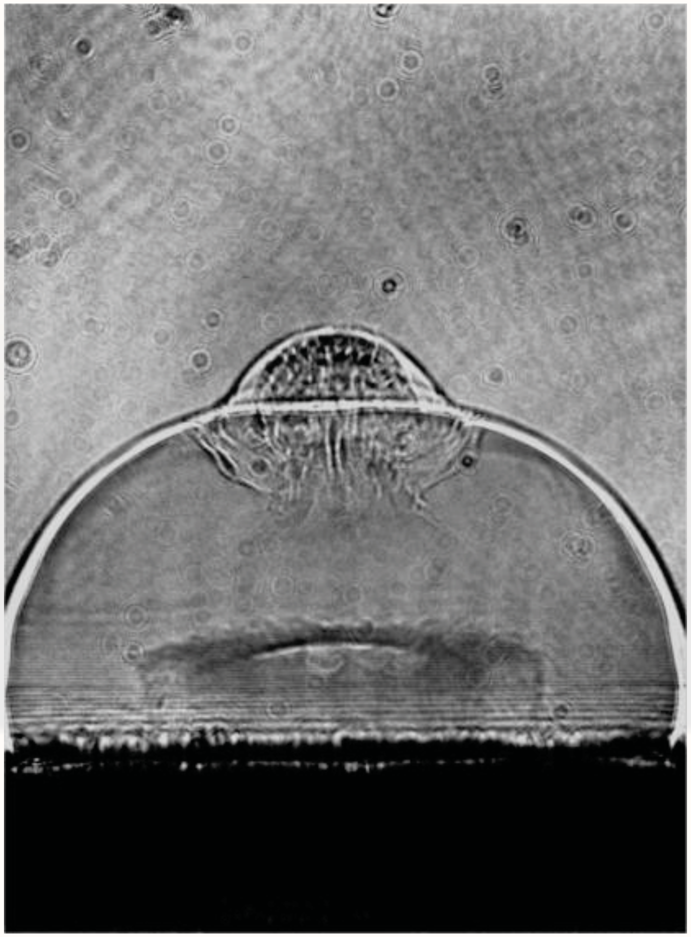


- **Ionized and shock fronts coupled without chemical reaction**

# Shadowgraph (1000-2500 mJ)

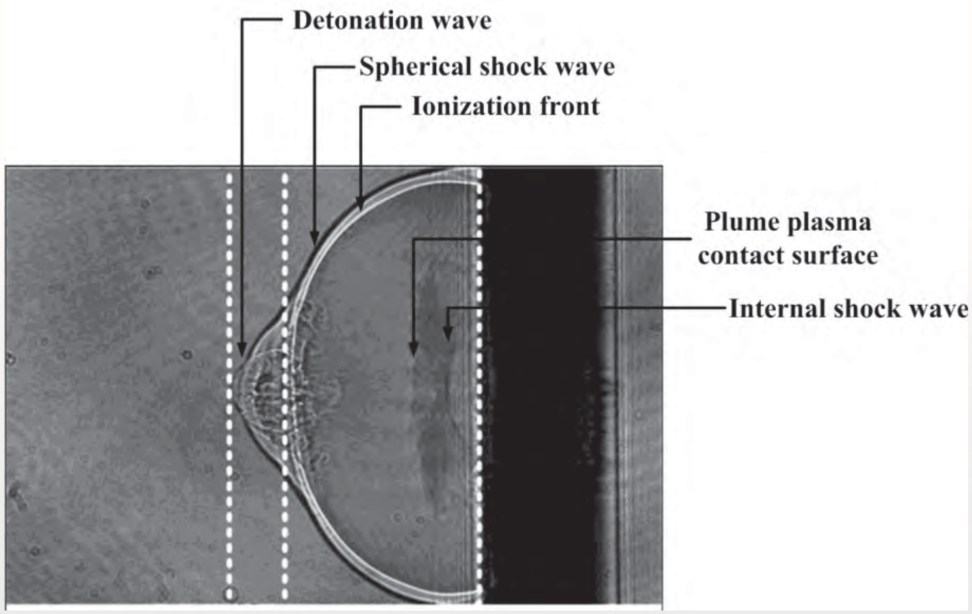



<Increasing delay times in 1 atm over an Al target>



- **Separation of shock and detonation fronts**

# Laser supported detonation velocity




- image resolution method (ratio of pixel and real length )

| Energy (mJ) | Detonation velocity (m/s) | SD | SDOM | %( $\frac{\sigma_{\bar{x}}}{\bar{x}} \times 100$ ) |
|---|---|---|---|---|
| 1000 | 1399 | ± 128 | ± 74 | 5.27 |
| 1500 | 1440 | ± 67 | ± 37 | 5.28 |
| 2000 | 1502 | ± 73 | ± 42 | 2.79 |
| 2500 | 1507 | ± 174 | ± 100 | 6.66 |

