Initiation of Hydrogen Detonation

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Onset of Detonation

- **Direct initiation** by rapid deposition of energy
  - Blast wave
  - Shock reflection
  - Shock focusing

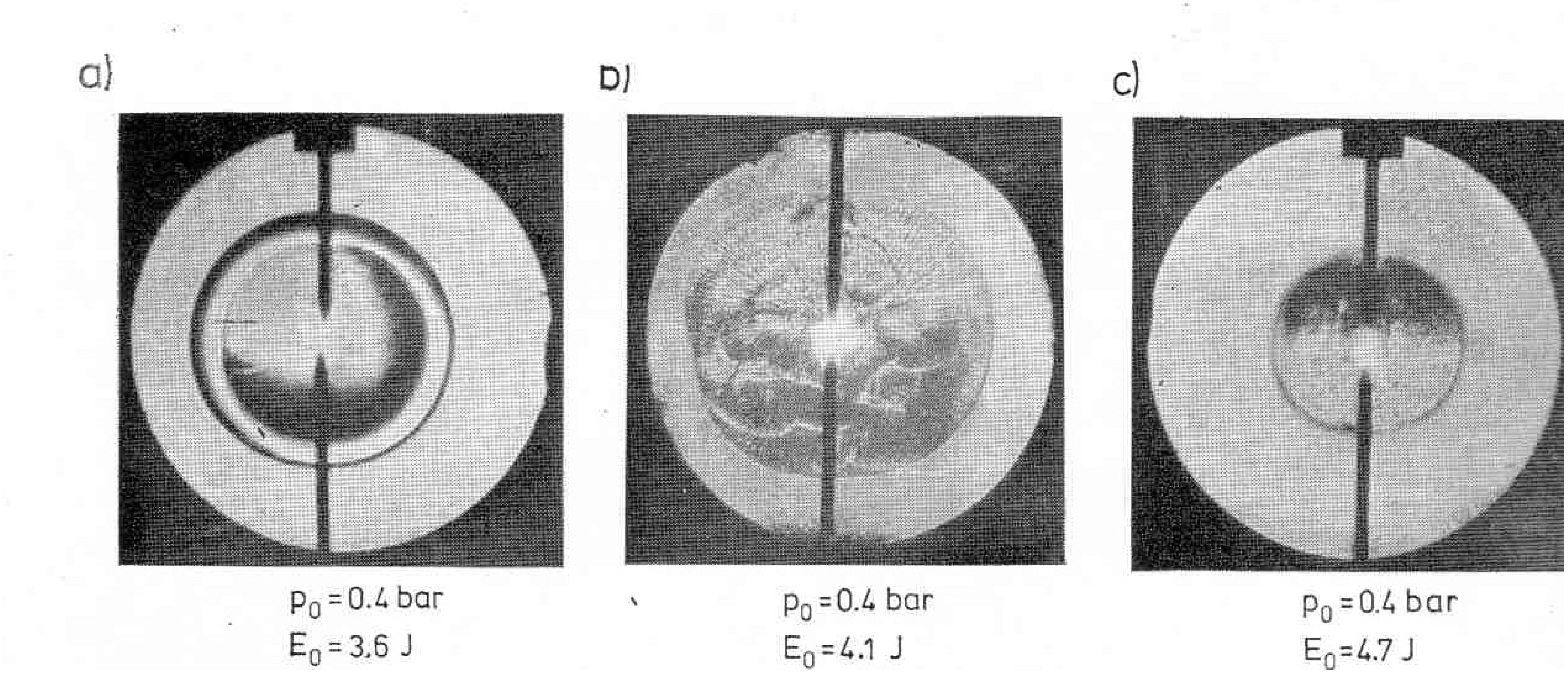
- **Indirect initiation** through the acceleration of a series of progressively more reactive states
  - SWACER - Synchronized initiation
    - Flash Photolysis
    - Turbulent mixing
  - DDT – Deflagration to Detonation Transition

Outline

- Direct initiation by rapid energy release
- Direct initiation by shock reflection
- Direct initiation by shock focusing
- SWACER – synchronized initiation
- DDT – Deflagration to Detonation Transition

Direct initiation of detonation

Stoichiometric hydrogen-chlorine mixture; a) subcritical; b) critical; c) supercritical



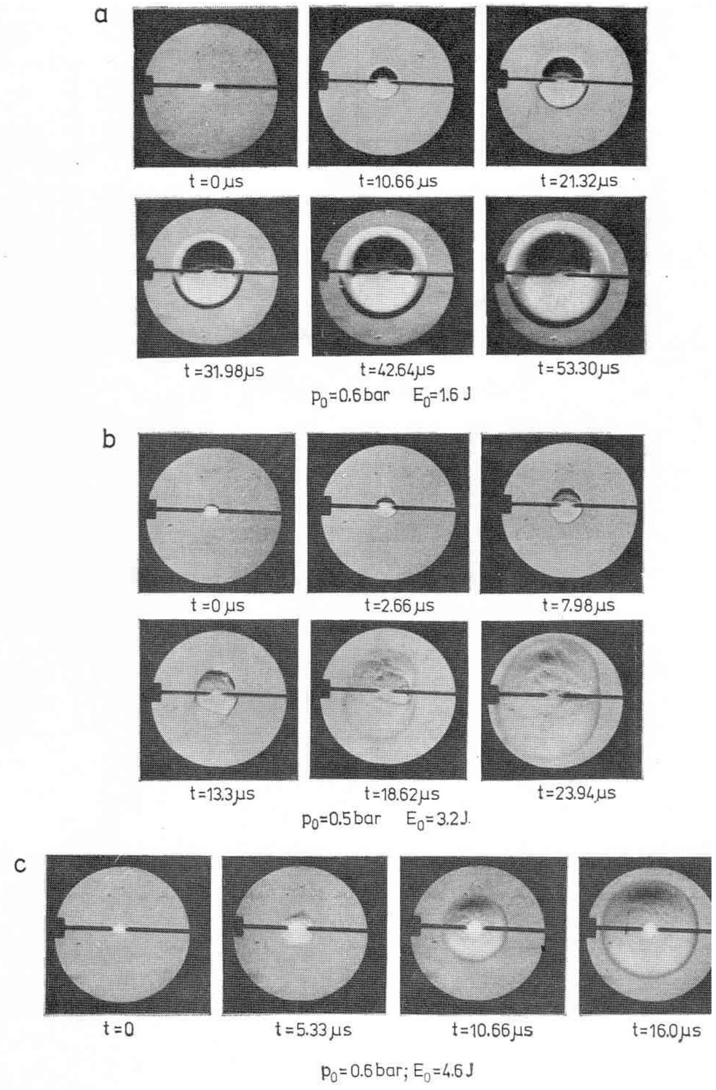
a) $p_0 = 0.4$ bar, $E_0 = 3.6$ J

b) $p_0 = 0.4$ bar, $E_0 = 4.1$ J

c) $p_0 = 0.4$ bar, $E_0 = 4.7$ J

(Teodorczyk et al. 1978)

Direct initiation of detonation



Stoichiometric hydrogen-chlorine mixture;

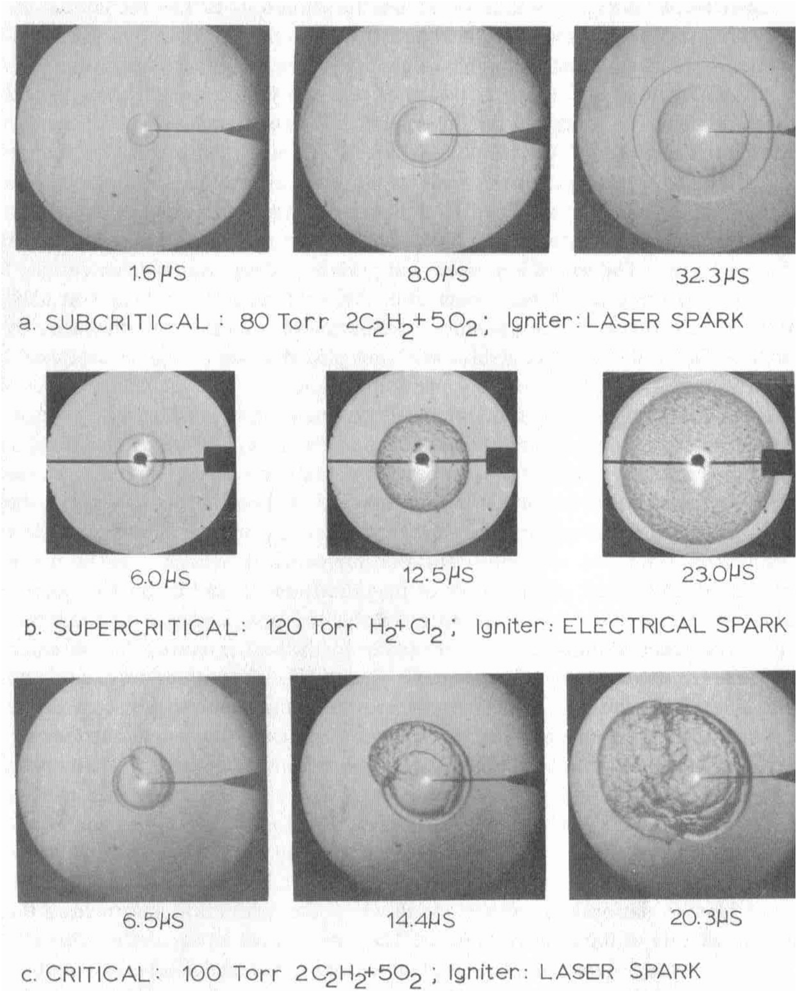
a) subcritical;

b) critical;

c) supercritical

(Source: Teodorczyk et al. 1978)

Direct initiation of detonation



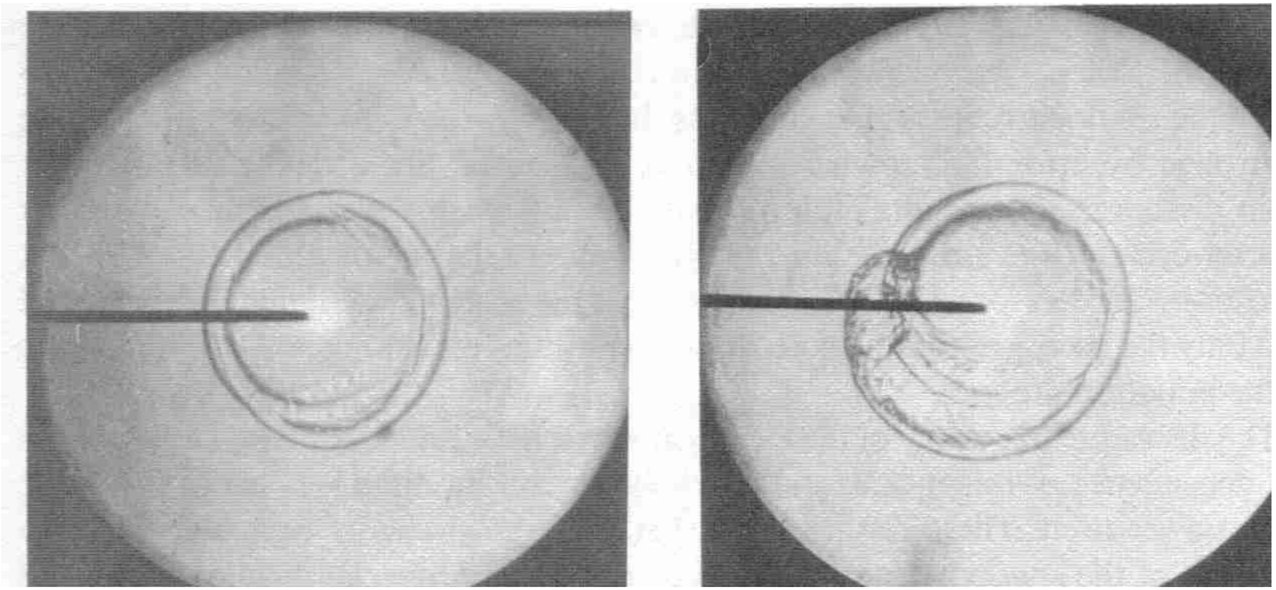
a) subcritical; acetylene-oxygen; laser spark

b) supercritical; hydrogen-chlorine, electric spark

c) critical; acetylene-oxygen, laser spark

(Source: Lee et al. 1977)

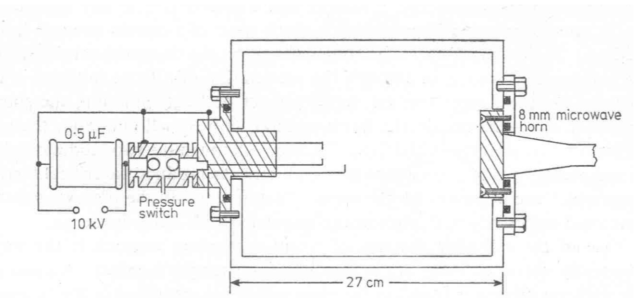
Direct initiation of detonation

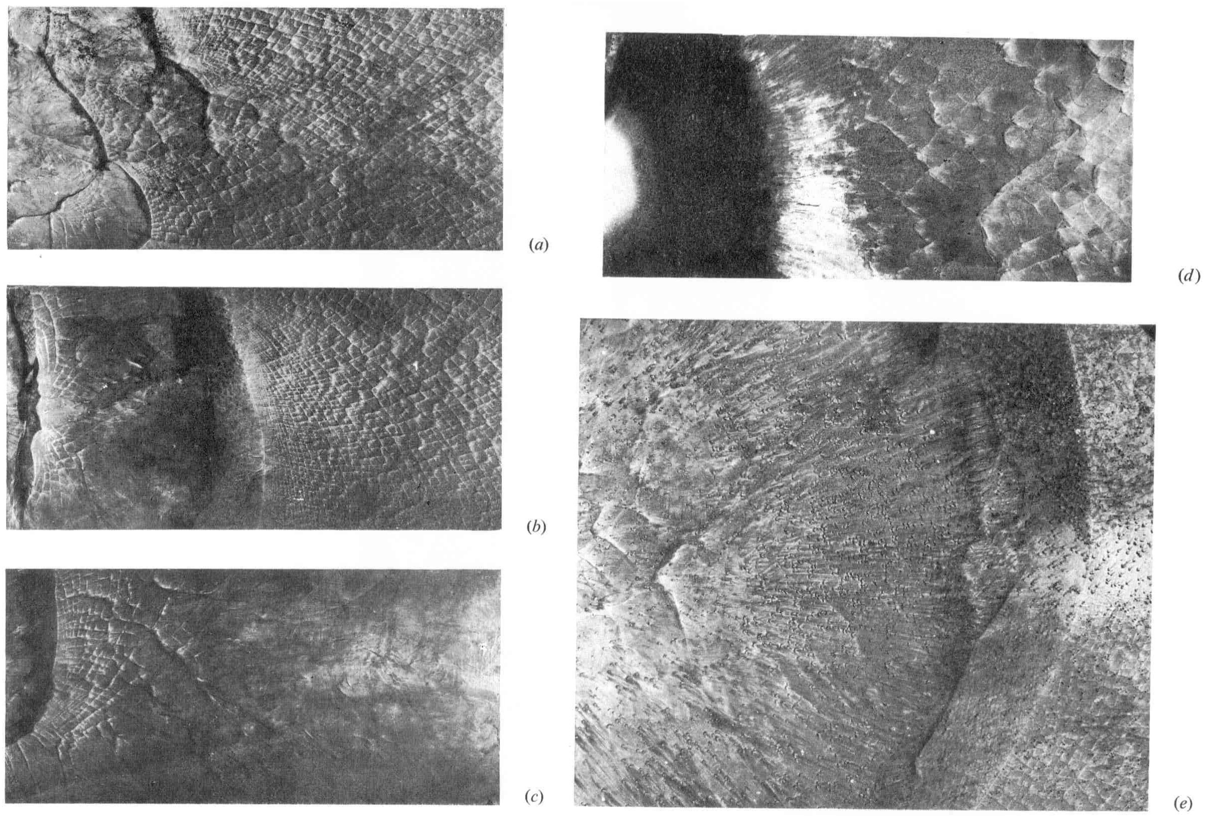


Onset of detonation at the end of the
quasi-steady period of the critical regime.
Stoichiometric C_2H_2-O_2 at 100 torr,
ignition by laser spark

(Source: Lee et al. 1977)

Direct initiation of detonation



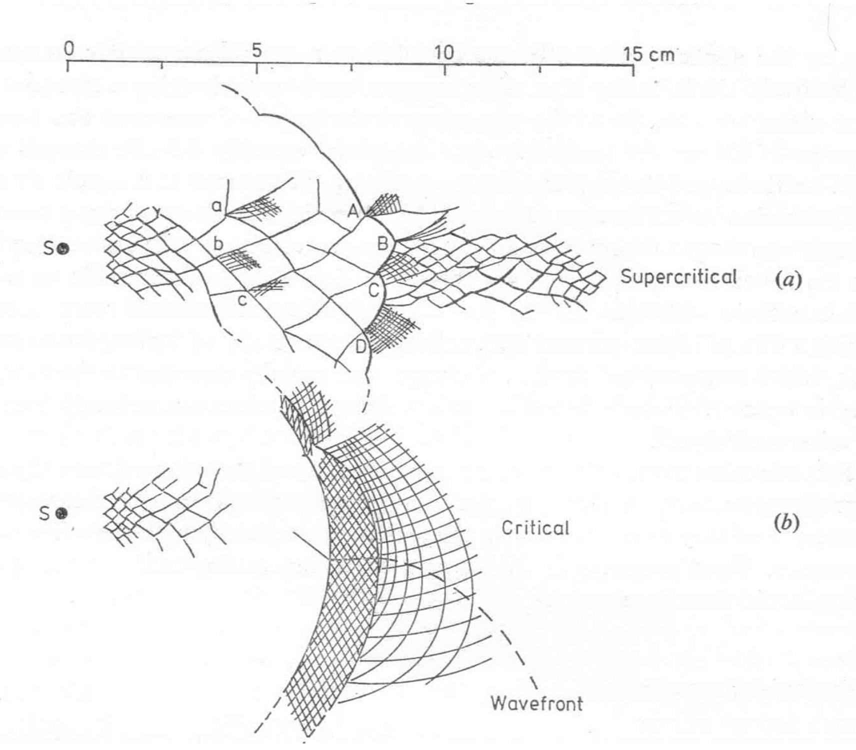


Smoked foil records of initiation of spherical detonations.
Exploding wire, 25 J energy
$2C_2H_2+5O_2+3Ar$

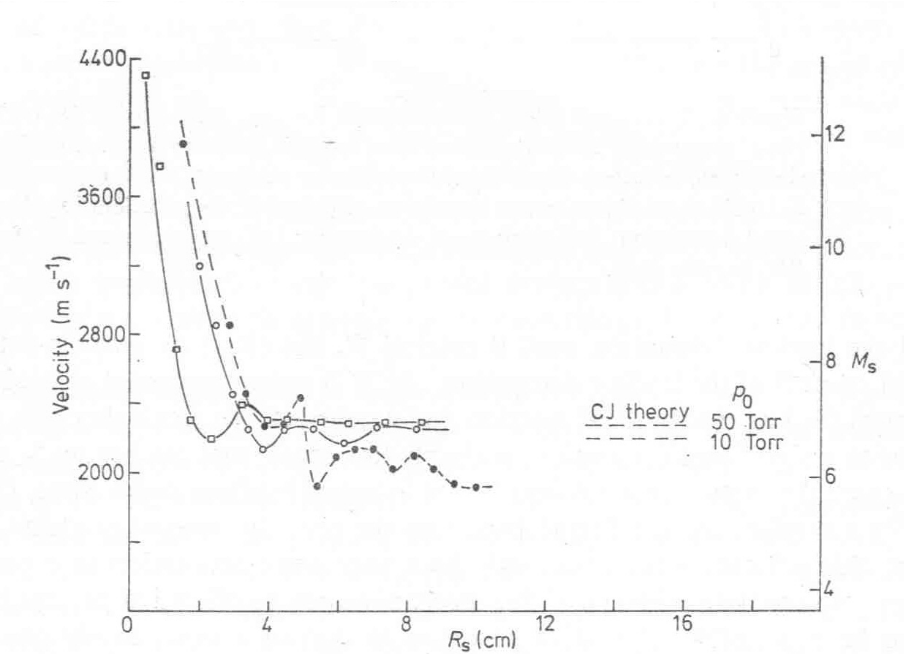
(a) 60 Torr;
(b) 55 Torr;
(c) 51 Torr, wave failure occurs.
(d) lead azide source, 31 Torr;
(e) details ofcritical initiation using exploding wire