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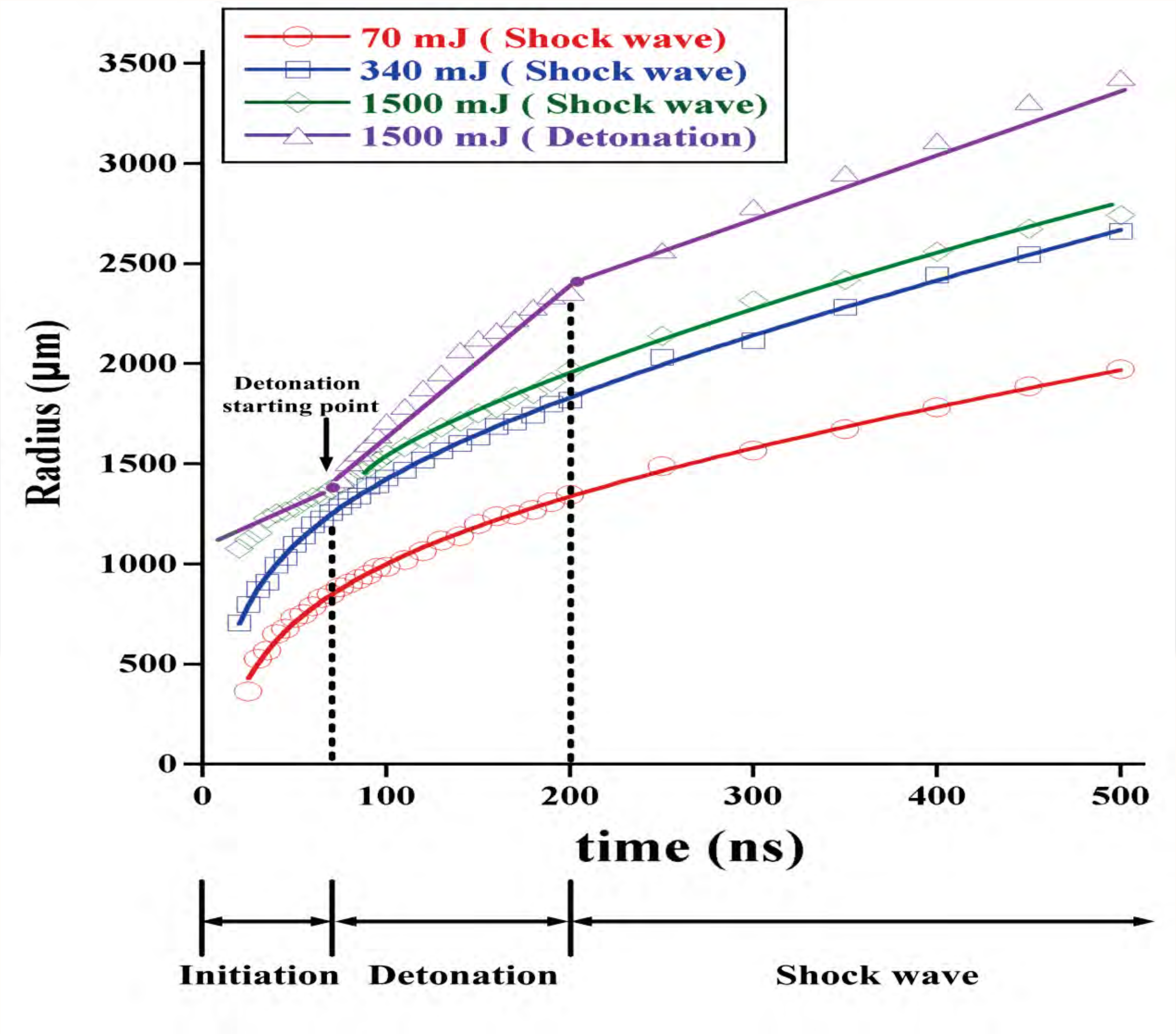
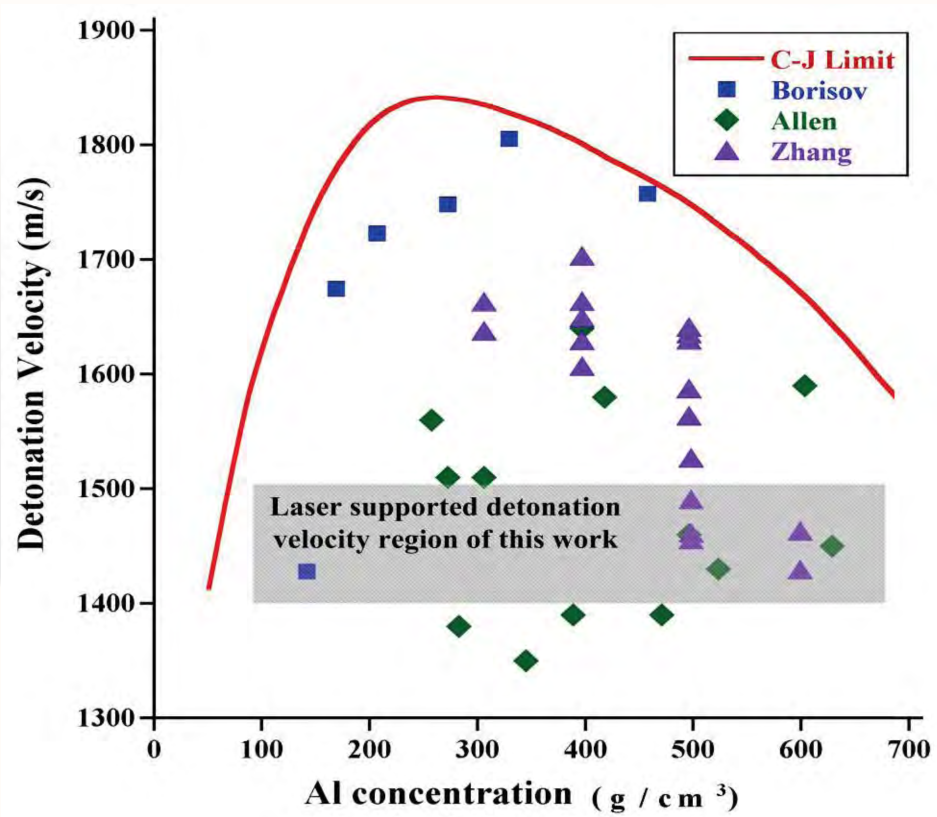
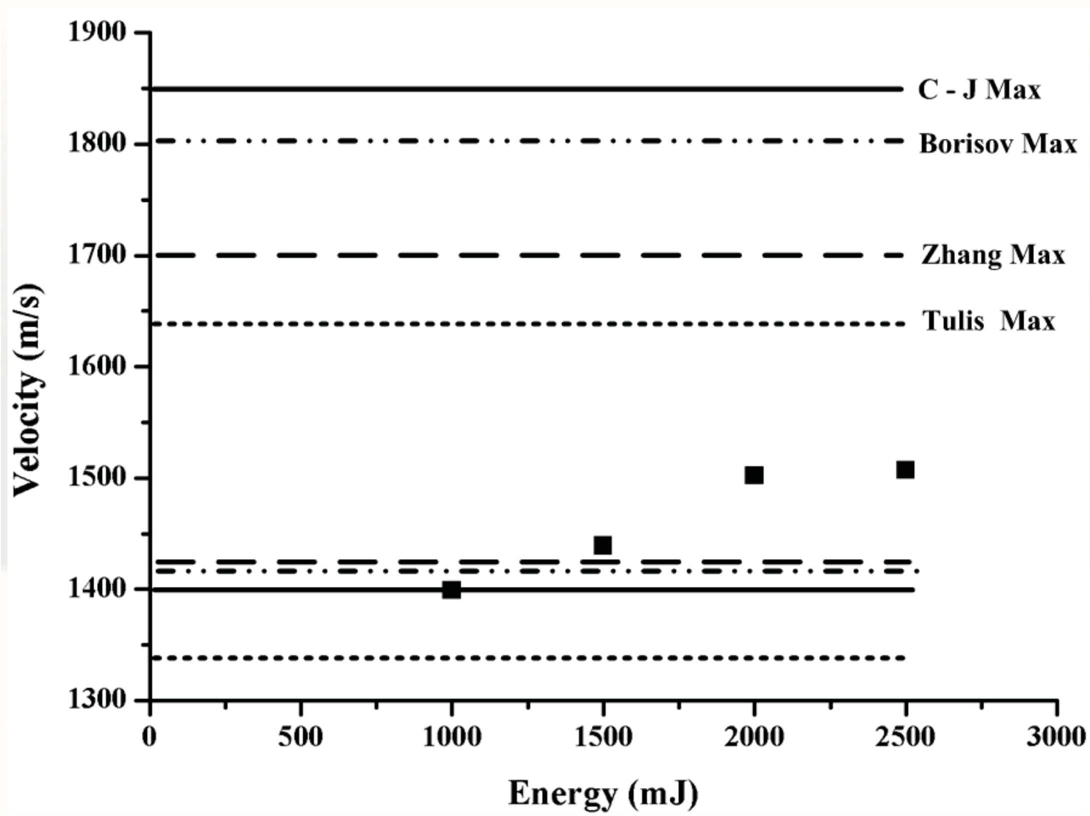
- **Time – Radius of propagation**



- **Al powder detonation vs. Laser supported detonation of Al sample comparison**



# Laser supported detonation pressure

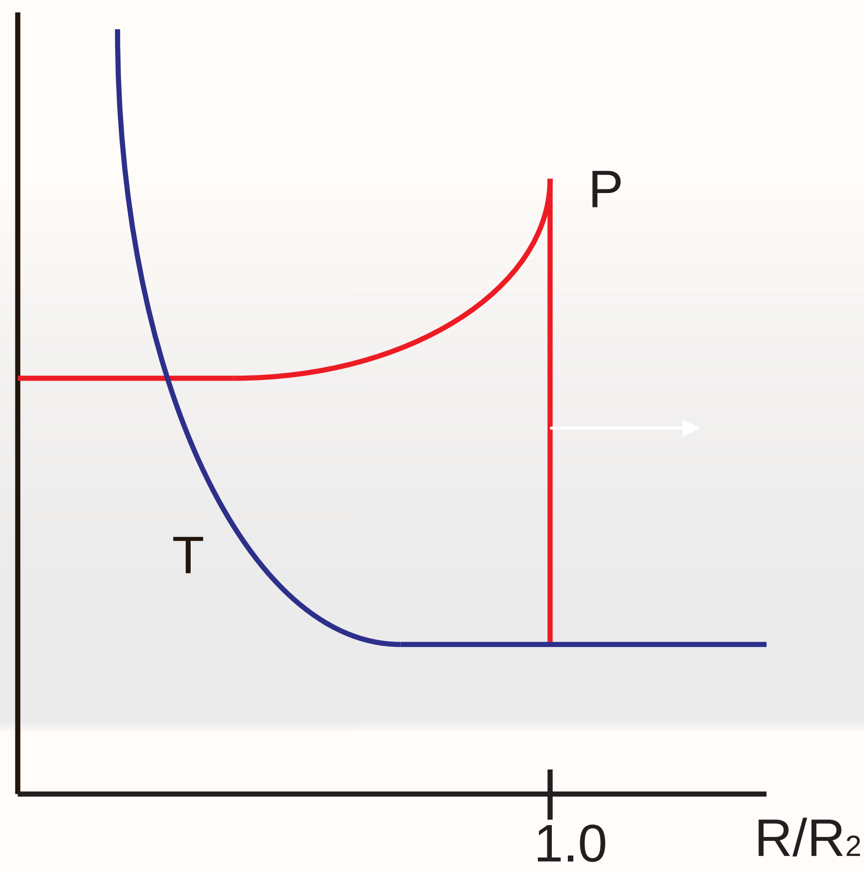
$$p_s = \frac{\rho_o V_s^{\,2}}{\gamma_{metal} + 1}$$

[ $\rho_s$: the density of the detonation wave]
[ $P_s$ : the pressure of the detonation wave]
[ $V_s$ : the detonation wave velocity]
[ $\gamma_{metal}$ : the specific heat ratio of metal]
[ $\rho_0$: the density of the ambient gas]

| Energy (mJ) | Detonation pressure (pa) | SD | SDOM | %( $\frac{\sigma_{\bar{x}}}{\bar{x}} \times 100$) |
|---|---|---|---|---|
| 1000 | 981772 | ± 12833 | ± 7409 | 0.39 |
| 1500 | 1039616 | ± 6727 | ± 3884 | 0.71 |
| 2000 | 1132298 | ± 7281 | ± 4204 | 0.37 |
| 2500 | 1139751 | ± 17474 | ± 10089 | 0.89 |

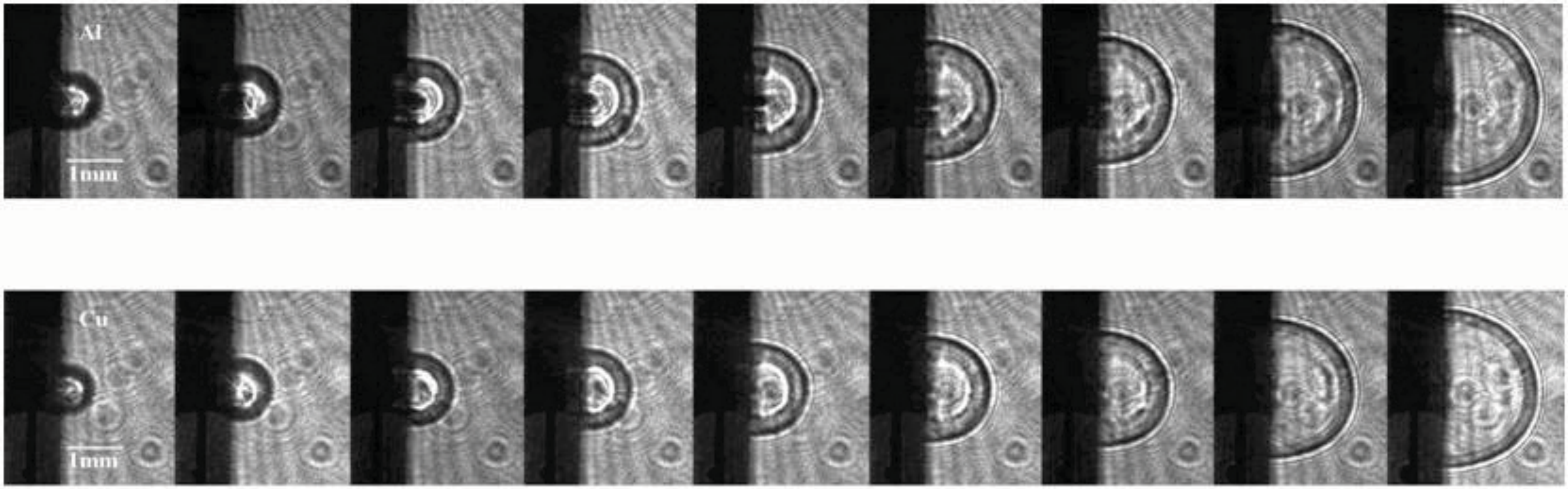
# Laser supported explosion (Sedov-Taylor Theory)

- Explosive melting and evaporation of solids
- Metals (with significant melt phase) undergo phase explosion upon high energy irradiation
- Classical Sedov-Taylor point source explosion theory seems to work here
- Hydrodynamic modeling of Laser explosion
- Ignition of energetic matter (space propulsion and weapons) via laser