(Source: Edwards et al. 1978)

Direct initiation of detonation



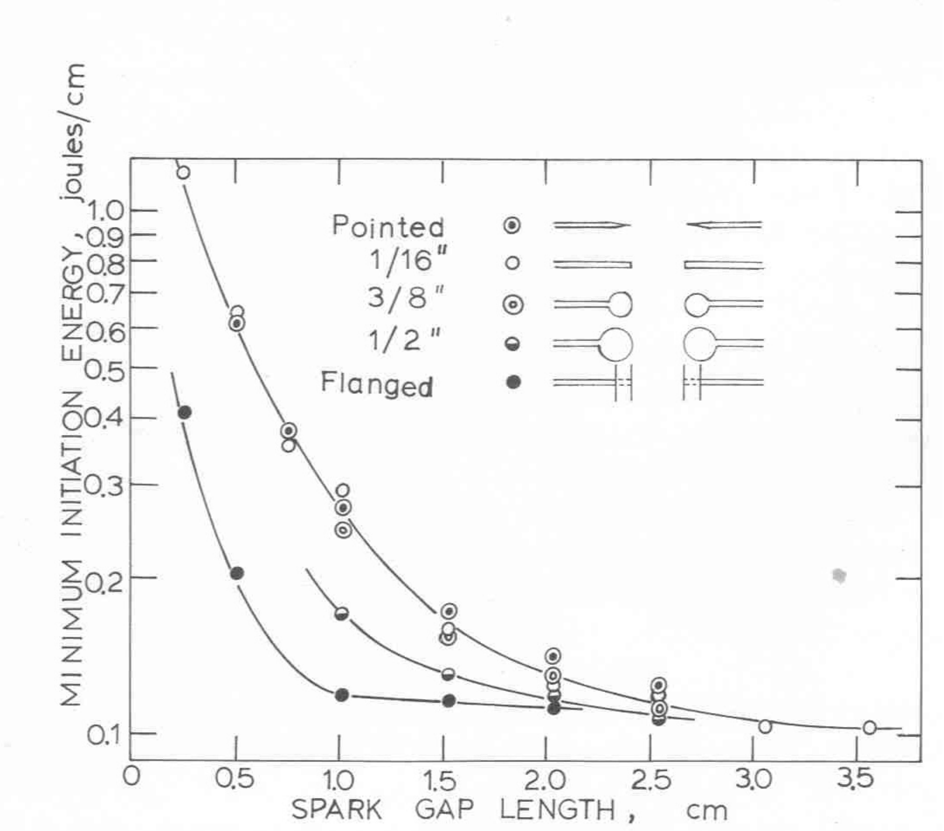
(a) supercritical and (b) critical initiation, using exploding wire;



45 mg lead azide.Initial pressure, p_0: ( ) 50 Torr; (ο) 30 Torr; (•) 15 Torr,

(Source: Edwards et al. 1978)

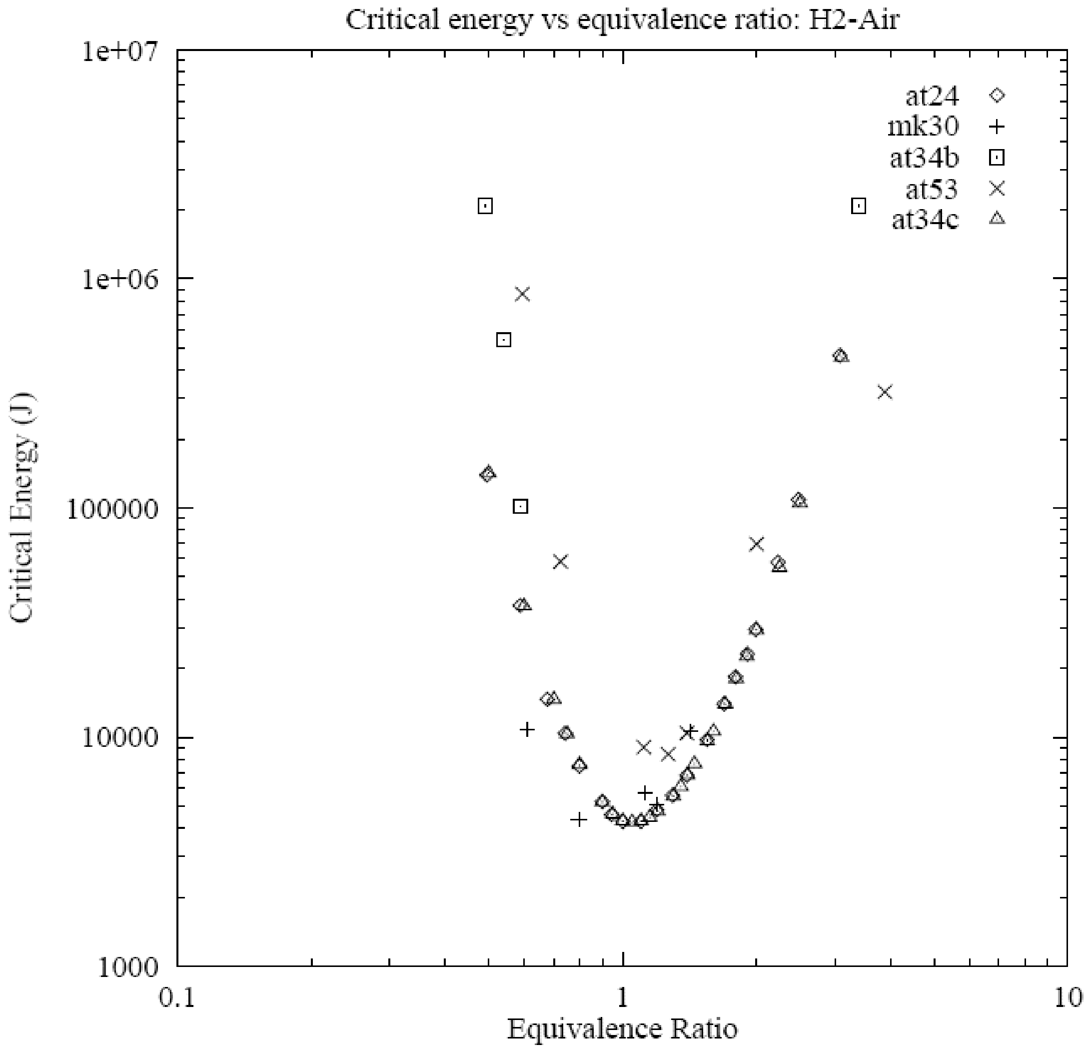
Direct initiation of detonation



critical energy for direct initiation of spherical detonations in stoichiometric C2H2-O2 at 100 torr

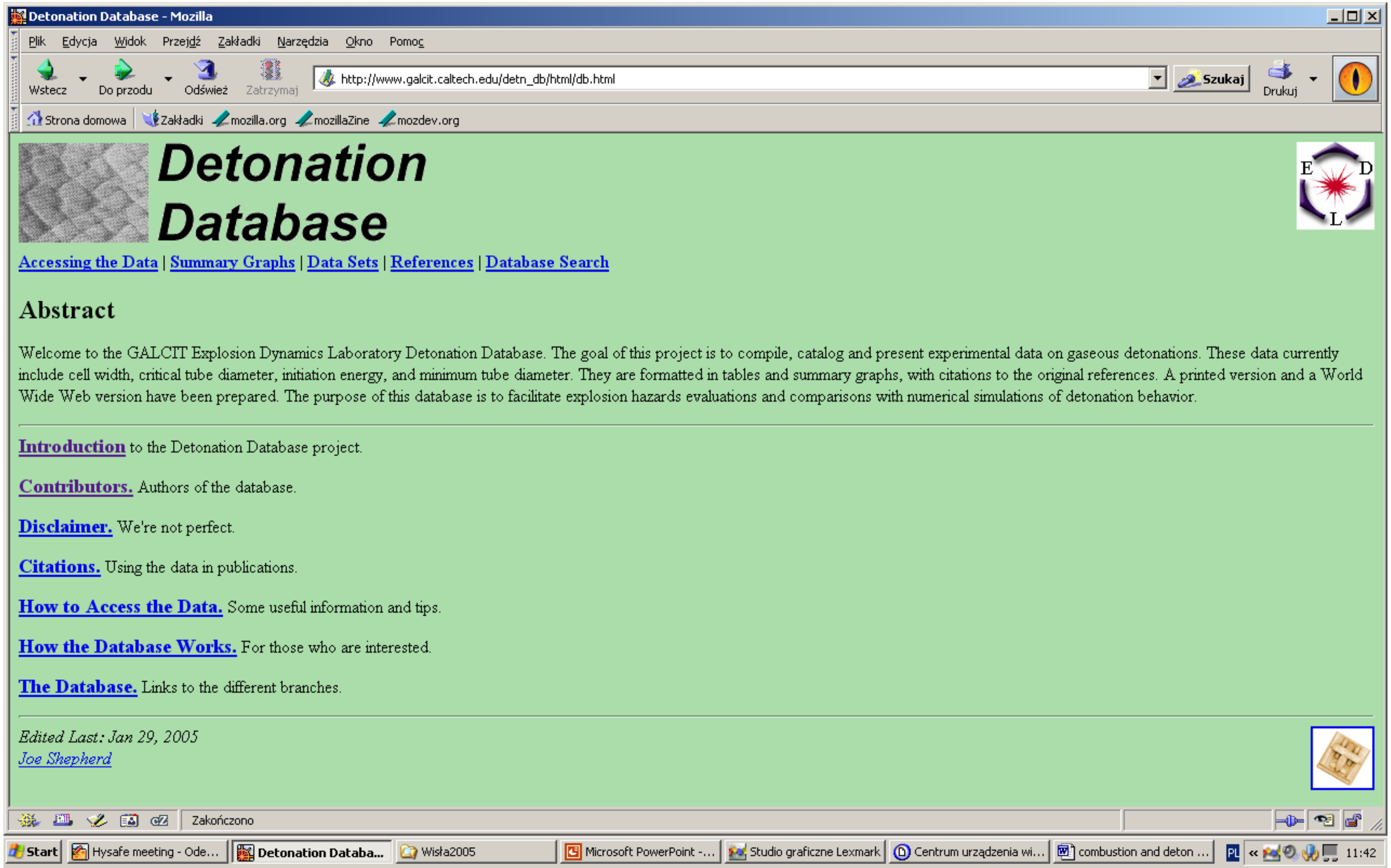
(Source: Matsui & Lee, 1976)

Direct initiation of detonation



From detonation database

Detonation database



Detonation Database

Accessing the Data | Summary Graphs | Data Sets | References | Database Search

Abstract

Welcome to the GALCIT Explosion Dynamics Laboratory Detonation Database. The goal of this project is to compile, catalog and present experimental data on gaseous detonations. These data currently include cell width, critical tube diameter, initiation energy, and minimum tube diameter. They are formatted in tables and summary graphs, with citations to the original references. A printed version and a World Wide Web version have been prepared. The purpose of this database is to facilitate explosion hazards evaluations and comparisons with numerical simulations of detonation behavior.

Introduction to the Detonation Database project.

Contributors. Authors of the database.

Disclaimer. We're not perfect.

Citations. Using the data in publications.

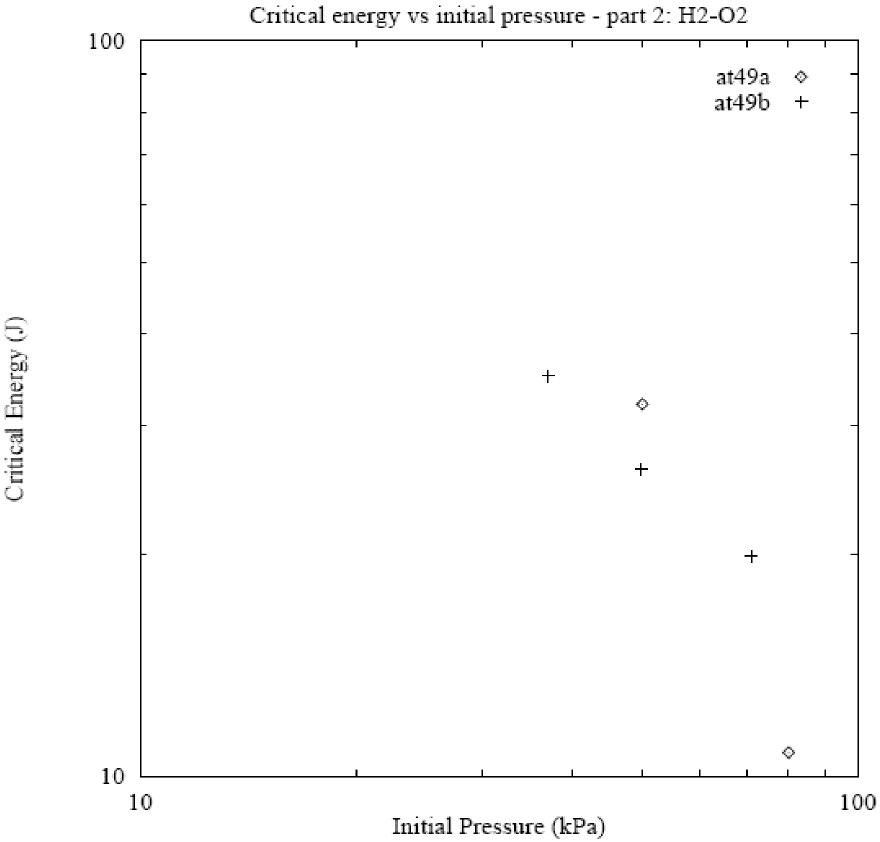
How to Access the Data. Some useful information and tips.

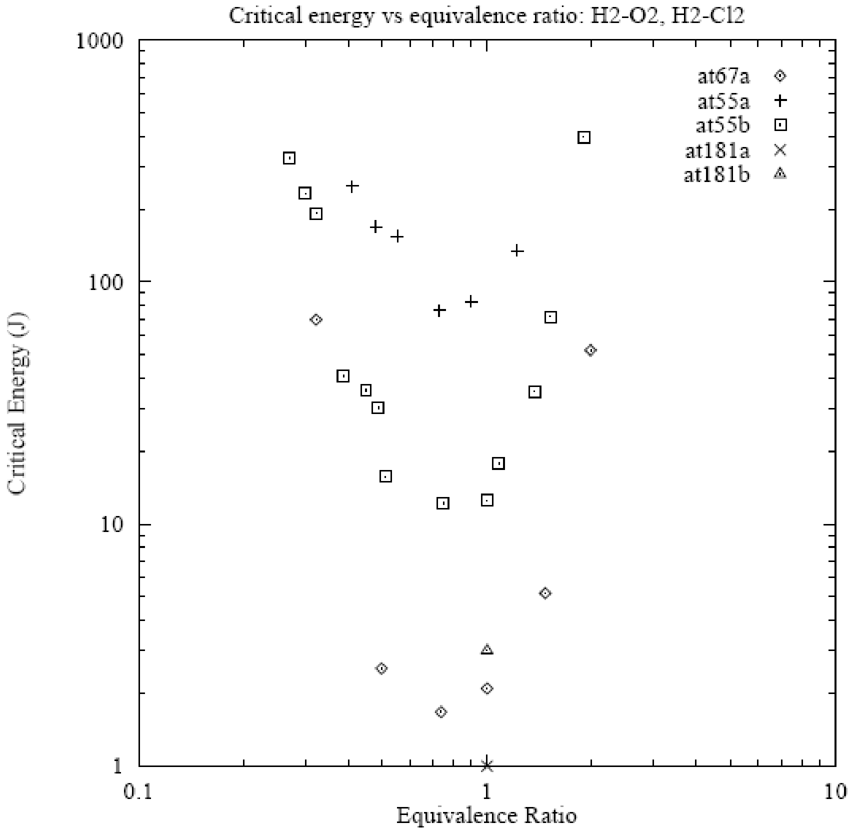
How the Database Works. For those who are interested.

The Database. Links to the different branches.

Edited Last: Jan 29, 2005
Joe Shepherd

Direct initiation of detonation





at49a: T=293 K;

at49b: T=123 K;

Direct initiation of detonation

Critical energy of initiation:

$$E_c = \frac{2197}{16}\pi\rho_0 V_{CJ}^2 I\lambda^3$$

ρ_2 - initial density of the mixture

V_{CJ} - Chapman-Jouget detonation velocity

λ - cell size

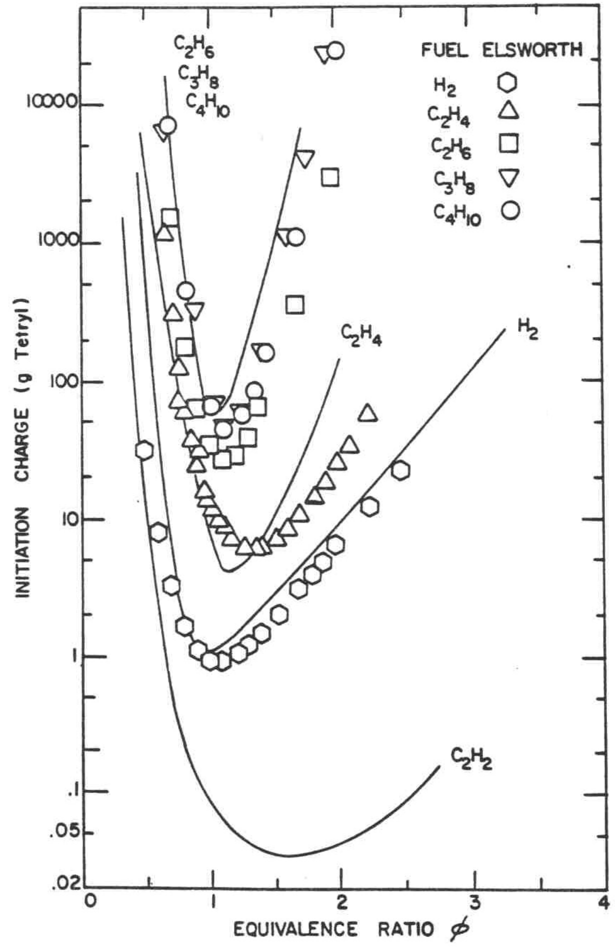
I – energy integral (table 2)

Energy integral I of H_2-air mixture *(Guirao et al. 1982)*

% H_2	I	% H_2	I
15	0.64765	45	0.76532
20	0.74232	50	0.71585
25	0.87237	55	0.67299
29.6	0.99306	60	0.63518
30	0.99527	65	0.60108
35	0.91458	70	0.58742
40	0.82589	75	0.54058