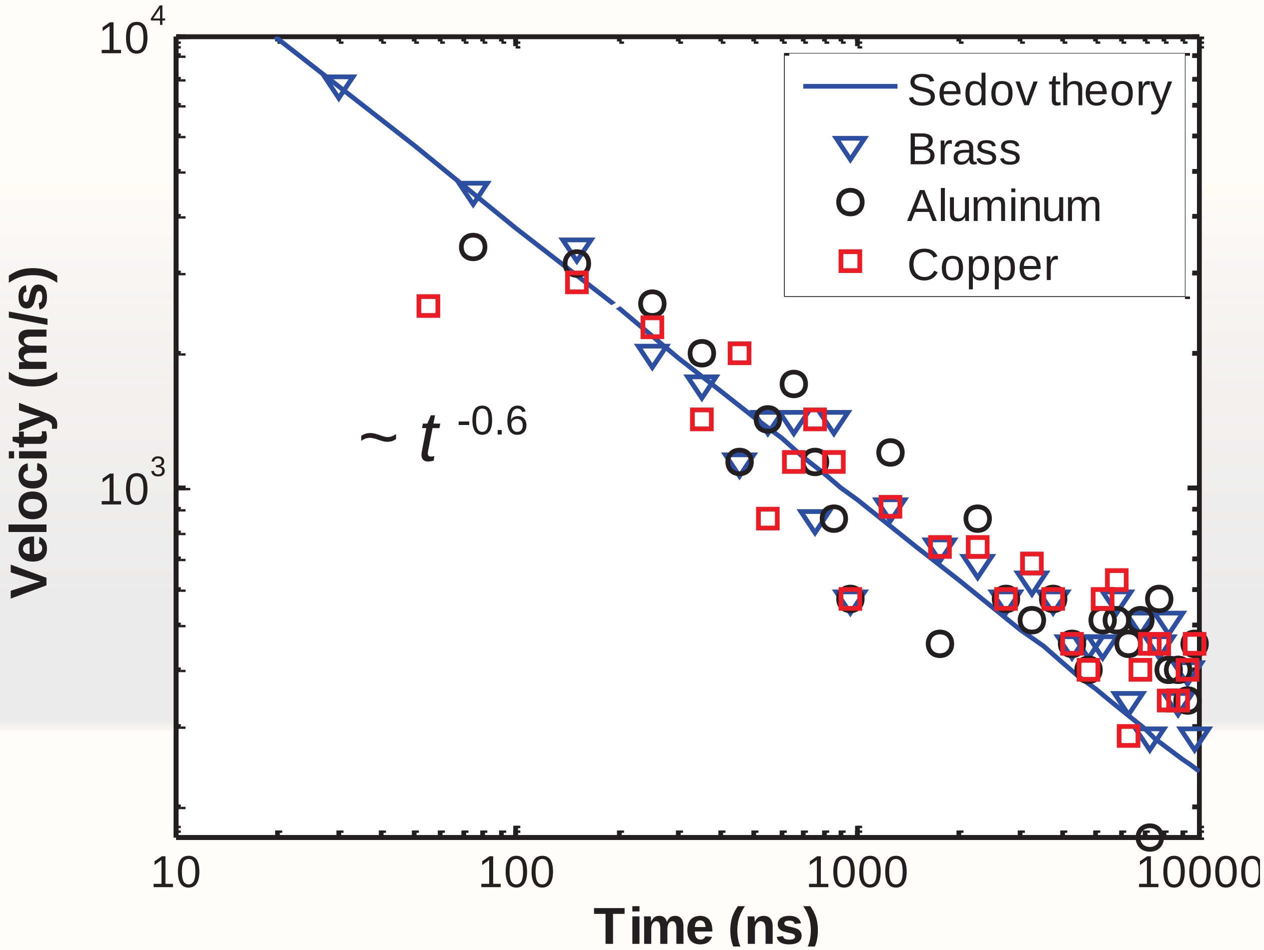

**Point-source Blast Wave**

# Developing spherical blast wave using laser ablation of aluminum and copper




**The Sequent shock wave images of Aluminum and Copper by 20mJ/pulse laser incident intensities shown in the increasing order of time elapse (30, 50, 70, 90, 120, 160, 200, 300, 400ns).**

# Velocity of metal phase explosion wave



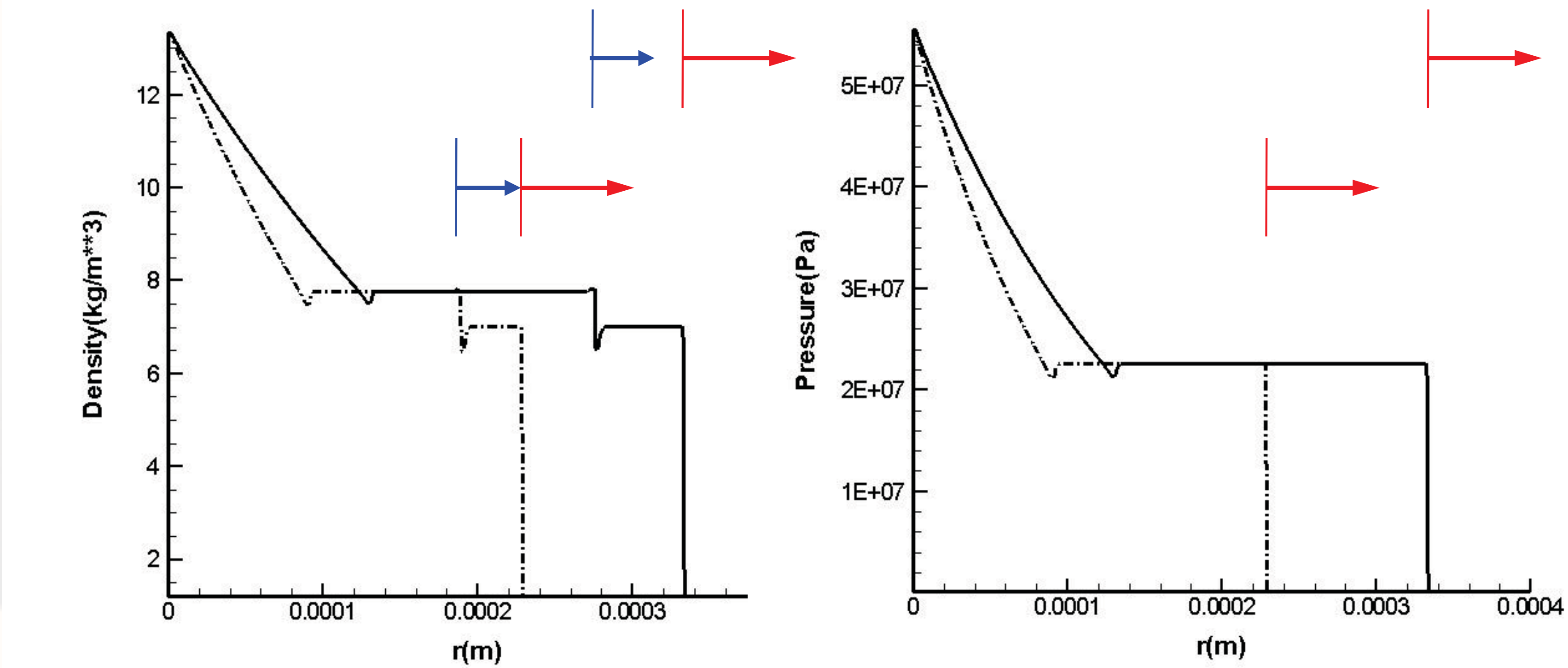

(Shown 1mm-thick metal at 200 mJ/pulse)

**Velocities follow the theoretical $t^{-0.6}$ - curve**

$$v = \lambda_0 \left( \frac{E}{\rho_{air}} \right)^{0.2} 0.4 \quad t^{-0.6}$$

# Micro explosion structure identified

Hot (vaporized) metal vapor / shocked (plasma) air / ambient air




- **Images at two different instances (22 ns apart), suggesting shock velocity of 4500 m/s**
- **This says that early-on profiles are given by the solution of Euler equations for metal vapor-air shock interaction**

# Structure of Riemann confirms initial blast wave profile

- **Theoretical Hugoniot properties of laser induced shock state during the first 1000 ns of 20 mJ/pulse beam.**
- **Shock speed is measured (~4500 m/s), other variables are estimated from strong shock approximation**
- **Calculations show the shocked states behind the initial planar explosive wave at 75ns is reproduced**

| | Shock speed $u_s$(m/s) | Density[1] $\rho_s$ (kg/m$^3$) | Pressure[2] $p_s$ (MPa) |
|---|---|---|---|
| Time (75 ns) | | | |
| Aluminum | 4571 | 7.76 | 22.5 |
| Brass | 4571 | | 22.5 |
| Copper | 3429 | | 12.7 |
| Time (150 ns) | | | |
| Aluminum | 2857 | 7.76 | 8.8 |
| Brass | 3429 | | 12.7 |
| Copper | 3143 | | 10.6 |
| Time (950 ns) | | | |
| Aluminum | 571 | 7.76 | 0.35 |
| Brass | 510 | | 0.35 |
| Copper | 510 | | 0.35 |

[1] $\rho_s = \rho_{air}(\gamma+1)/(\gamma-1), \rho_{air} = 1.29$ kg/m$^3$, $\gamma = 1.4$ for air
[2] $p_s = 2\rho_{air}u_s^2/(\gamma+1)$

# Flame acceleration (DDT)

$$\frac{P_2}{P_1} = \frac{2\gamma M_s^2}{\gamma+1} - \frac{\gamma-1}{\gamma+1}$$

$$\frac{\rho_2}{\rho_1} = \frac{\left(\frac{\gamma+1}{\gamma-1}\right)\frac{P_2}{P_1}+1}{\left(\frac{\gamma+1}{\gamma-1}\right)+\frac{P_2}{P_1}}$$

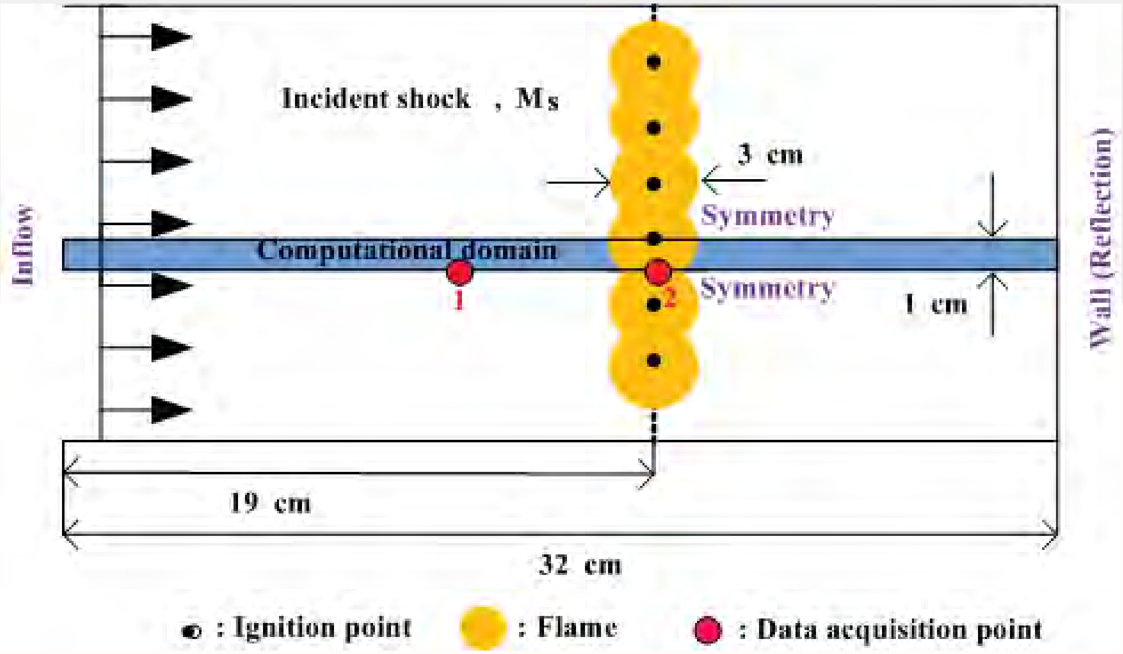
$$\frac{T_2}{T_1} = \frac{\left(1+\frac{\gamma-1}{2}M_s^2\right)\left(\frac{2\gamma}{\gamma-1}M_s^2-1\right)}{\frac{(\gamma+1)^2}{2(\gamma-1)}M_s^2}$$

| Parameter & Property | Acetylene-air mixture | Ethylene-air mixture |
|---|---|---|
| Initial pressure ($P_0$) | 1.33 X $10^4$Pa | 1.33 X $10^4$Pa |
| Initial temperature ($T_0$) | 293K | 293K |
| Initial density ($\rho_0$) | 1.58 X $10^{-1}$kg/$m^3$ | 1.58 X $10^{-1}$kg/$m^3$ |
| Specific heat rate (γ) | 1.25 | 1.15 |
| Molecular weight (M) | 29 X $10^{-3}$kg/mol | 29 X $10^{-3}$kg/mol |
| Pre-exponential factor (A) | 1 X $10^9$$m^3$/(kg s) | 3.2 X $10^8$$m^3$/(kg s) |
| Activation energy ($E_a$) | 29.3$RT_0$ | 35.3514$RT_0$ |
| Chemical energy release (q) | 35.0$RT_0$/M | 48.824$RT_0$/M |
| Transport constants ($\nu_0$=$\mu_0$=$D_0$) | 1.3 X $10^{-7}$kg/(s m $K^{0.7}$) | 7.0 X $10^{-8}$kg/(s m $K^{0.7}$) |
| Adiabatic flame temperature | 2340K | 2625K |
| Adiabatic flame density | 1.98 X $10^{-2}$kg/$m^3$ | 1.77 X $10^{-2}$kg/$m^3$ |
| Incident shock intensity | 1.2 | 1.9 |

# Acetylene-air mixture

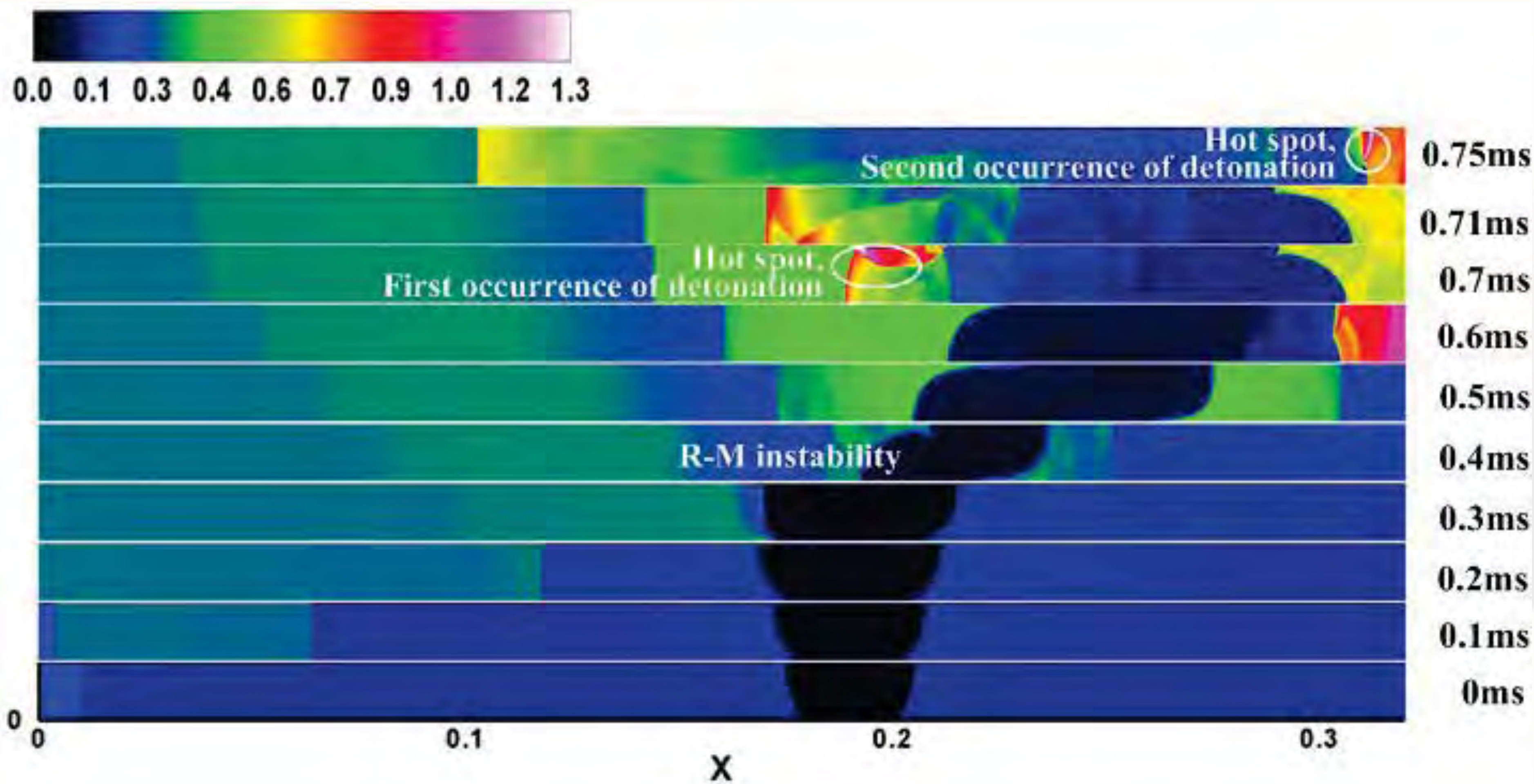

**Experimental schlieren image**

[*T. Scarinci, etc., 1993*]