Direct initiation of detonation

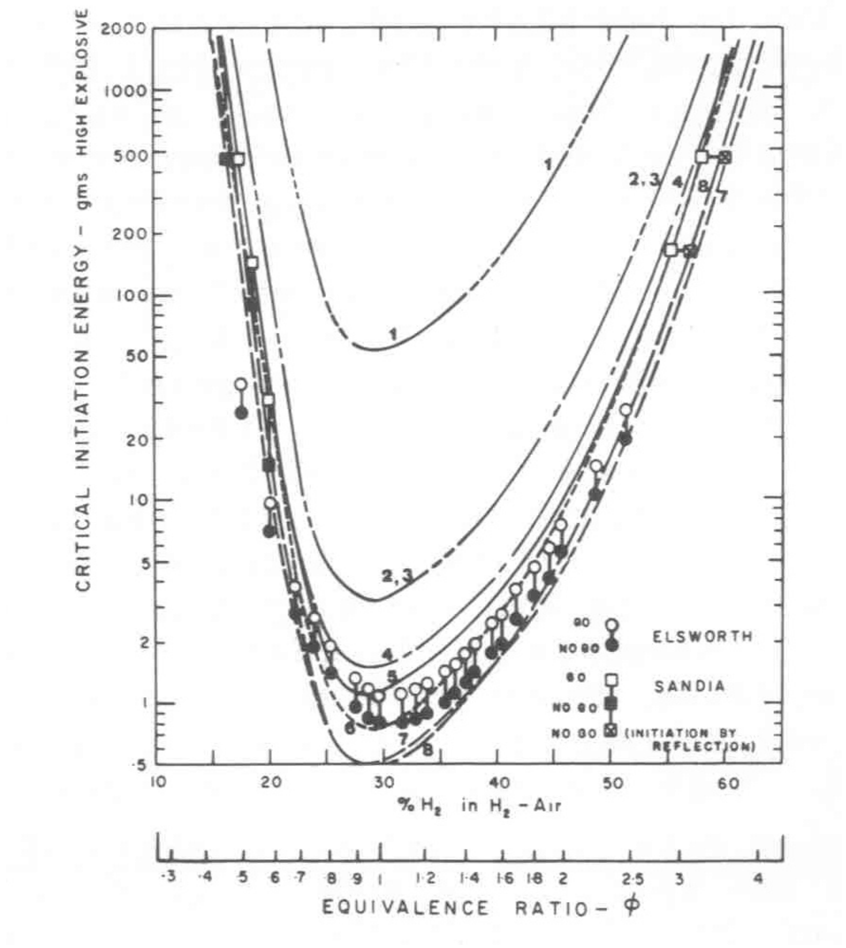
Fuel-Air Mixtures ($T_o = 300$ K, $P_o = 1$ atm



Model vs. Experimental data

Direct initiation of detonation

Models vs. Experimental data

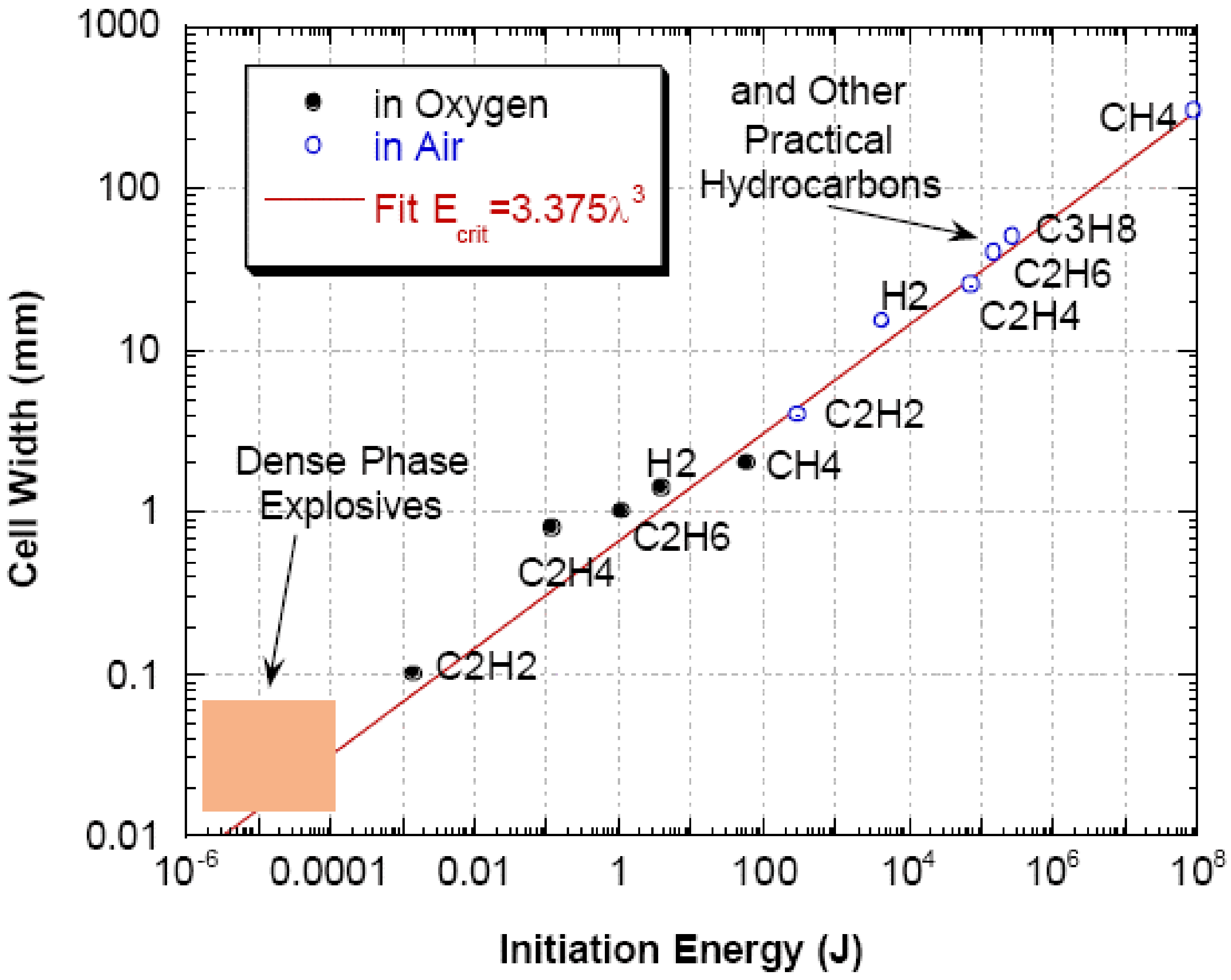


Theoretical curves:

1 – Edwards (1976a) hydrodynamic thickness model;
2 – Lee et al. (1982) blast model; l
3 - Lee et al. (1983) hydrodynamic thickness model;
4 – detonation kernel model;
5 – surface energy model;
6 – cell energy model;
7 – chemical energy model;
8 – work done model.

(Benedick et al. 1986)

Direct initiation of detonation



(Schauer et al. 2005)

Direct initiation of detonation - numerical

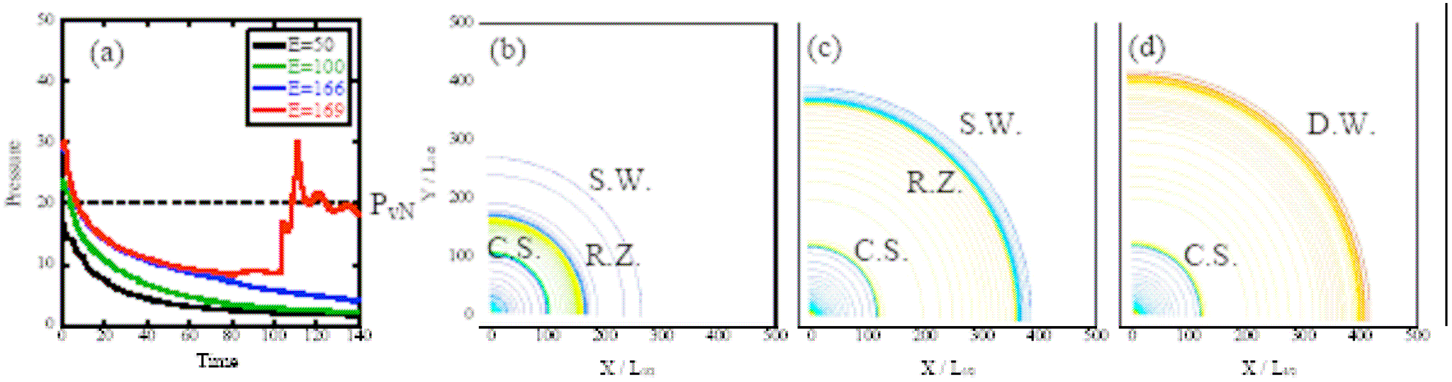


Fig.3 (a) shock pressure histories on the line of X=Y (P_{vN}=20.03). Temperature distributions of (b) E=50x10^6, (c) E=166x10^6 and (d) E=169x10^6 at t=110 with circular grid. 20 points/$L_{1/2}$ and 1 point/deg. are set. (D.W. : Detonation Wave, S.W. : Shock wave, R.Z. :Reaction Zone, C.S. : Contact Surface)

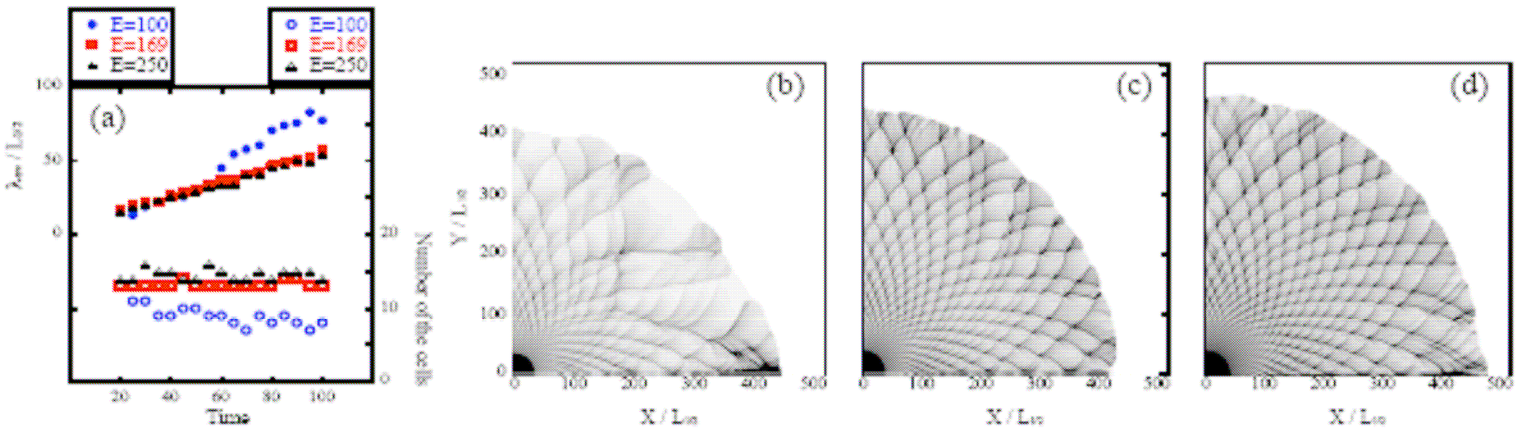
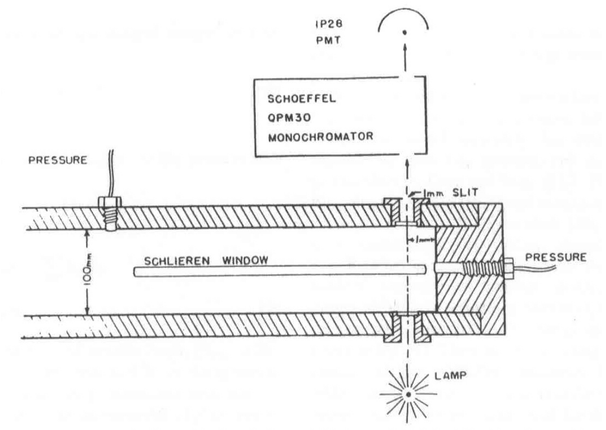
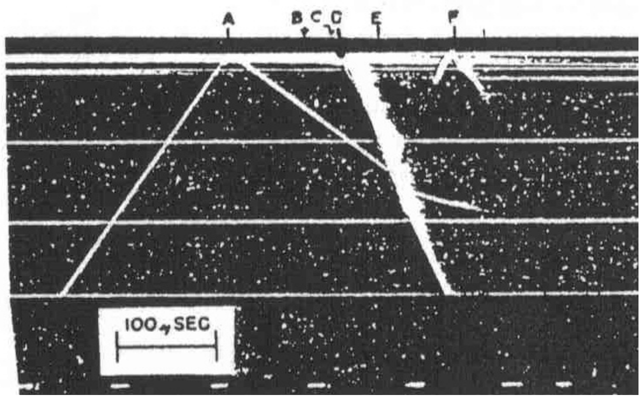


Fig.5 (a) Evolution of the averaged cell width and the cell number. The maximum pressure distributions of (b) E=100x10^6, (c) E=169x10^6 and (d) E=250x10^6. 10 points/$L_{1/2}$ are set in X and Y directions.

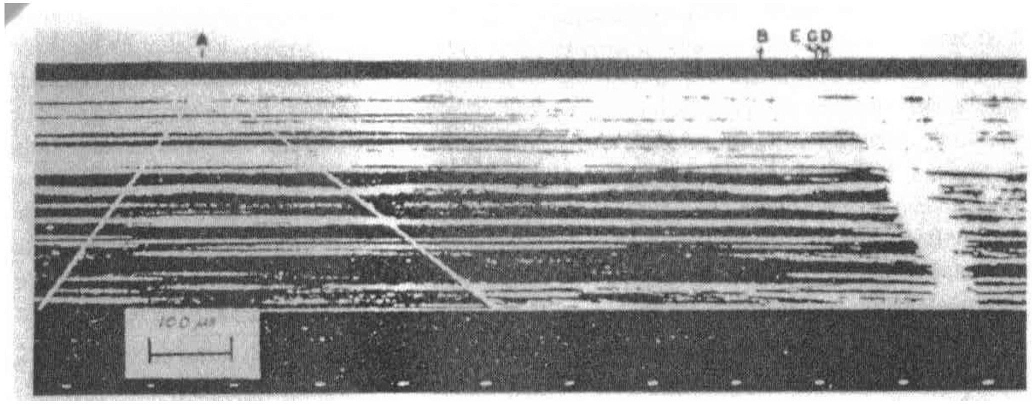
Source:
Nirasawa & Matsuo
21st ICDERS, July 23-27, 2007, Poitiers

Strong and weak ignition behind reflected shock





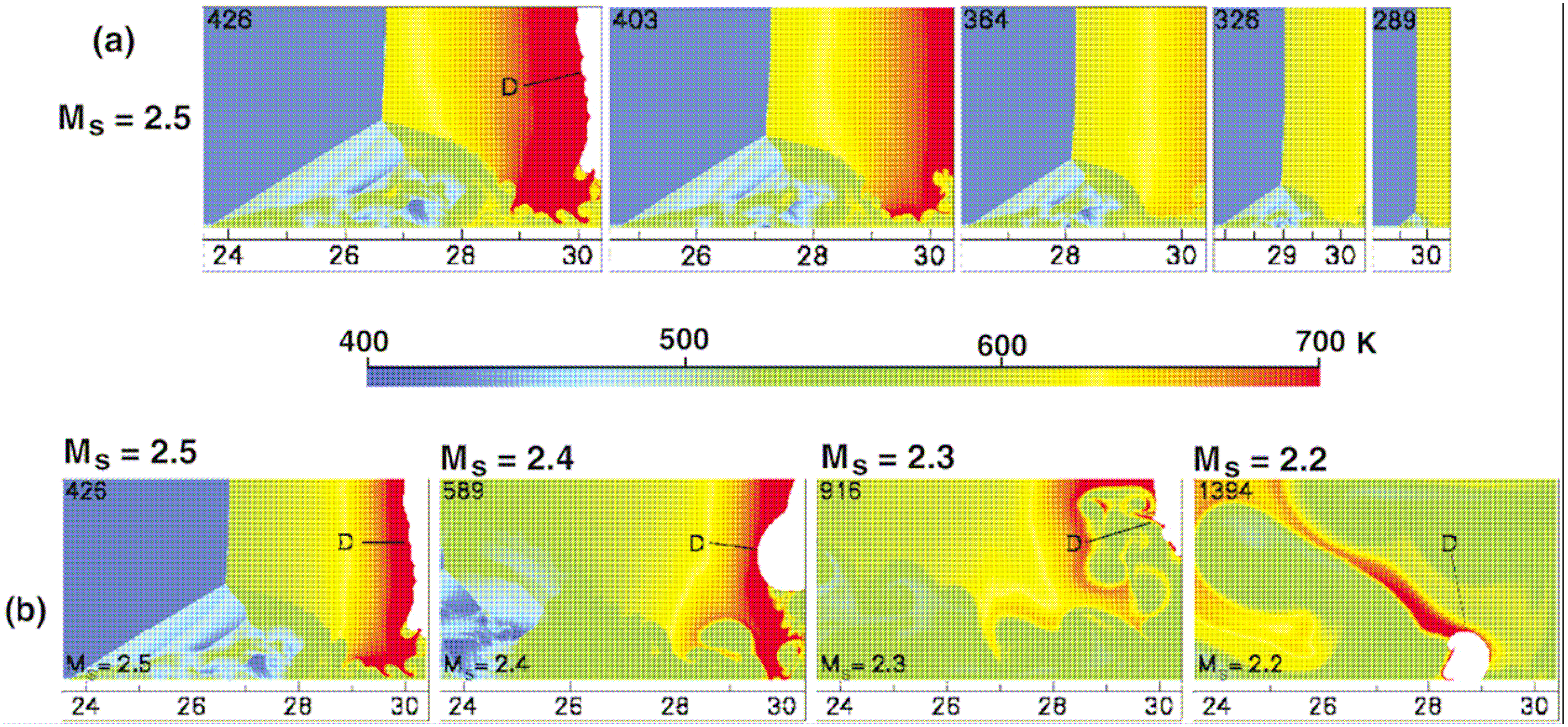
Strong ignition;
$2H_2+O_2+7Ar$



Weak ignition;
$8H_2+2O_2+90Ar$

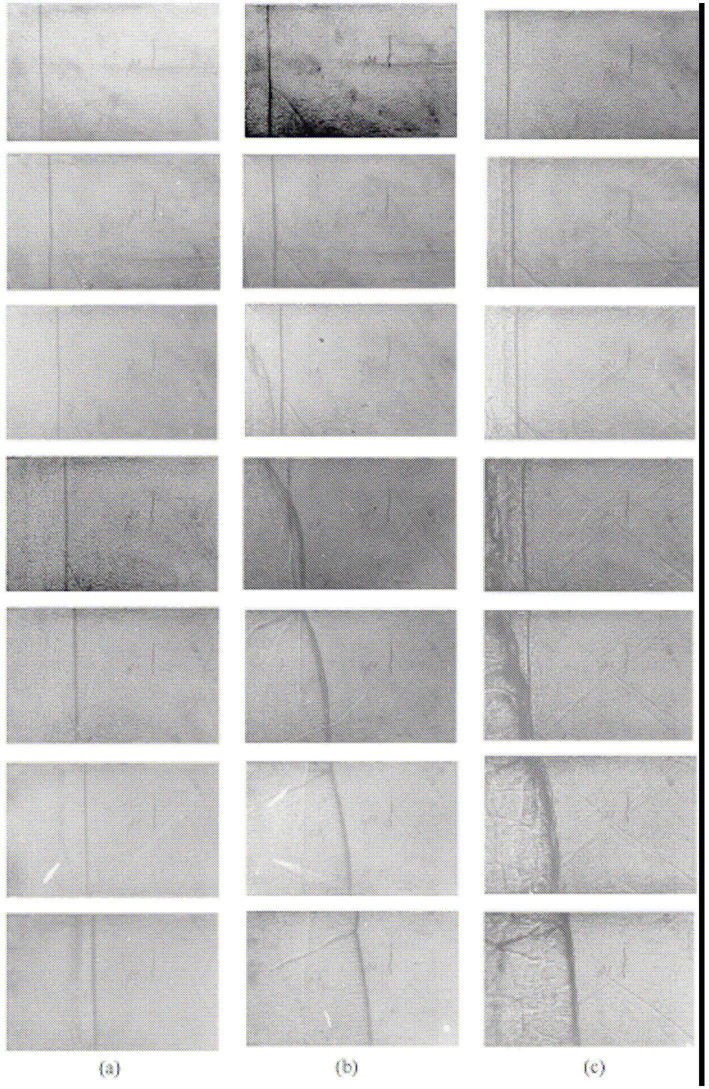
(Cohen & Larsen, 1967)

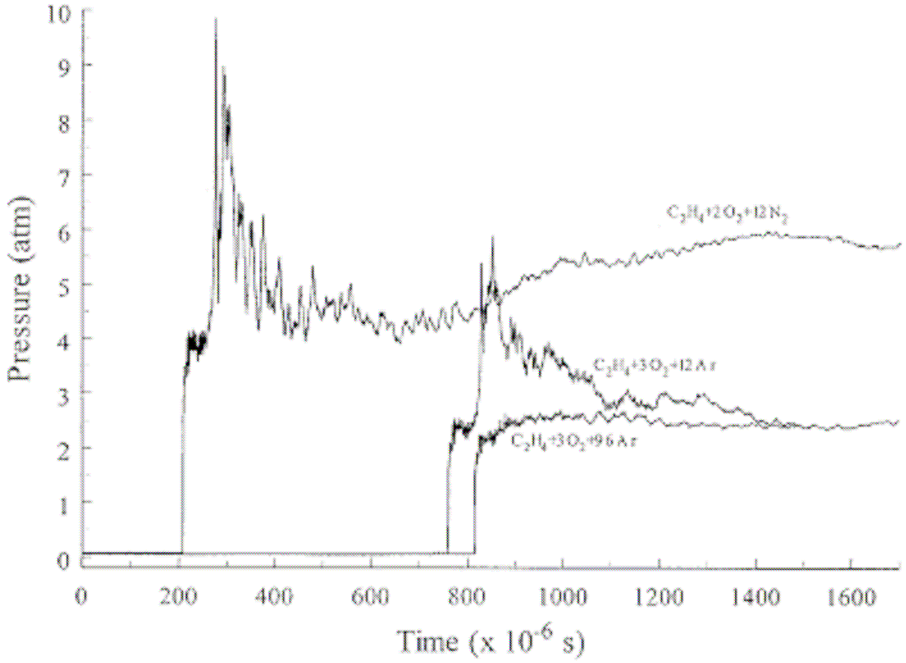
Reflected shock initiation of detonation



(Gamezo et al., 2001)

Reflected shock initiation of detonation





(a) $C_2H_4 + 3O_2 + 96Ar$ (incident shock Mach number 2.65),
(b) $C_2H_4 + 3O_2 + 12Ar$ (incident shock Mach number 2.64),
(c) $C_2H_4 + 3O_2 + 12N_2$ (incident shock Mach number 3.11).