**2D numerical domain**

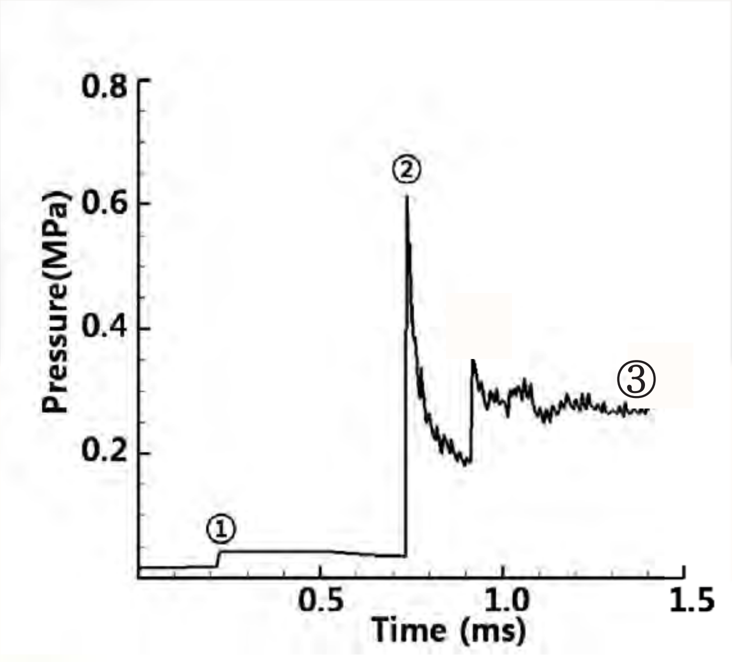
# Acetylene-air mixture



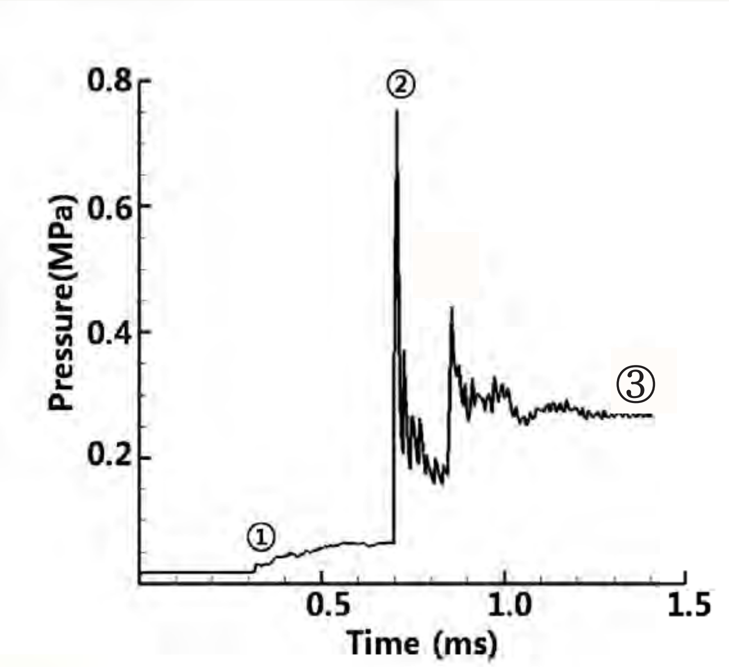

**Time sequences of density fields under M=1.2 incident shock interacting with an acetylene-air flame**

# Calculated pressure histories

- Gages
  ① Incident shock wave propagates from left to right.
  ② Pressure peak shows detonation occurrence.
  (peak pressure: 0.6~0.8MPa, velocity: 1887m/s)
  ③ Pressure is stabilized after detonation (0.27MPa).