Initial pressure 0.0526 bar; 10 μs frame spacing.

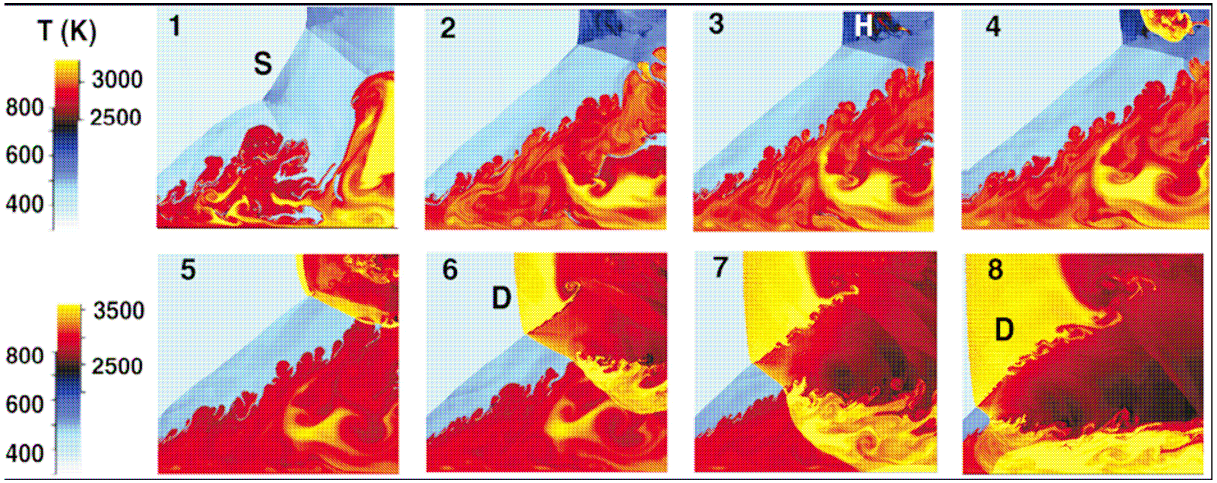
(Brown & Thomas, 1999)

Shock initiation of detonation

S – shock wave *H – hot spot*

D - detonation

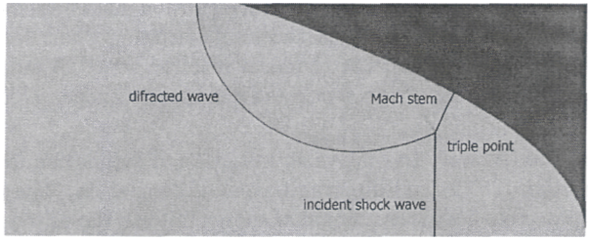
437 µs *485 µs* *496 µs* *503 µs*

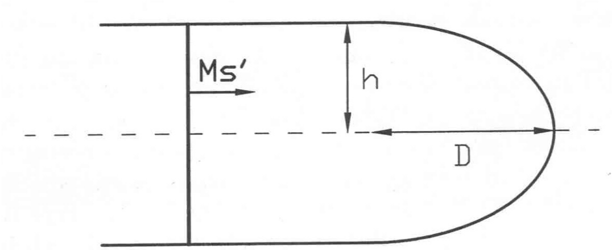


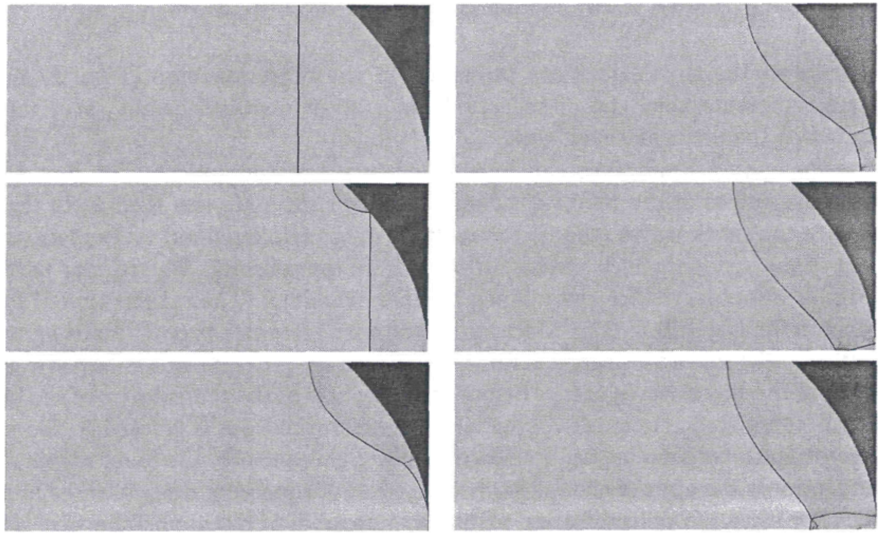
507 µs *515 µs* *524 µs* *533 µs*

(Gamezo et al. 1978)

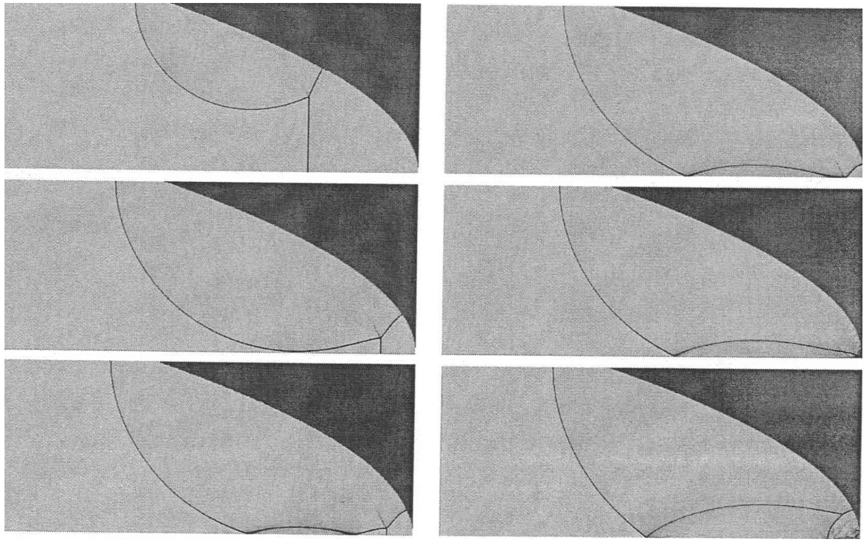
Detonation initiation by shock focusing





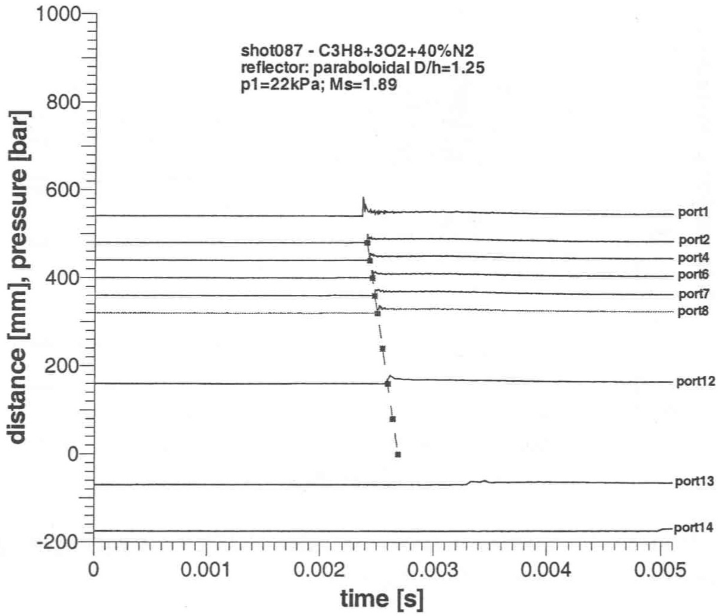


(a) (b)

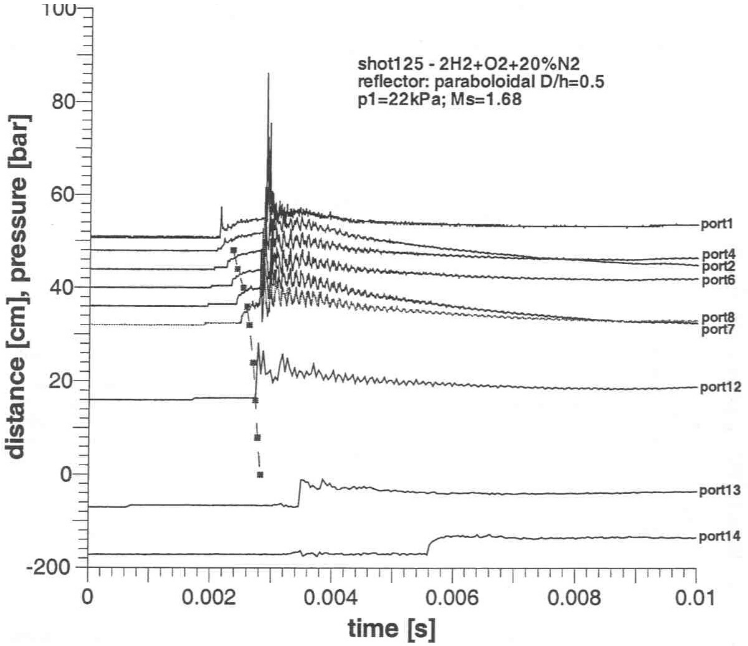


(Buraczewski & Shepherd, 2000)

Detonation initiation by shock focusing



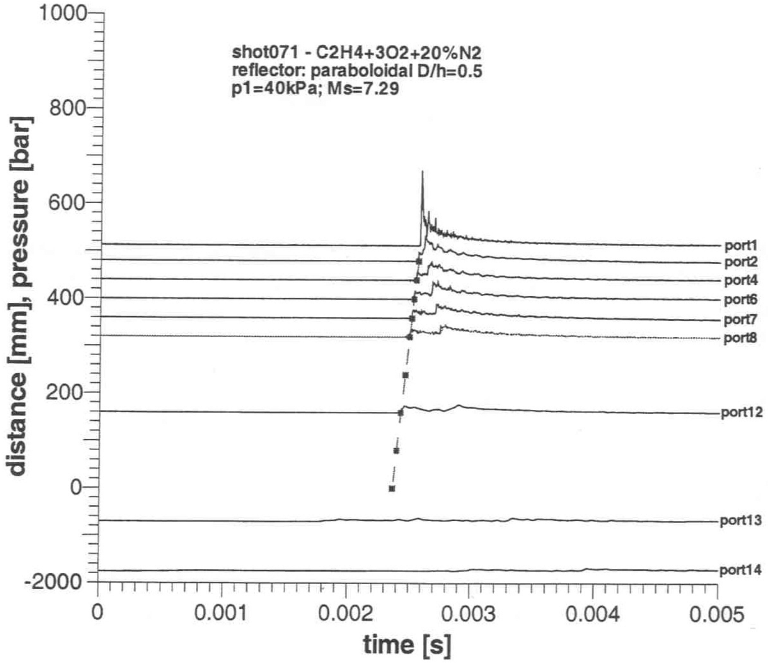
(a) Detonation initiation inside reflector; C3H8+5O2+40%N2; Ms = 1.89



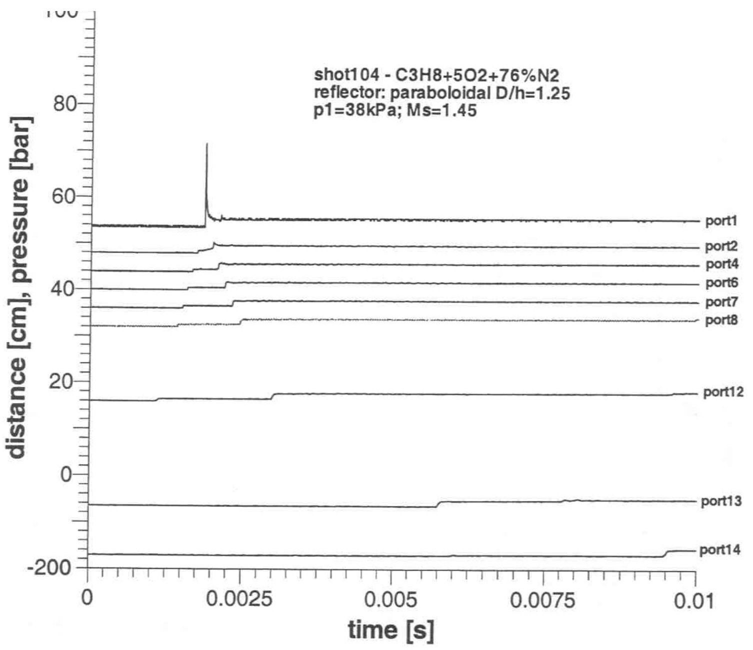
(b) DDT; H2+O2+20%N2; Ms = 1.68

(Buraczewski & Shepherd, 2000)

Detonation initiation by shock focusing



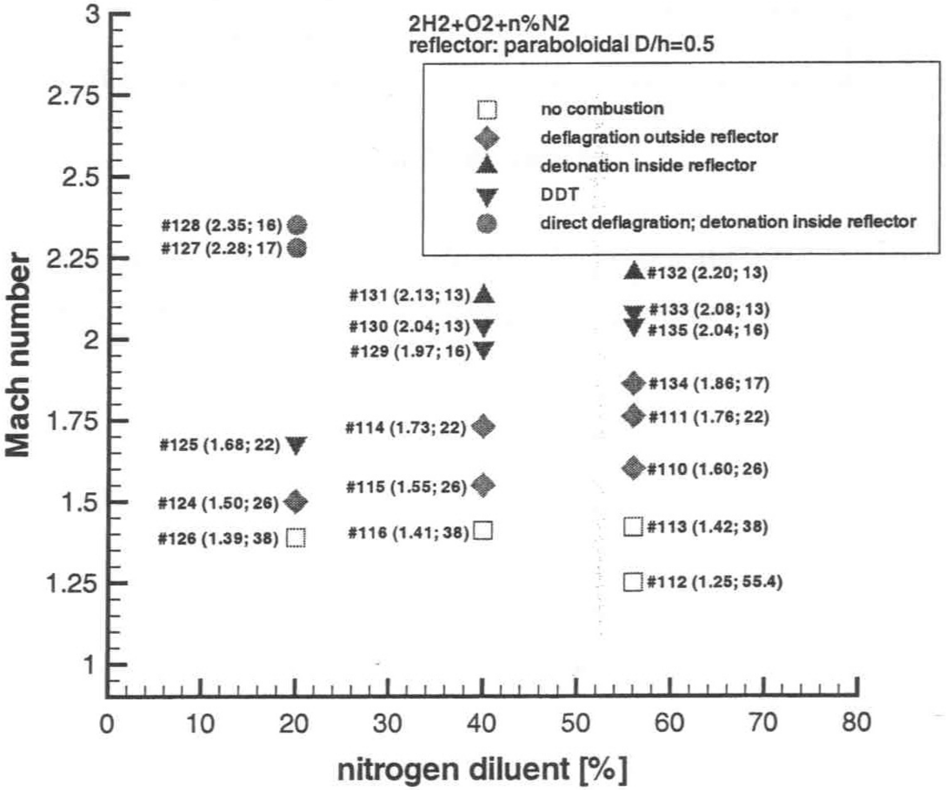
(a) Direct Detonation Initiation;
C2H4+3O2+20%N2; Ms = 1.41



(b) No combustion; C3H2+5O2+76%N2; Ms = 1.45

(Buraczewski & Shepherd, 2000)

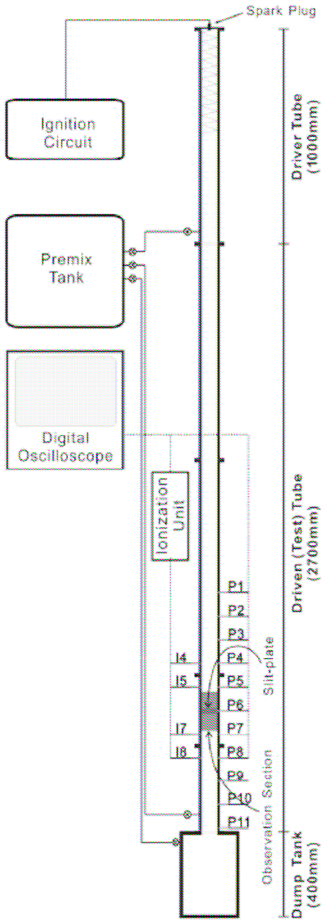
Detonation initiation by shock focusing

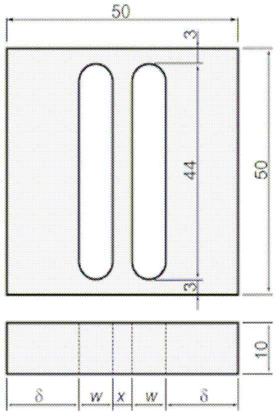


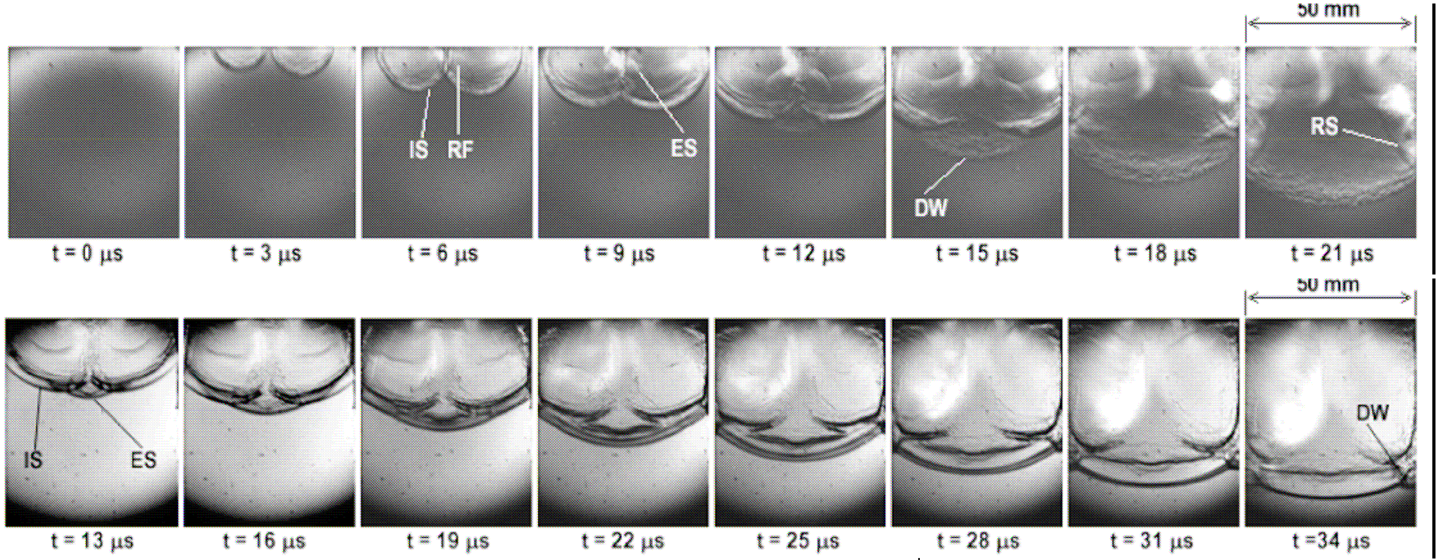
stoichiometric hydrogen-oxygen mixture
with varying nitrogen dilution for
paraboloidal reflector of D/h = 0.5.

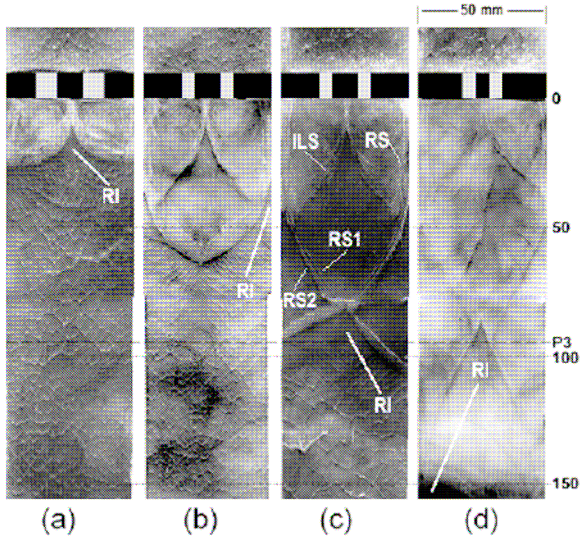
(Buraczewski & Shepherd, 2000)

Detonation initiation by shock collision









Source: Jayan Sentanuhady et al. 21st ICDERS, July 23-27, 2007 Poitiers

SWACER mechanism

SWACER – **S**hock **W**ave **A**mplification by **C**oherent **E**nergy **R**elease

(Lee & Moen, 1980)

- Turbulent mixing ⇒ temperature and concentration gradient – different induction times along the gradient (jet initiation of detonation)
- Ultraviolet irradiation ⇒ gradient of radicals (photochemical initiation)
- Accelerating energy release generates compression waves which are amplified to form a strong shock
- Close coupling between gasdynamics and exotermicity via compression waves

SWACER mechanism

D – detonation speed

U_{si} – spontaneous ignition wave speed

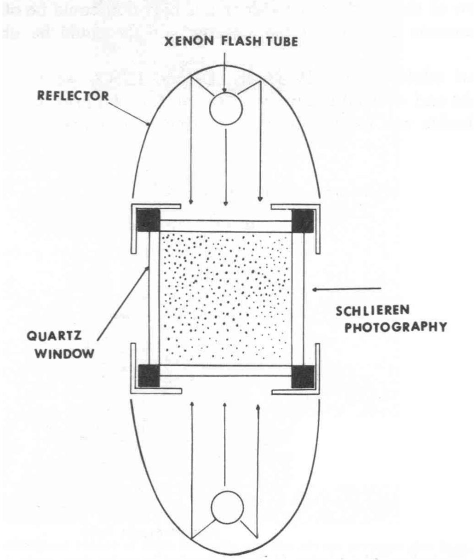
a – sound speed

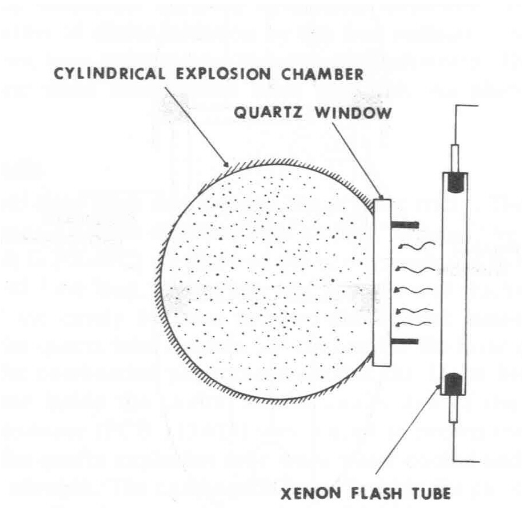
S_L – laminar flame speed

Zel'dovich (1980) proposed four different regimes:

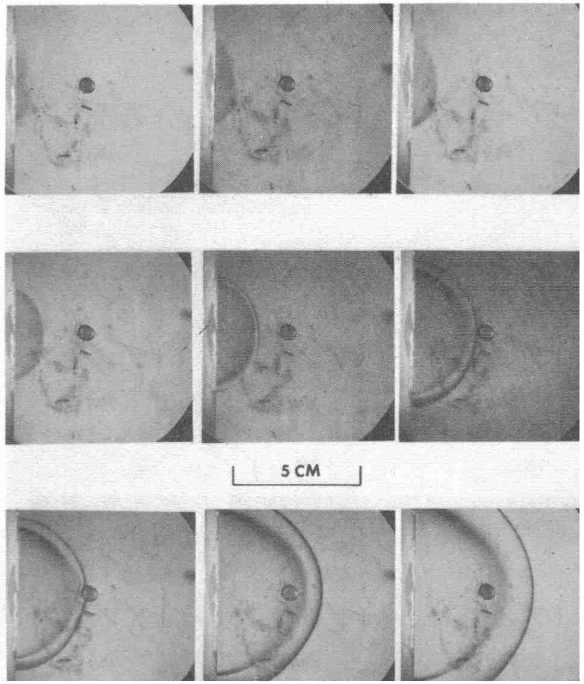
1. $U_{si} > D$: reaction wave is so rapid that it resembles a constant volume explosion
2. $a < U_{si} < D$: transition to detonation through synchronized initiation
3. $S_L < U_{si} < a$: reaction wave propagates with small pressure change across it because the compression wave run away
4. $U_{si} < S_L$: diffusion dominates, leading to the formation of laminar flame

Photochemical initiation of detonation

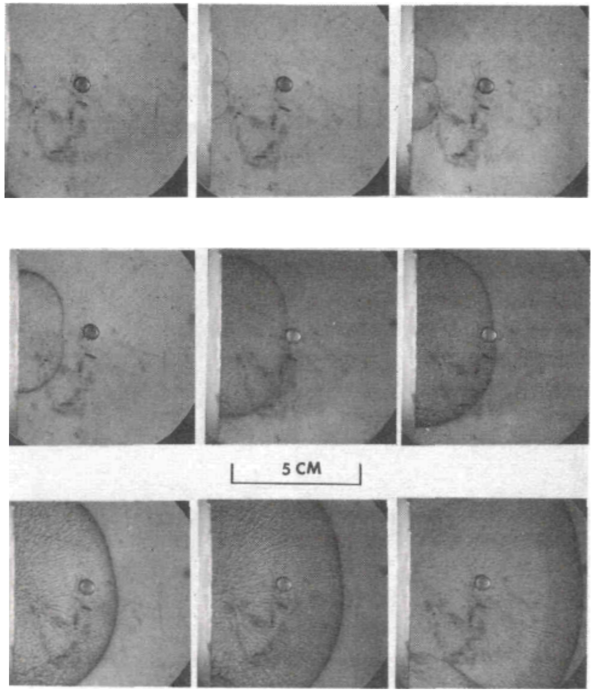




H_2-Cl_2 at 100 torr



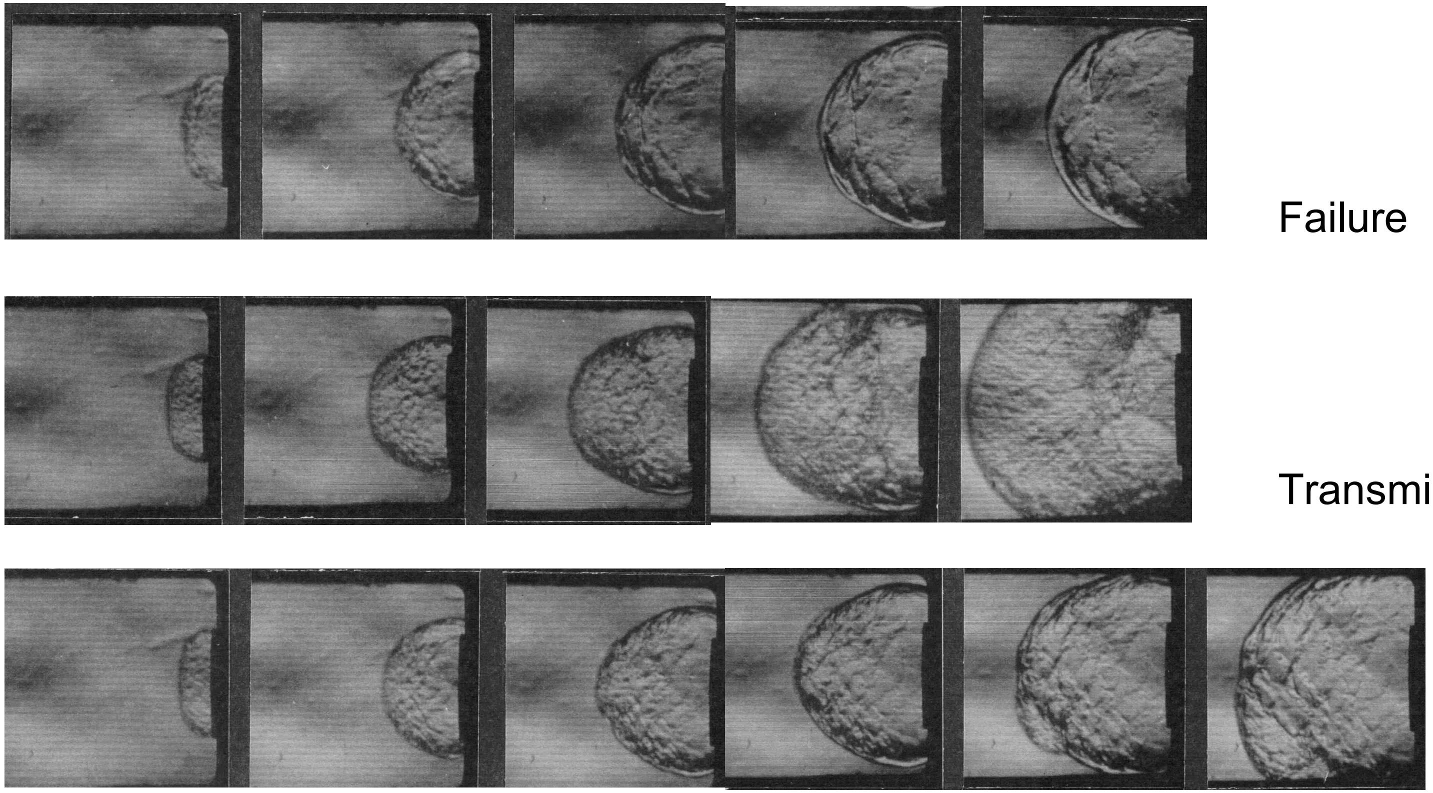
deflagration



detonation

(Lee et al. 1978)

Jet initiation of detonation



Failure

Transmission

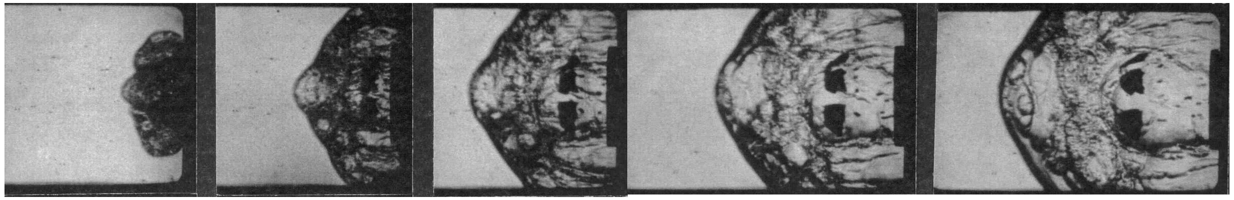
Re-initiation

Diffraction of planar detonation into unconfined space

(Inada et al., 1991)

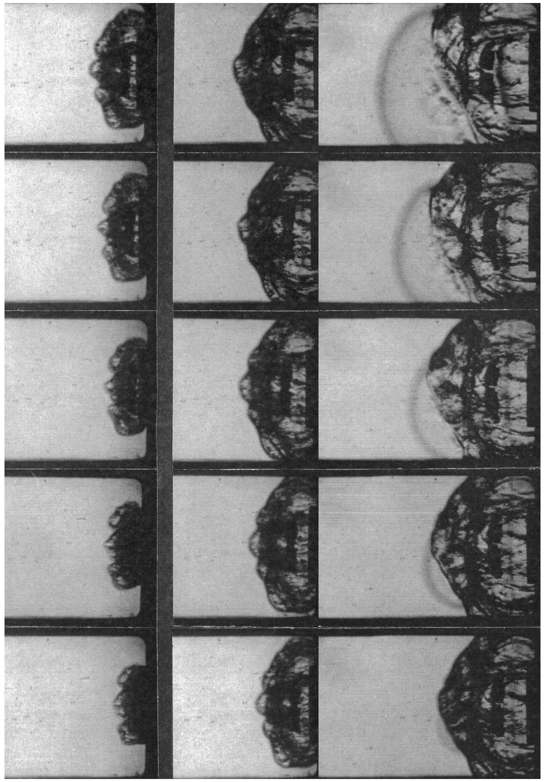
Jet initiation of detonation

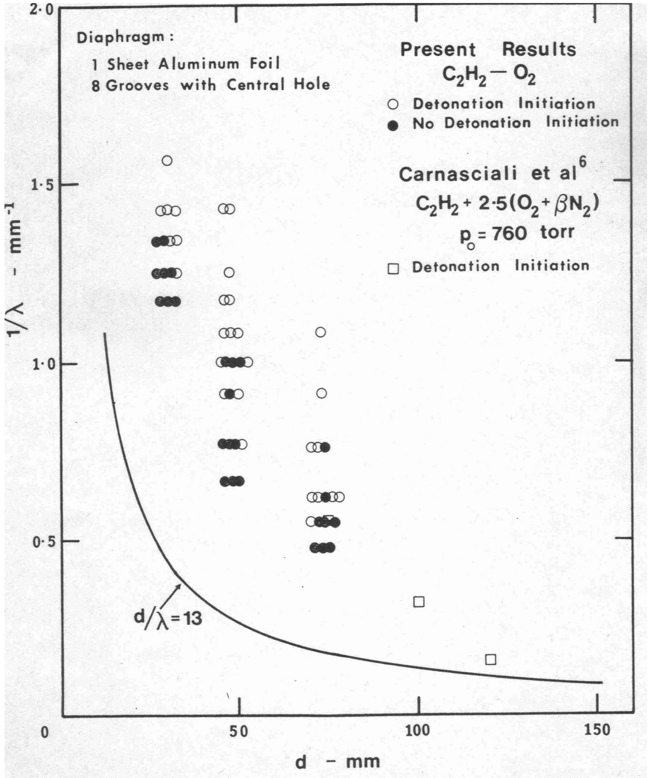
Failure



Initiation

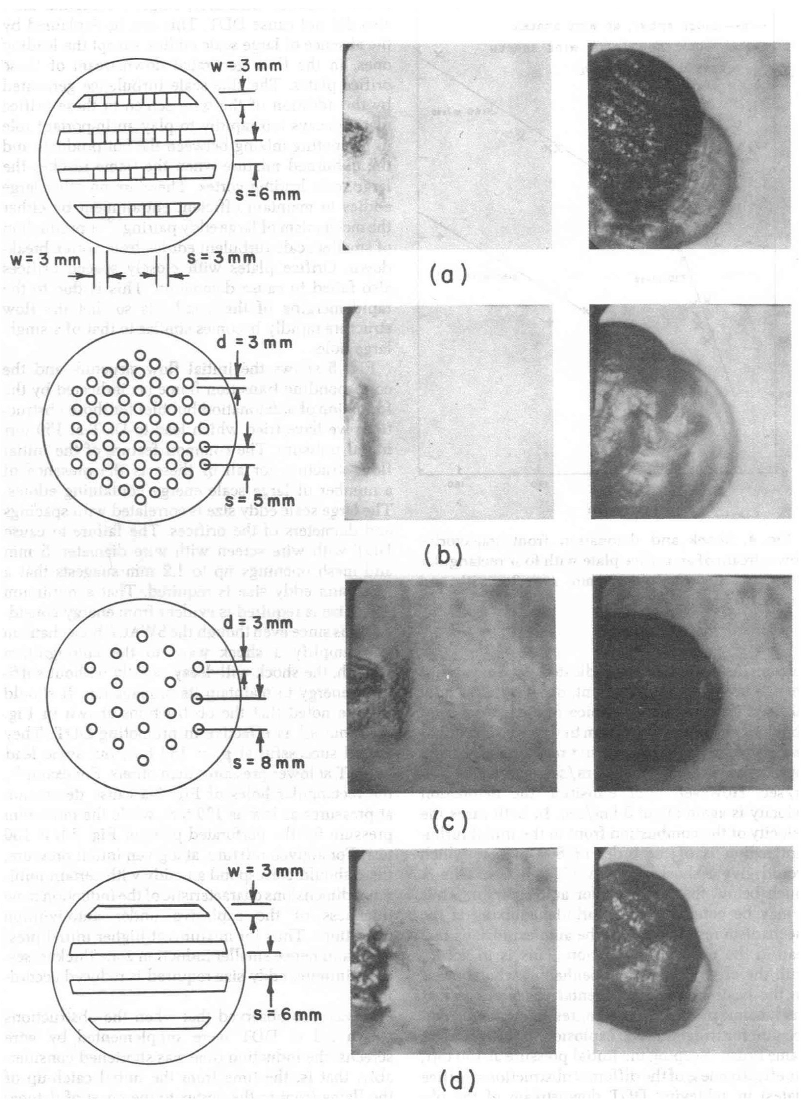
Turbulent
hot jet

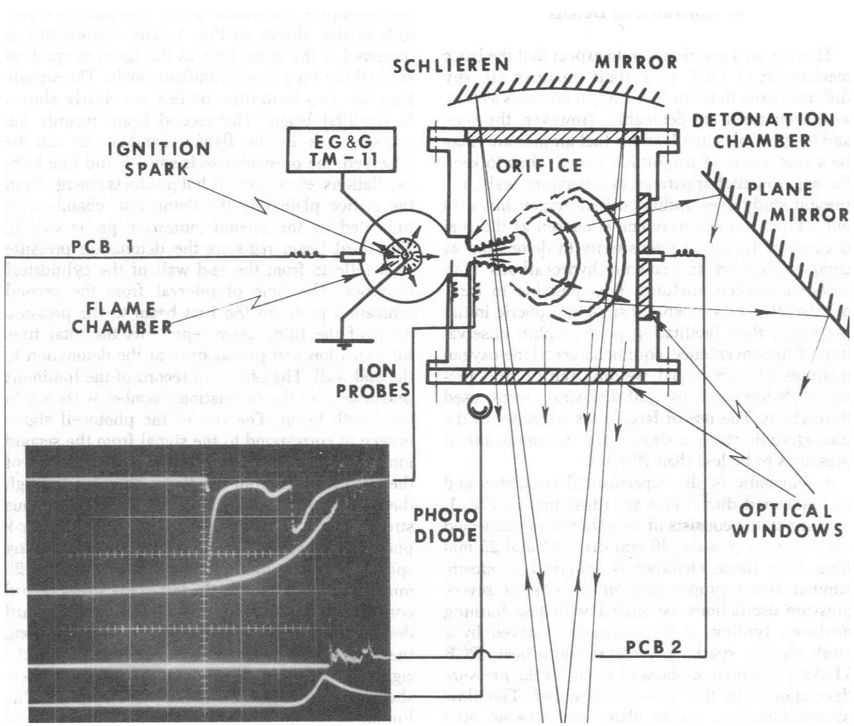




(Inada et al., 1991)