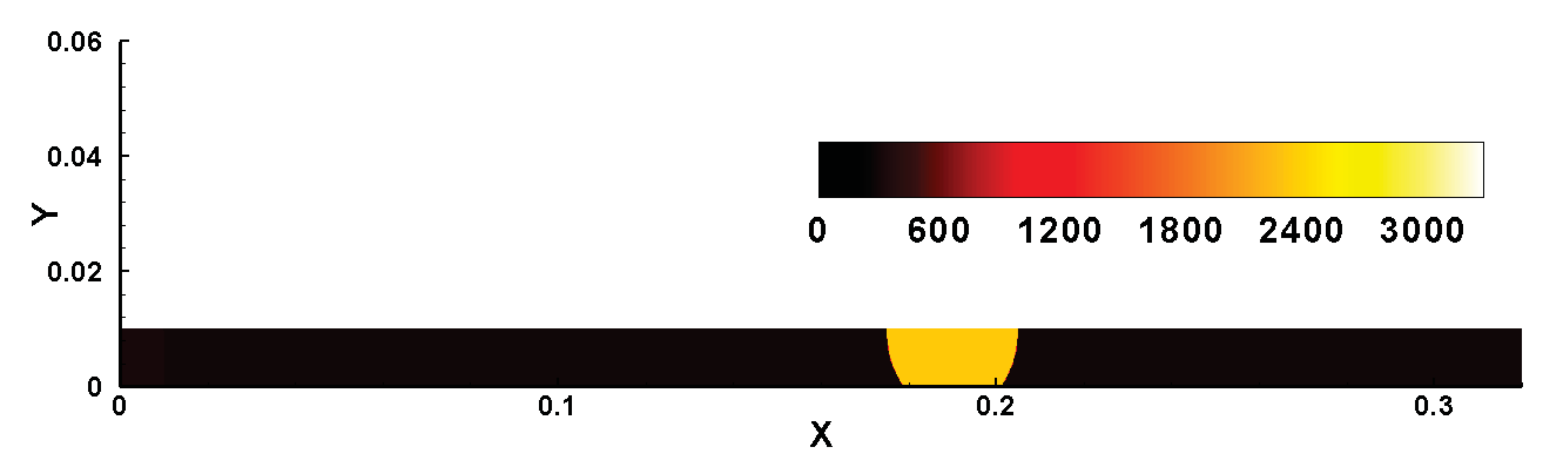



**Pressure history at gage 1**




**Pressure history at gage 2**

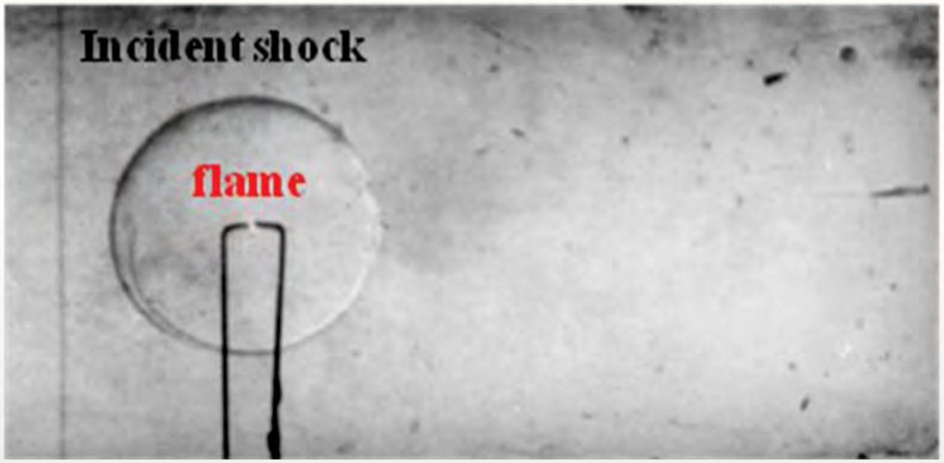
# Acetylene-air mixture




- Temperature

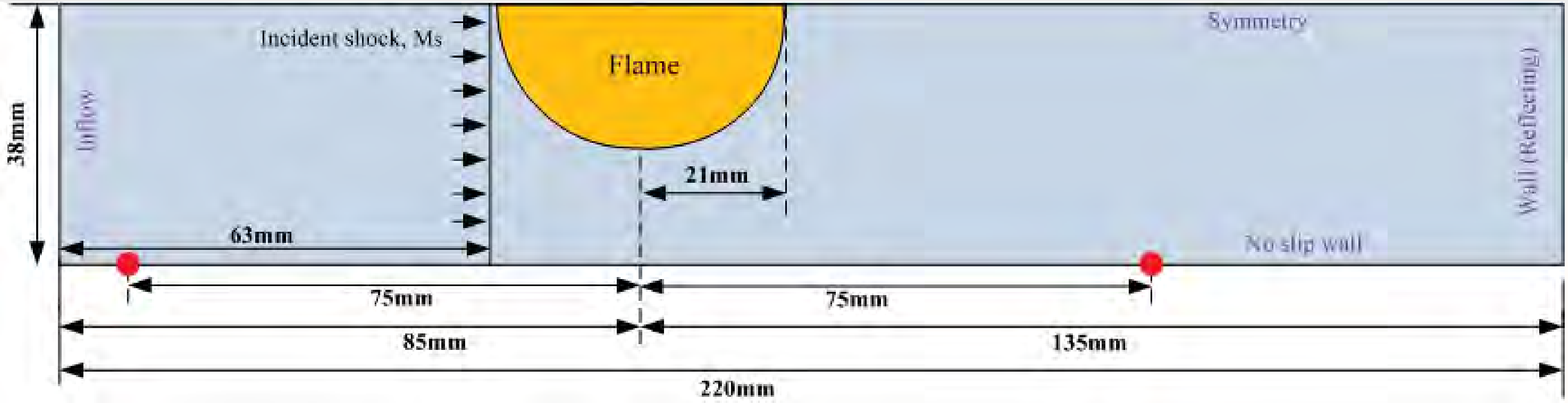
| | Reference value | Numerical value |
|---|---|---|
| Peak pressure | 805509Pa [0.8MPa] [*T. Scarinci, 1993*] | 0.6~0.8MPa |
| Pressure ratio | 19.5 [*I. Glassman, 1996*] | 20.3 |
| Detonation velocity | CJ Detonation velocity, 1870m/s [*A. M. Khokhlov, 1999*] | 1887m/s |

# Ethylene-air mixture – Initial Setup




**Experimental schlieren image**

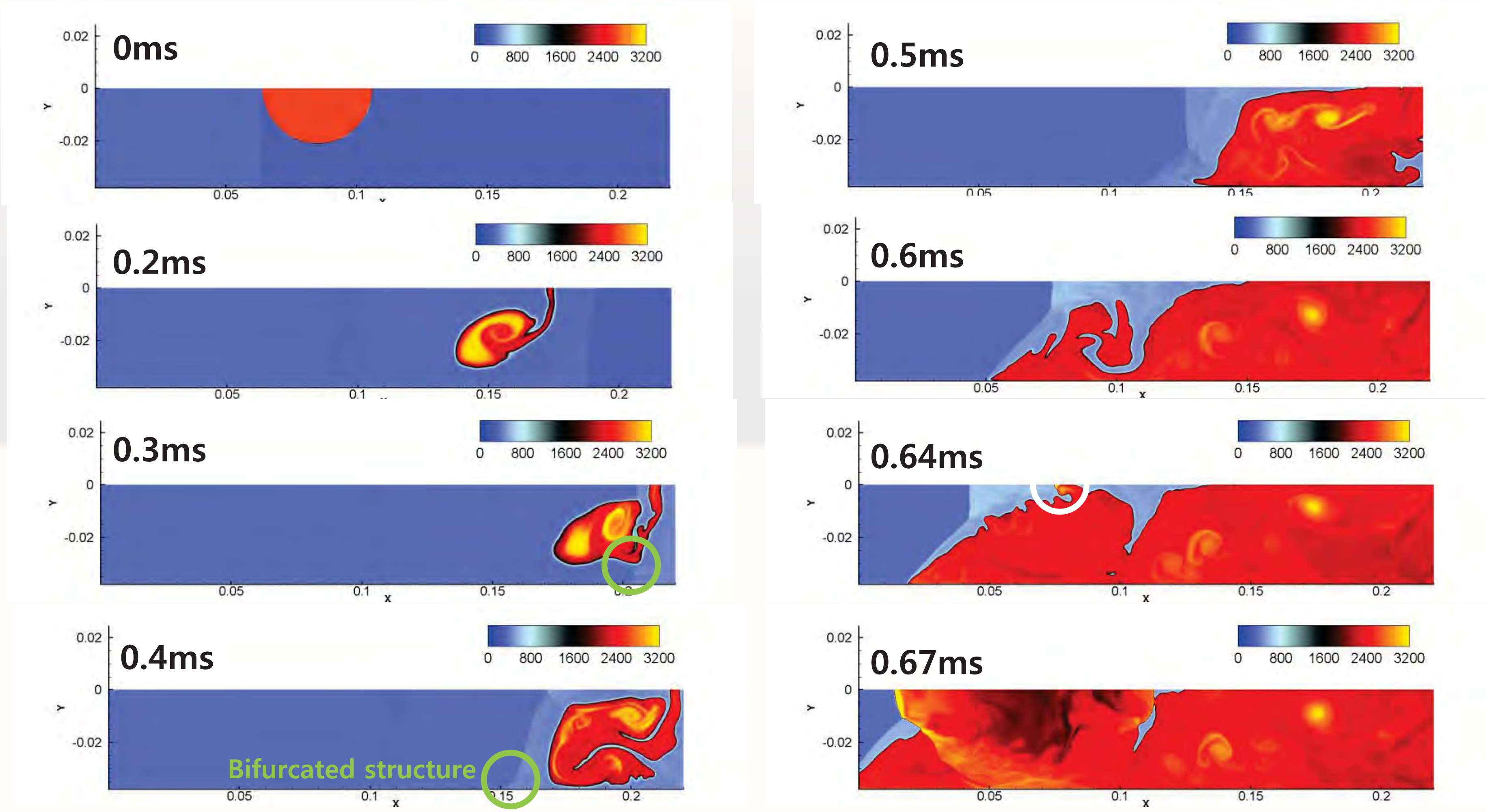
[G. *Thomas, etc., 2001*]




**2D numerical domain**

# Temperature: O: detonation occurrence)

- Flame surface is increased by flame instability (0.4ms)
- Bifurcated structure is formed by no slip boundary condition.
- Detonation is occurred at 0.64ms.



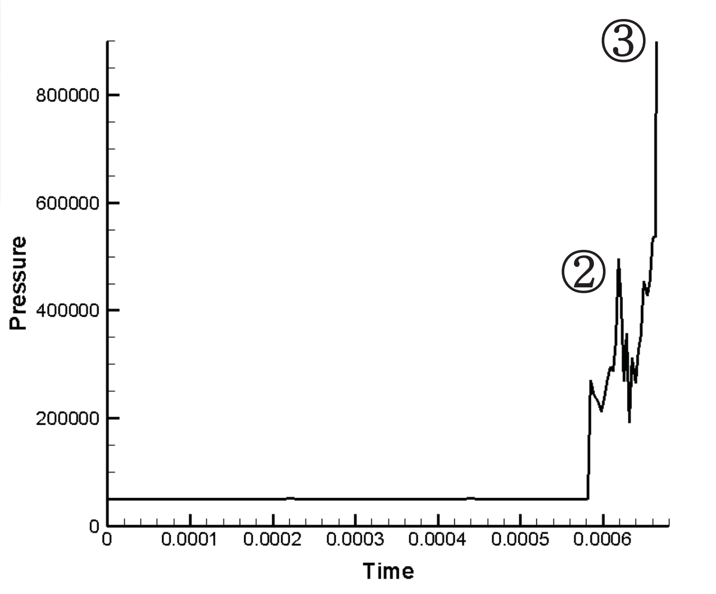
# Pressure histories

① **Incident shock wave(0.05MPa, 0.4825kg/m3, 363K) propagates from left to right.**

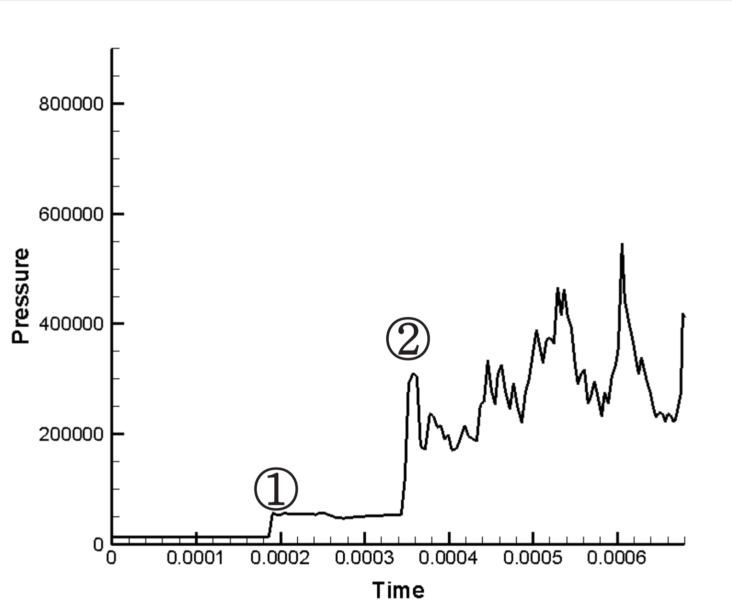
② **Pressure is increased by propagation of strange wave.**

**(Strange wave: a kind of reflection wave that is occurred between flame and wall and accompanies turbulent flame)**
**velocity~1500m/s, pressure ratio~10 [*G. Thomas, et al., 2001*]**

③ **Pressure peak(more than 0.8MPa) shows detonation occurrence.**

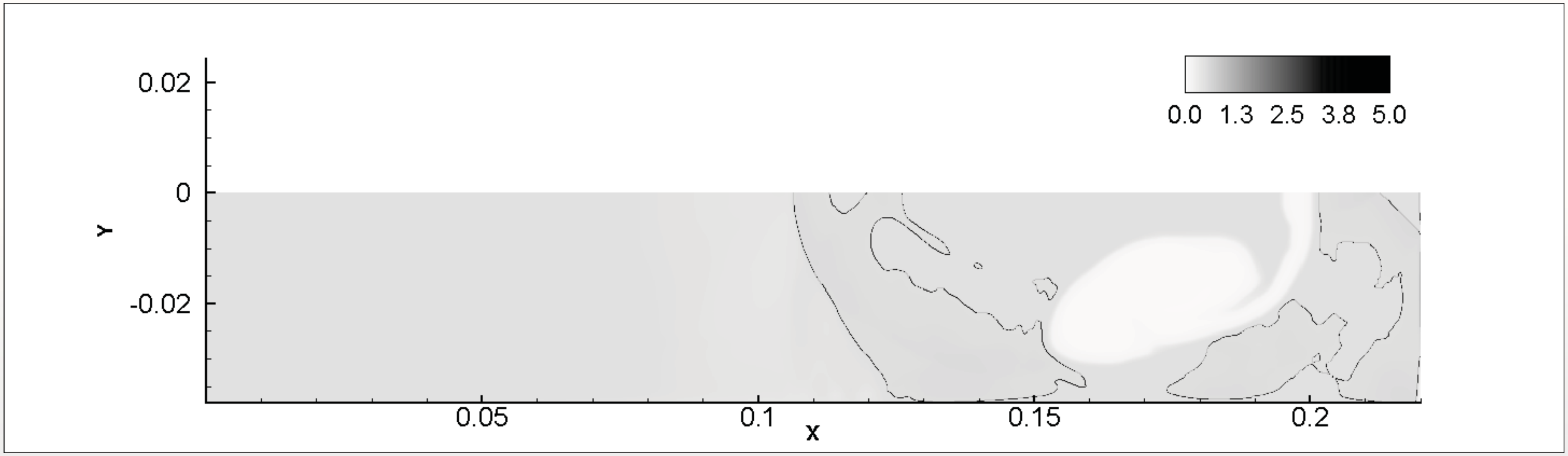



**Pressure history at gage 1**

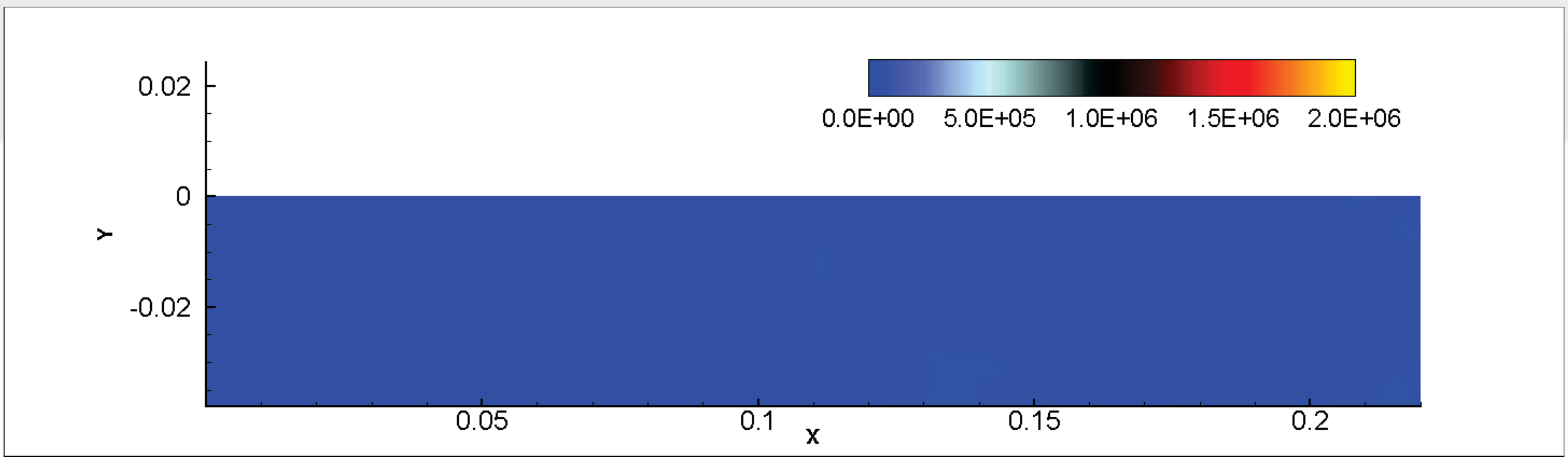



**Pressure history at gage 2**

# Density and Pressure (0.2~0.7 ms)




**Video clip of density field [unit: kg/m$^3$]**




**Video clip of pressure field [unit: Pa]**

# Summary

- **Hydrocode** development for simulation of energetic materials
  - Cook off test of Rocket Propellants, Explosives, Gaseous Fuels
  - Many more simulation capabilities not shown

- High power laser ablation experiment for studying **metal detonation in air**: Not in powder form, rather in a bulk.

- Flame acceleration research via DNS for understanding the origin of **Deflagration-to-Detonation** transition from a quiescent flame: rocket chamber instability, engine knock, gas pipe failure due to explosions, etc.