Jet initiation of detonation

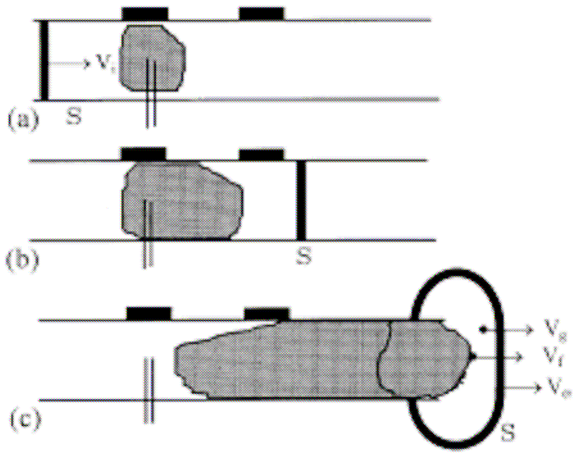


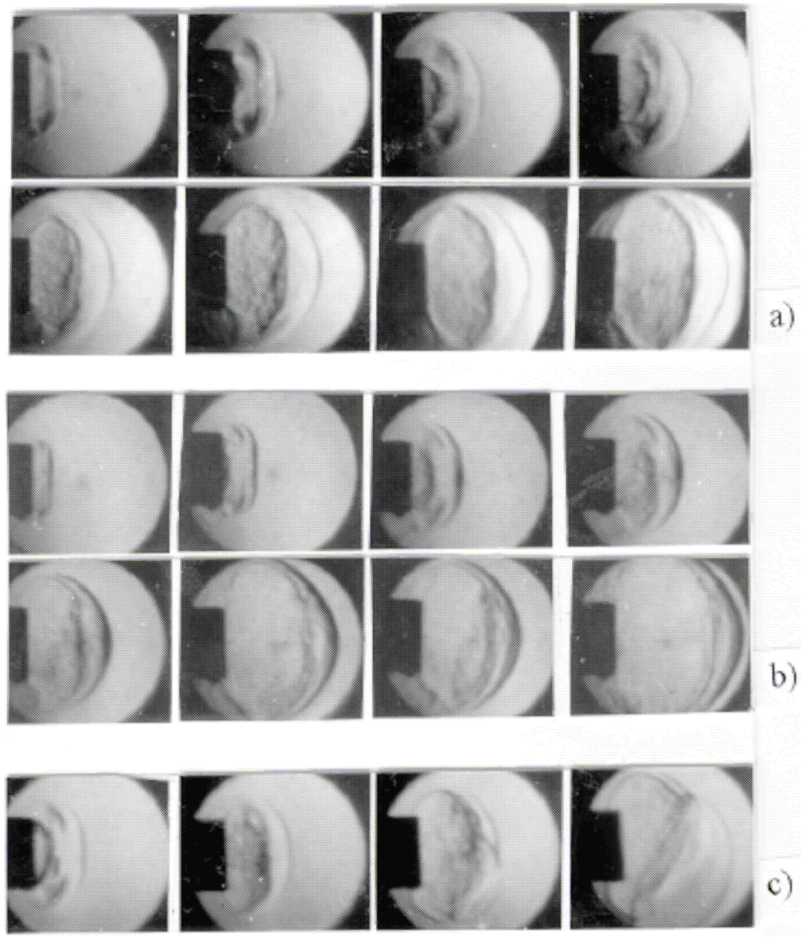


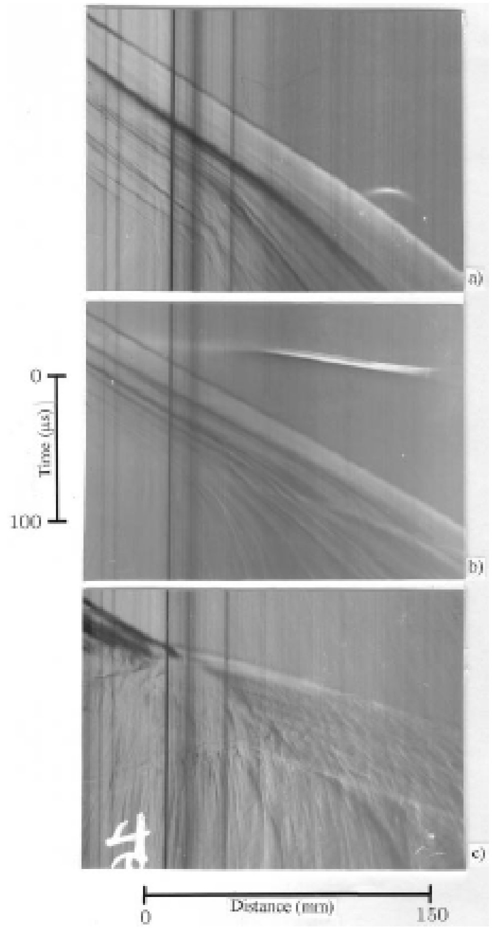
C2H2-O2, 150 torr

(Knystautas et al., 1978)

Jet initiation of detonation







C2H4-O2, 60 torr

(a) *failure,*

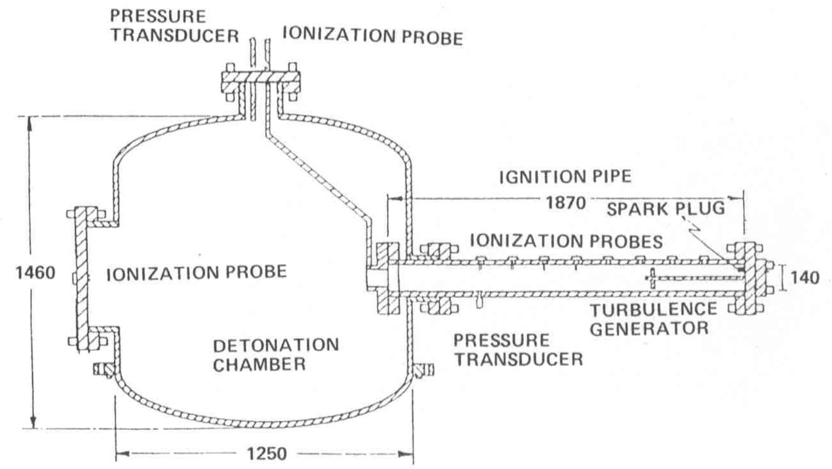
(b) *flame acceleration,*

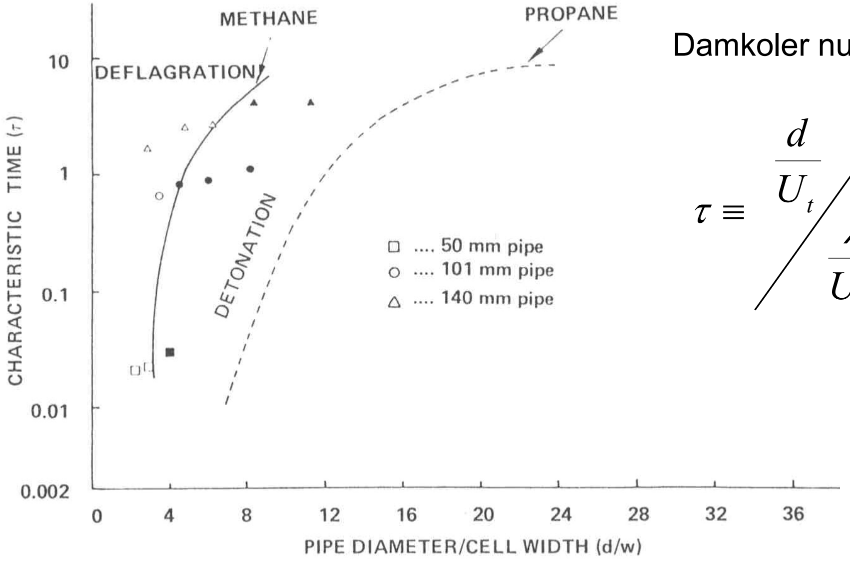
(c) *transition to detonation.*

$\Delta t = 10\ \mu s$,

(Thomas & Jones, 2000)

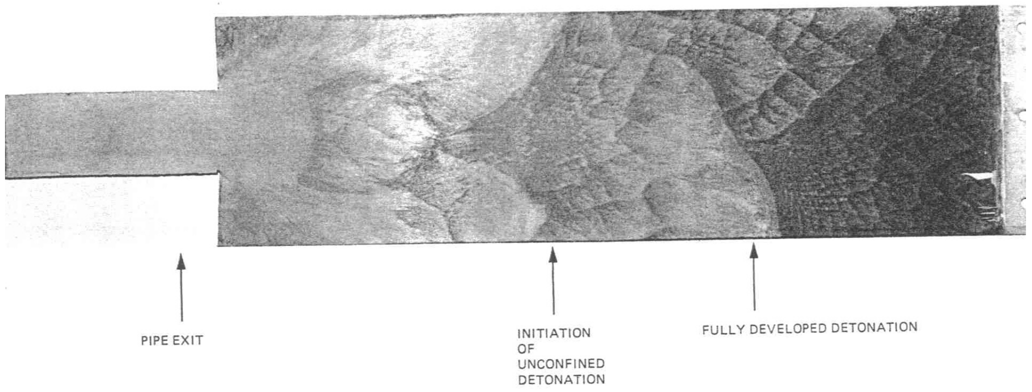
Jet initiation of detonation





Damkoler number

$$\tau \equiv \frac{d / U_t}{\lambda / U_d}$$



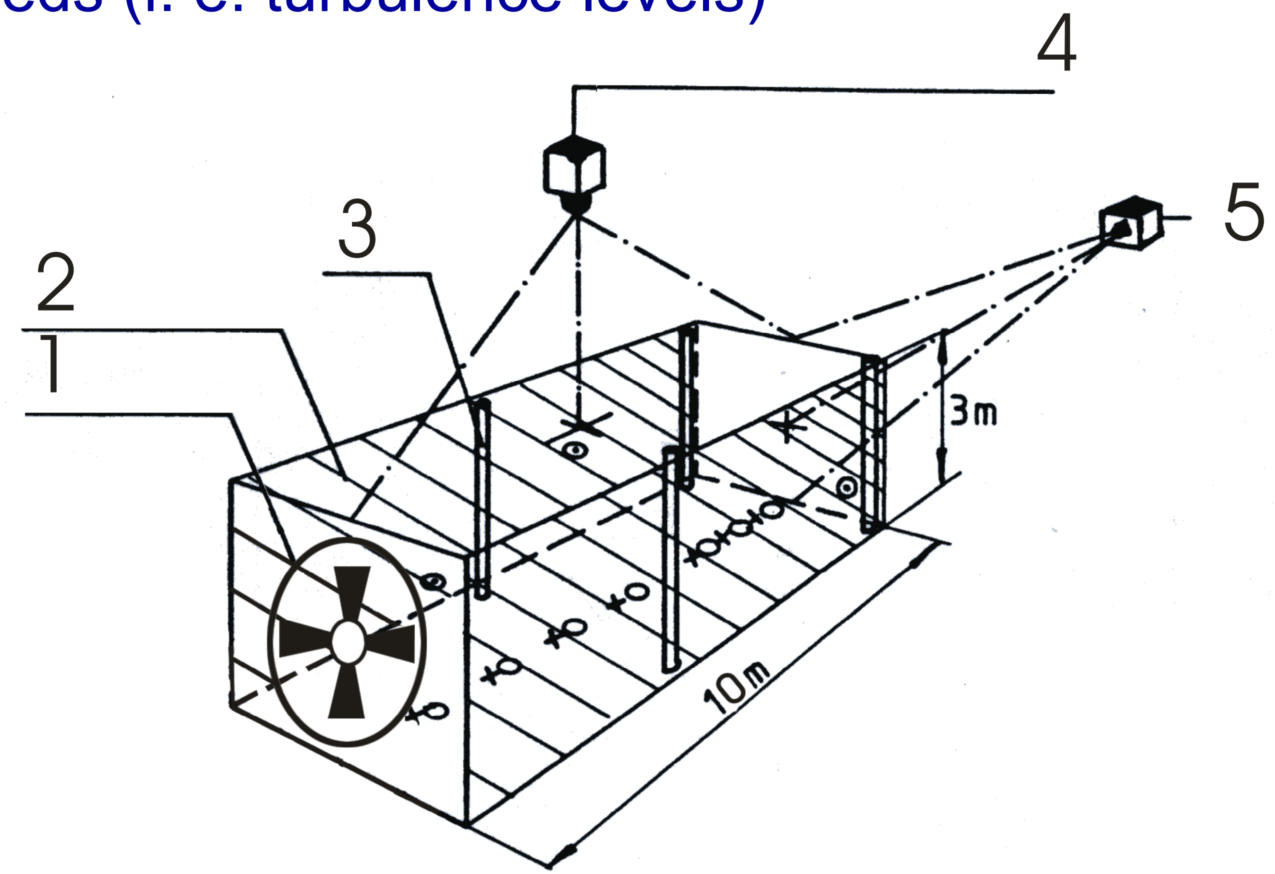
(Ungutt & Shuff, 1988)

Pipe diameter 50 mm for a stoichiometric propane-oxygen with 45.5% nitrogen, 0.4 bar

SWACER in large scale?

Turbulence plus partial confinement

Variable fan speeds (i. e. turbulence levels)



1 fan

2 partially confined hydrogen/air mixture

3 tube

4 Hycam- and Locam camera

5 Hycam camera

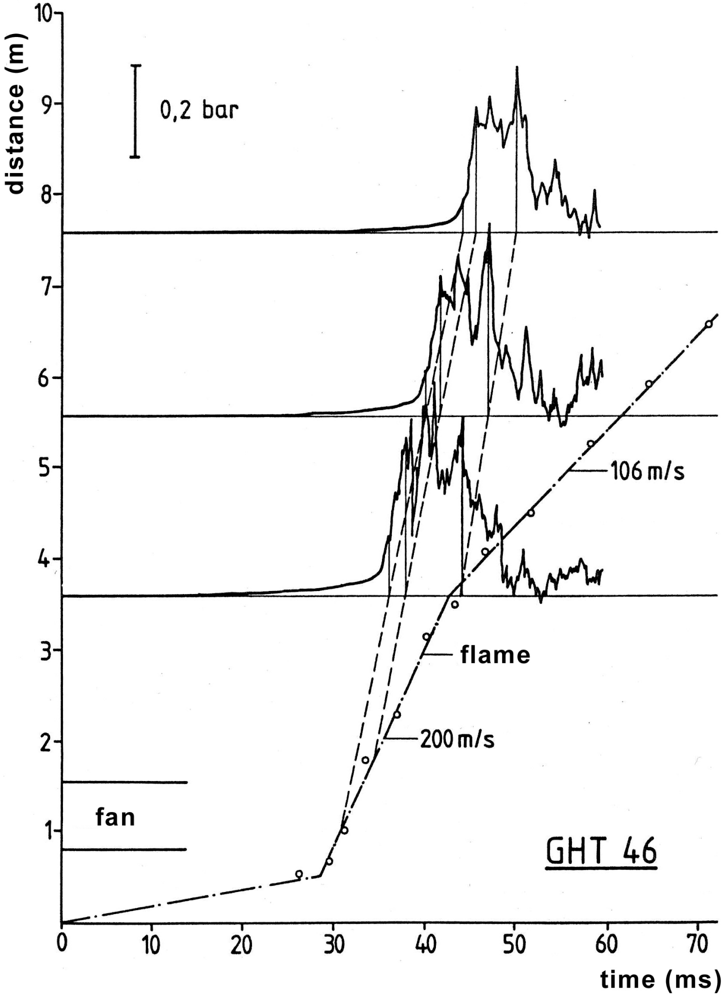
x, o: pressure transducers

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

SWACER in large scale?

Flame Propagation and Pressure/Time-History

Moderate fan speed
(i.e. turbulence level)

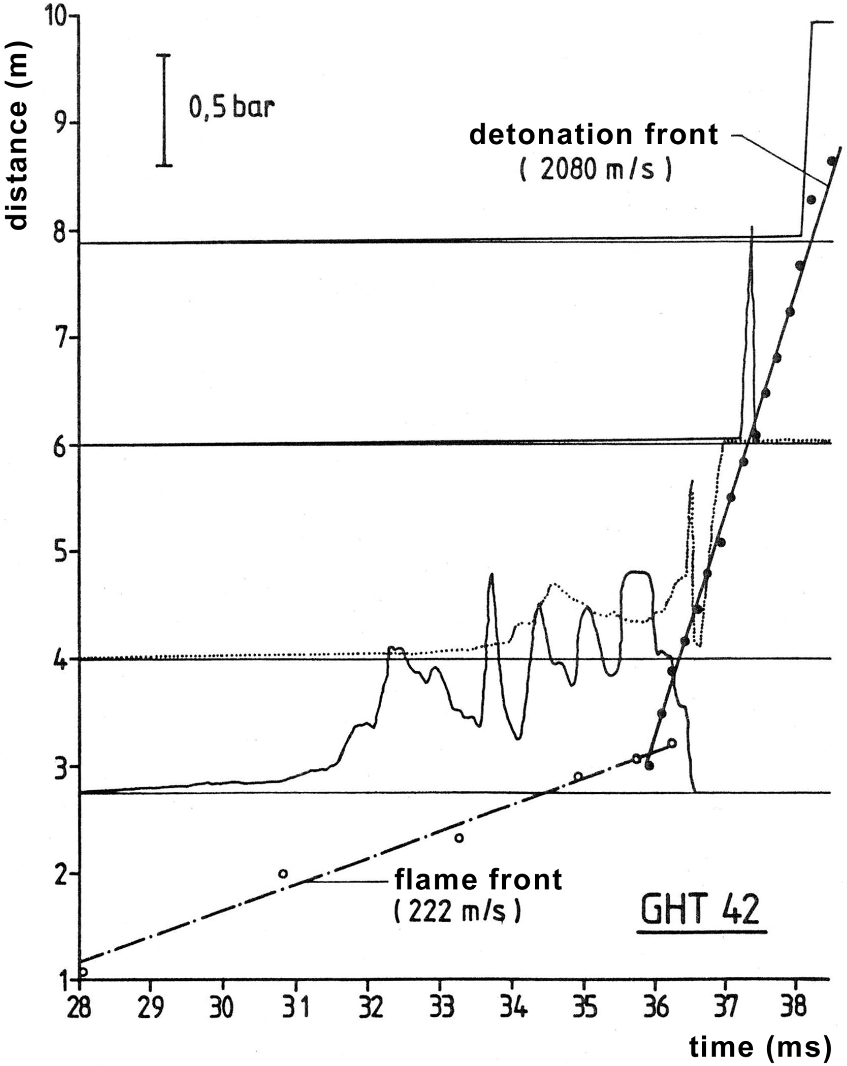


(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

SWACER in large scale?

For very high fan speed (i.e. turbulence level):

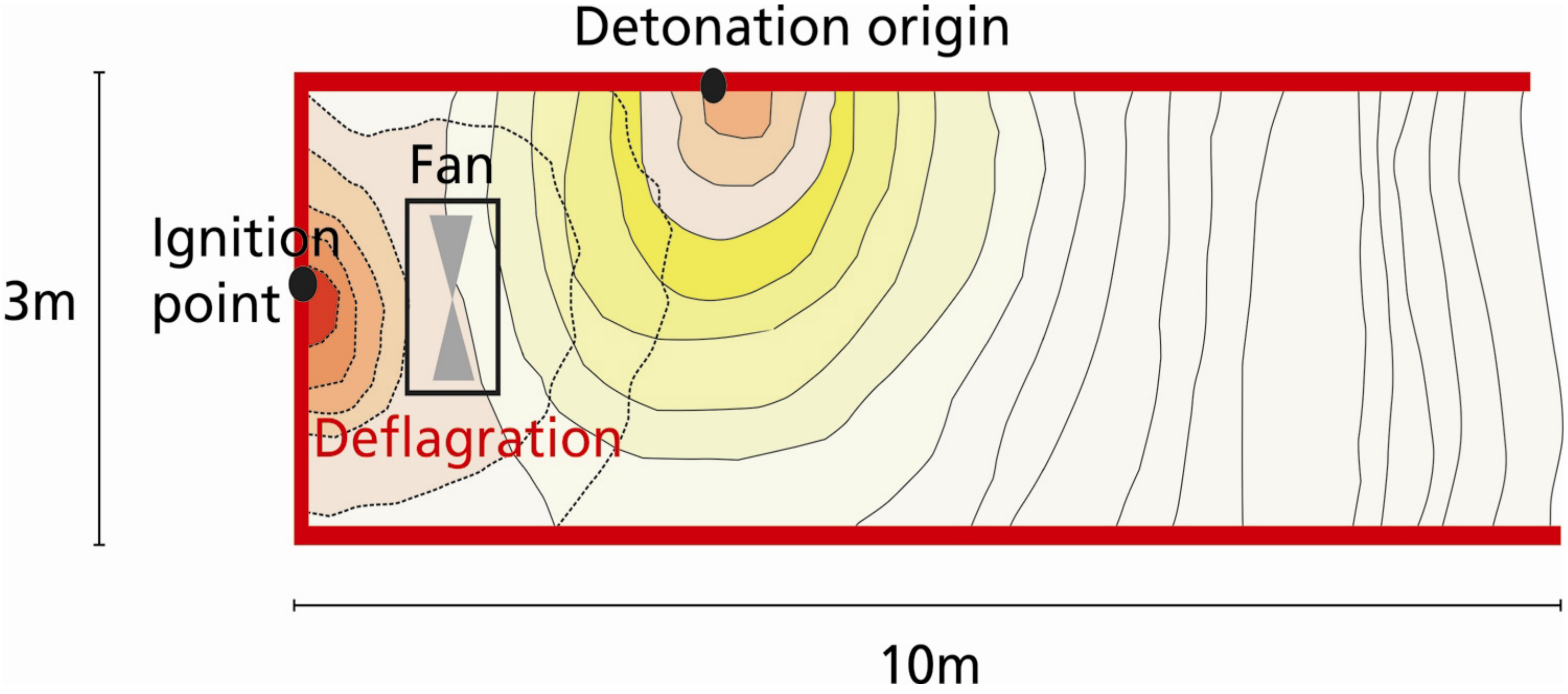
Deflagration to Detonation Transition



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

SWACER in large scale?

Detonation of a hydrogen/air mixture within a “lane”, simulated by two parallel walls (top view)



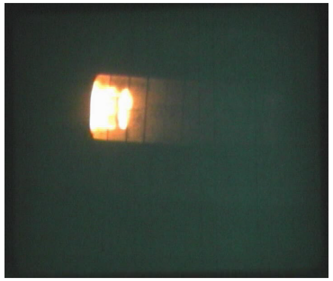
(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

SWACER in large scale?

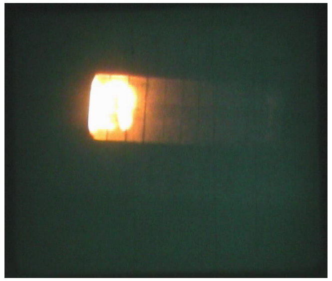
Detonation of a hydrogen/air mixture within a “lane”, simulated by 2 parallel walls (top view)

12 ms

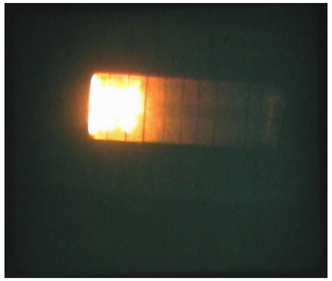
18 ms



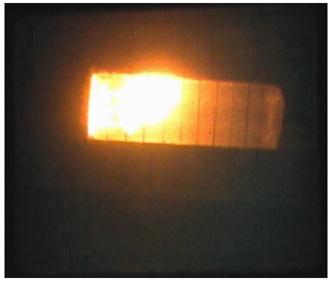
24 ms



30 ms



36 ms



42 ms

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

SWACER in large scale?

Detonation of a hydrogen/air mixture within a “lane”, simulated by 2 parallel walls (top view)

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

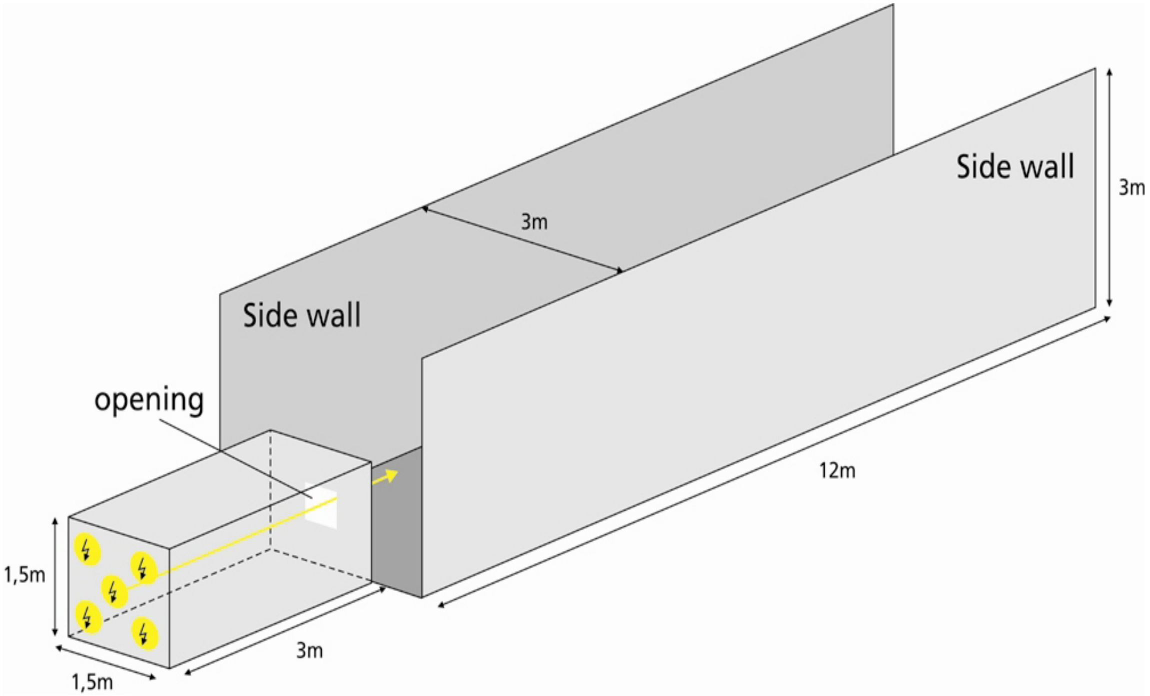
SWACER in large scale?

Test Site after Detonation

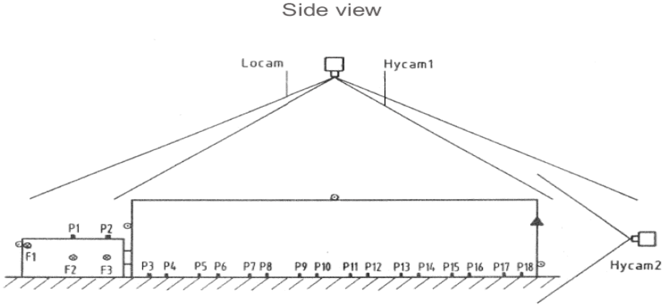
(Courtesy of dr Schneider from Fraunhofer
Institute Chemische Technologie)

Jet initiation of detonation in large scale

Test setup for igniting a hydrogen/air mixture by means of a flame jet within a “lane“, simulated by two parallel walls



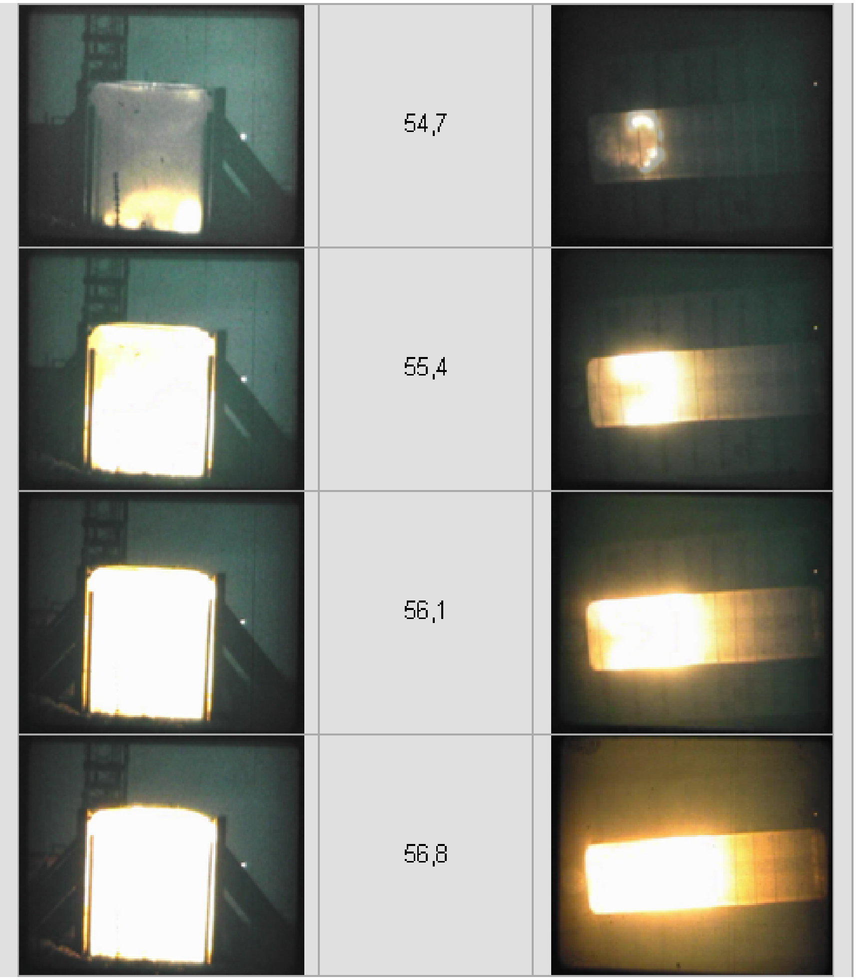
Ignition at rear end of box



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

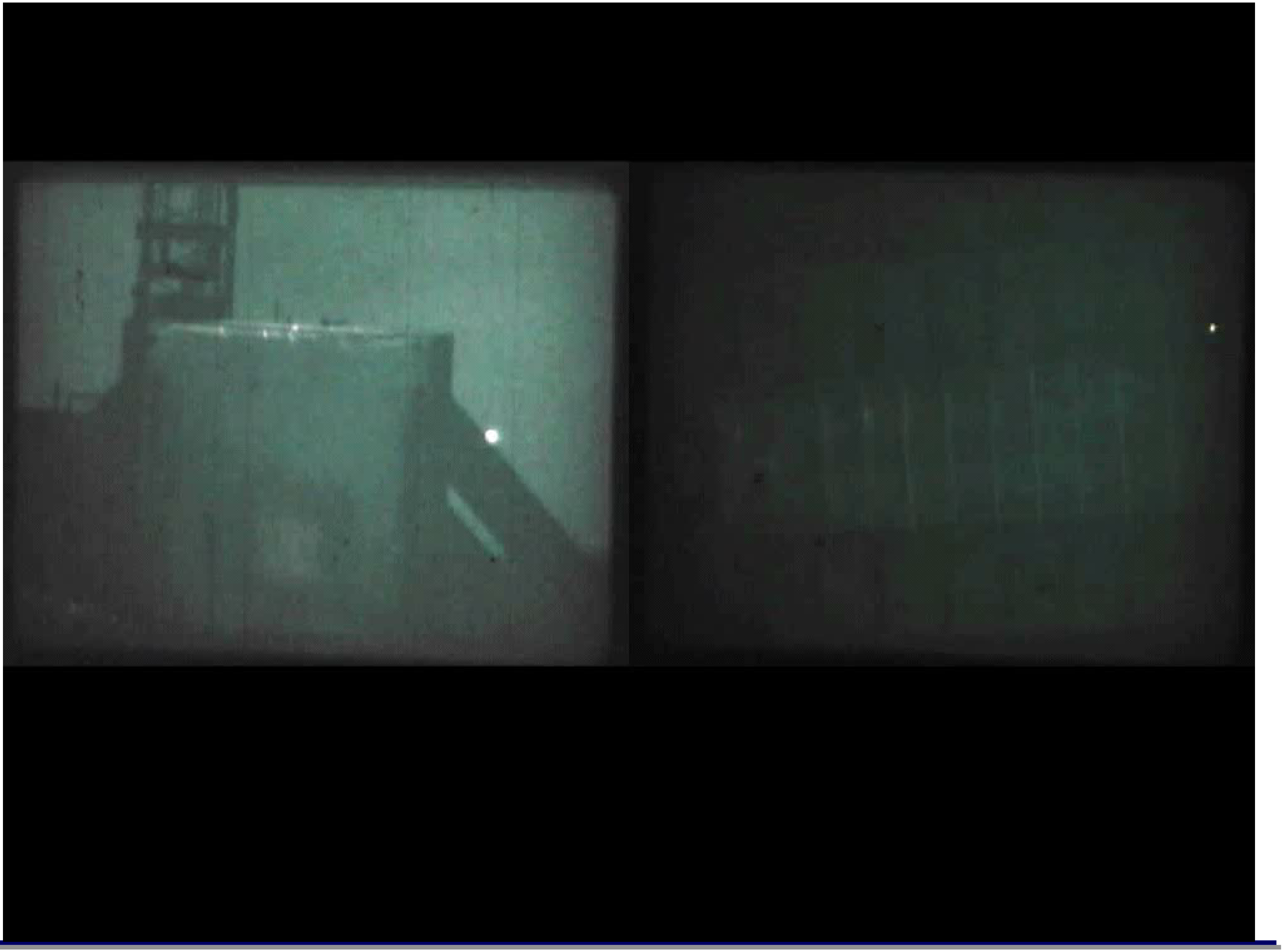
Jet initiation of detonation in large scale

Flame jet ignition of hydrogen air cloud within a “lane” with subsequent transition to detonation near the ground.



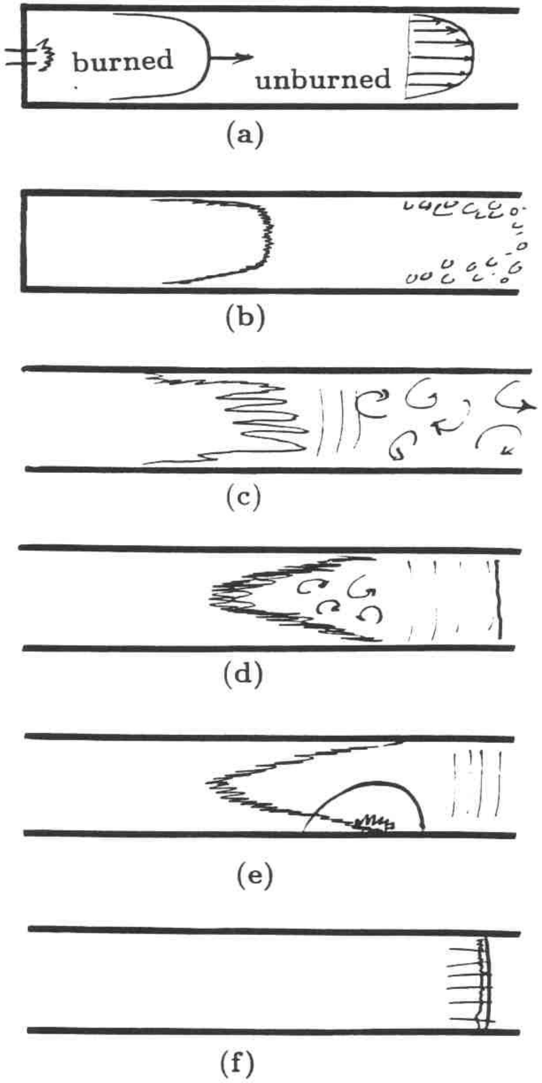
(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

Jet initiation of detonation in large scale



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

Progress of DDT event in a smooth tube



a) the initial configuration showing a smooth flame and the laminar flow ahead;

b) first wrinkling of flame and instability of the upstream flow;

c) breakdown into turbulent flow and a corrugated flame;

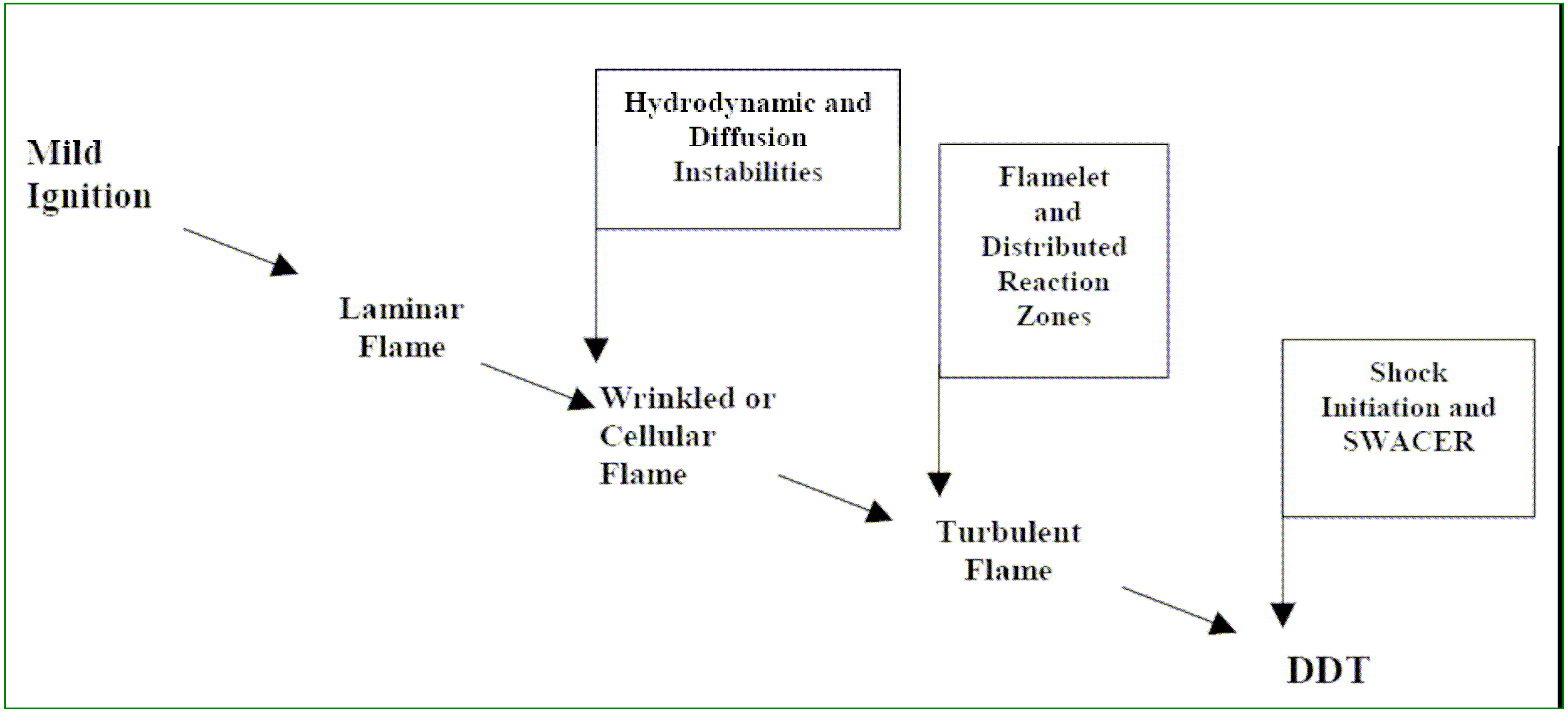
d) production of pressure waves ahead of the turbulent flame;

e) local explosion of a vertical structure within the flame;

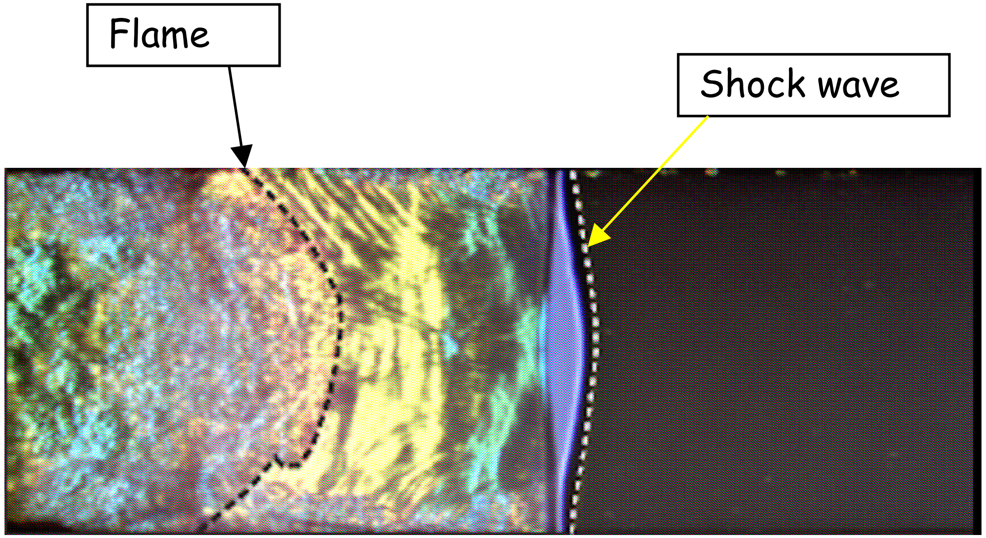
f) transition to detonation.

(Shepherd&Lee, 1992)

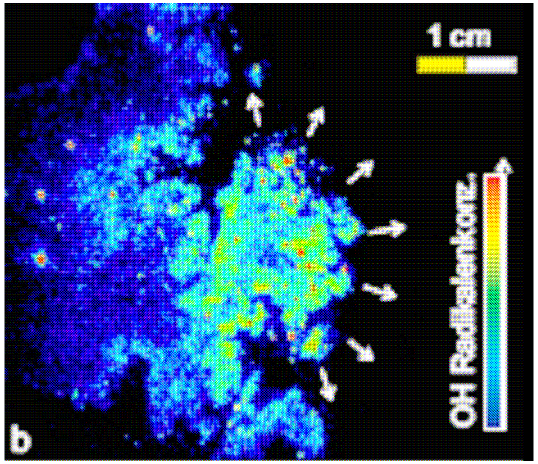
Regimes of flame propagation leading to DDT



Fast deflagration



Schlieren image of a fast deflagration wave (22% H2 in air), flame velocity 1200 m/s;



OH radical distribution of a fast deflagration wave, flame velocity 850 m/s, 17,5% H2 in air;

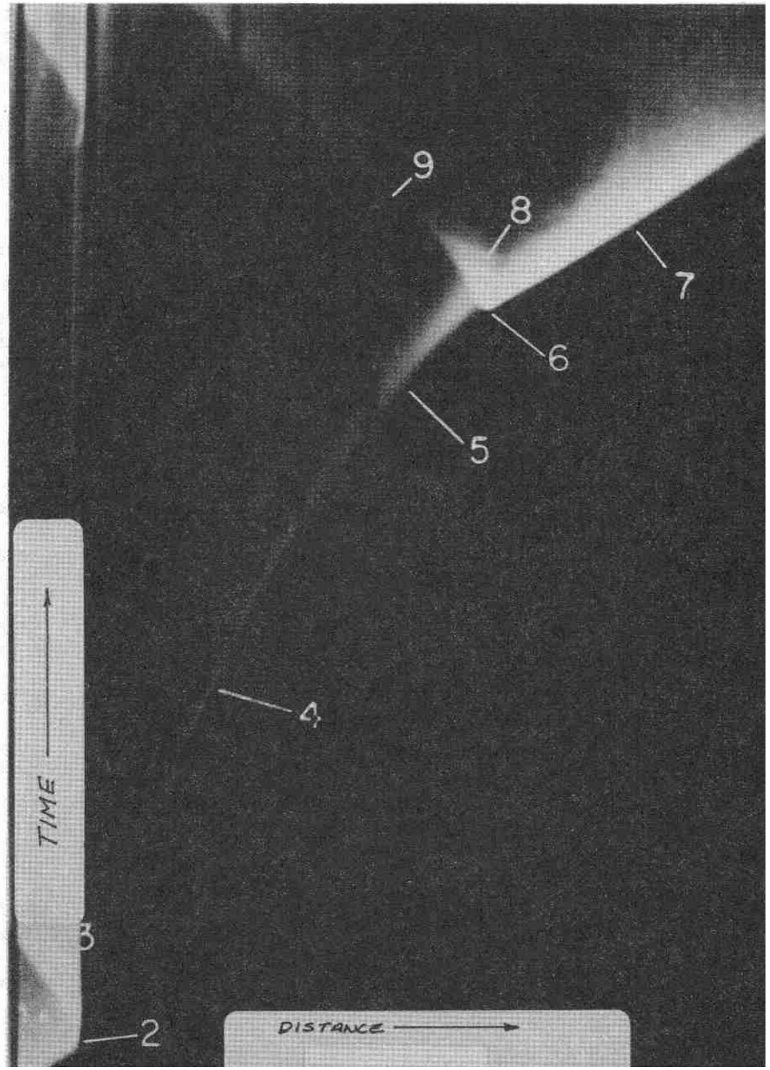
(Eder, 2001)

Transition distance to DDT

Depends on:

- Combustible mixture (chemistry and thermodynamics)
- Tube diameter – for hydrogen-air in smooth tube:
  - 8 m in 50 mm tube
  - 30 m in 400 mm tube
- Ignition source
- Obstacles, wall roughness
- Initial conditions
- ???

DDT in smooth tube



Streak direct photograph

4, 5 – accelerating flame

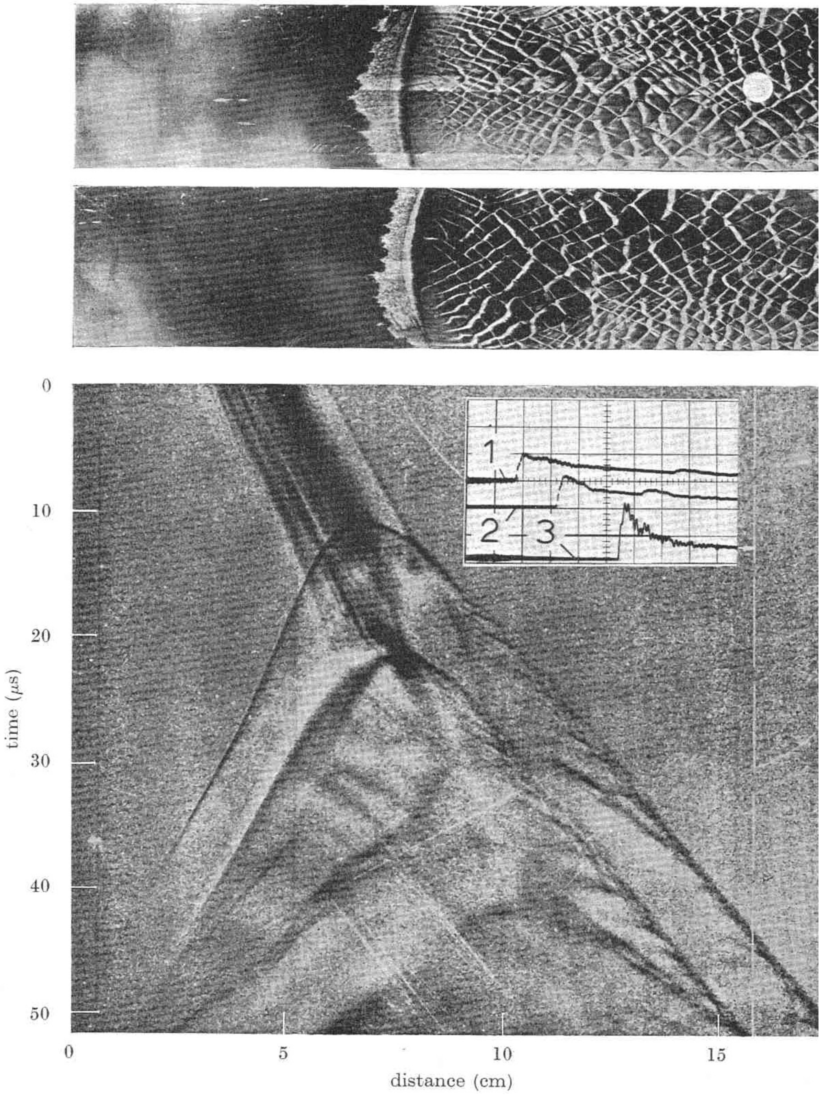
6 – explosion ahead of the flame

7 – detonation

8, 9 – retonation wave

(Lee, 1978)

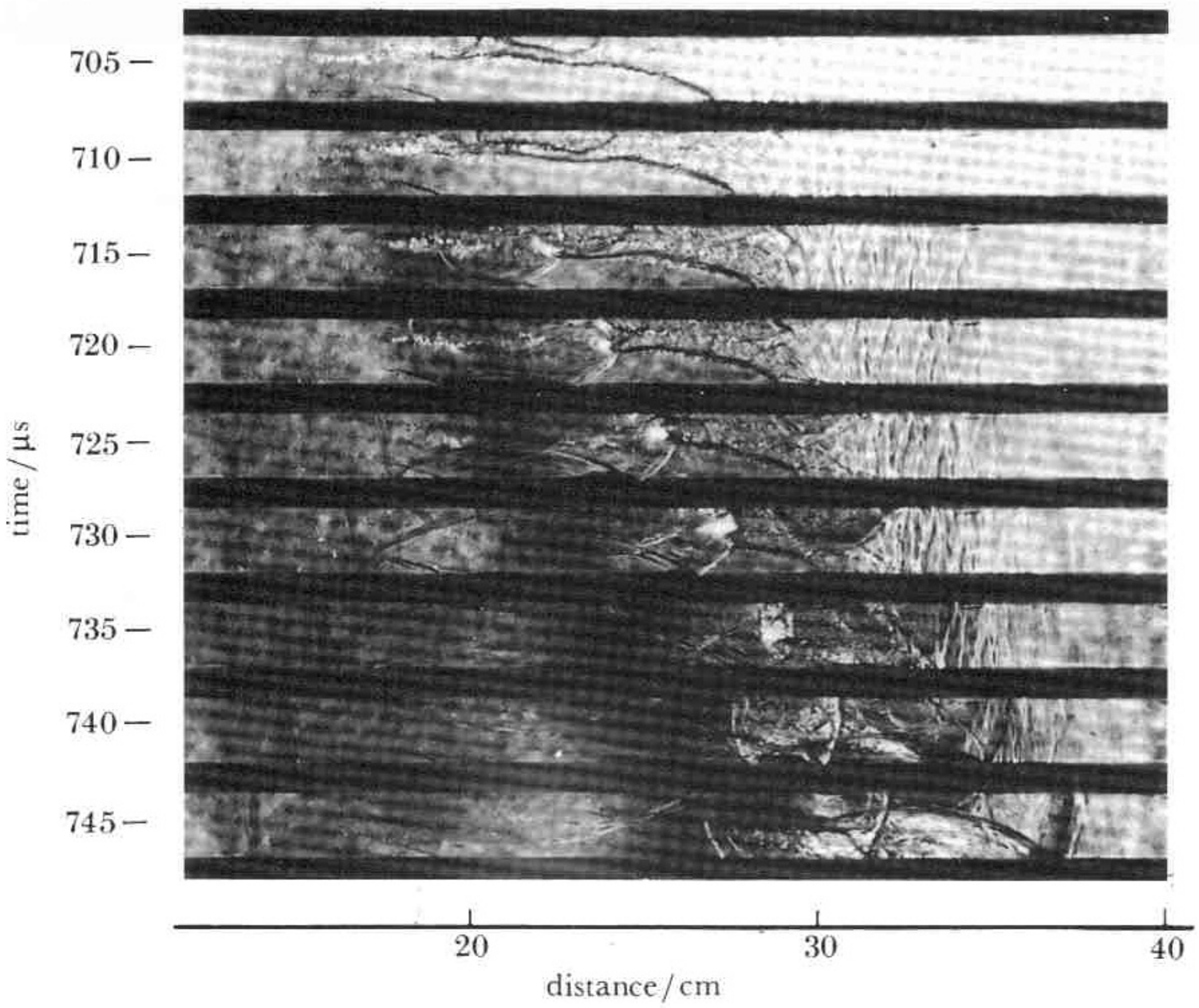
DDT in smooth tube



Streak schlieren photograph

(Myer&Oppenheim, 1965)

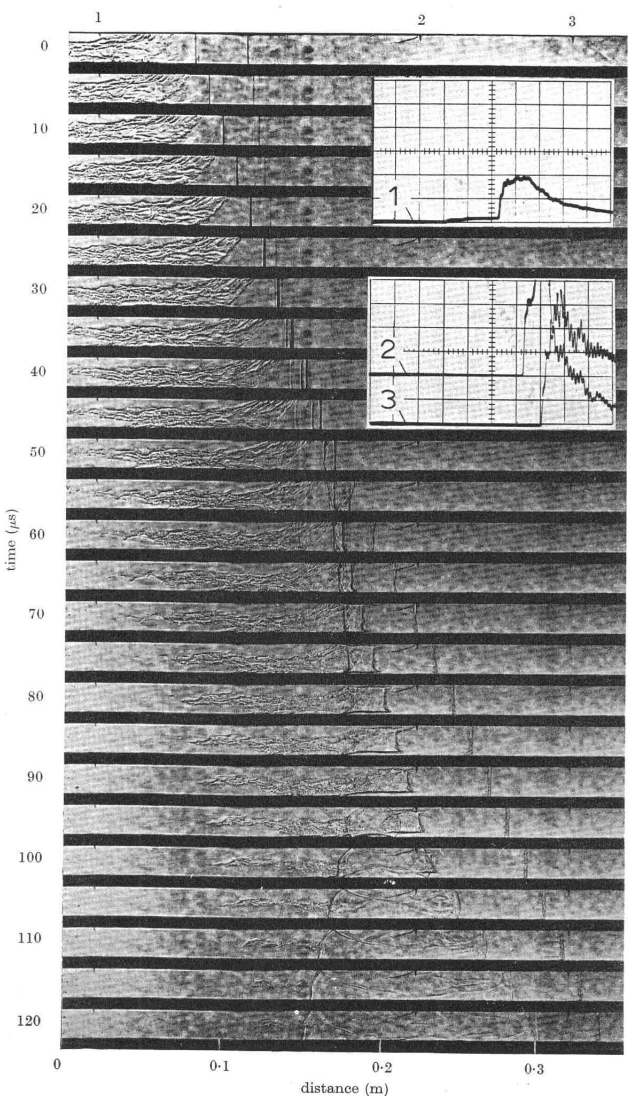
DDT in smooth tube

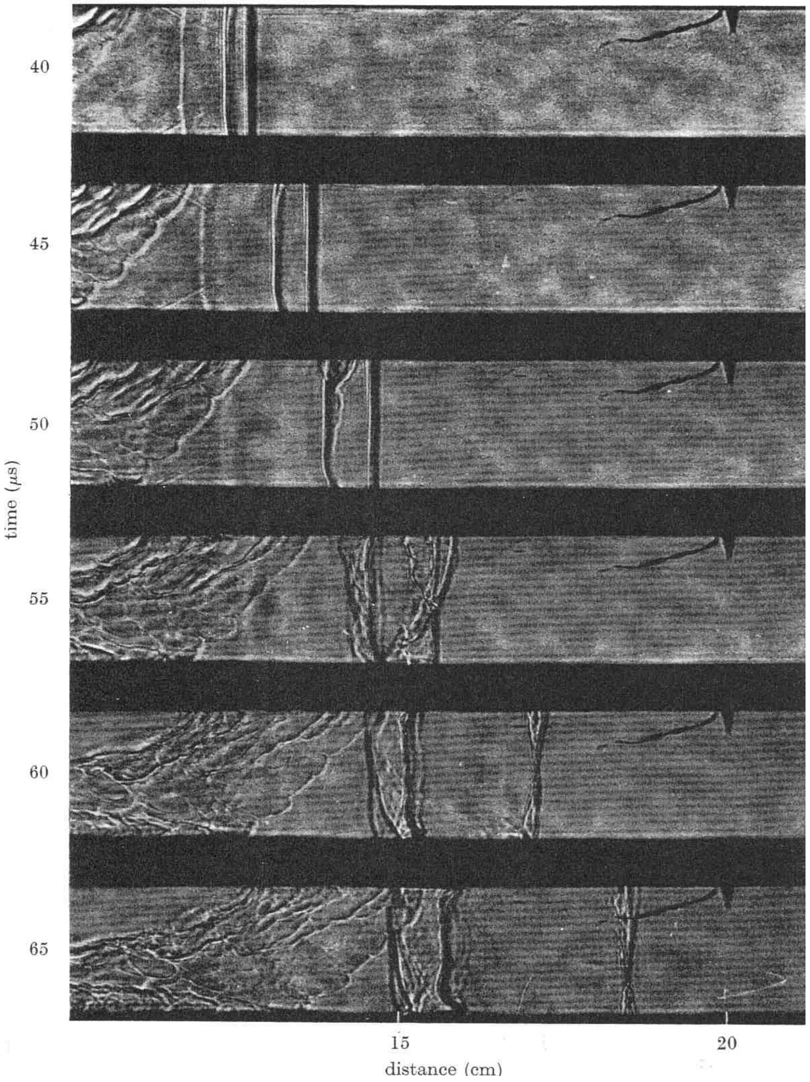


Schlieren framing photographs by rotating mirror camera

(Myer&Oppenheim, 1965)

DDT in smooth tube

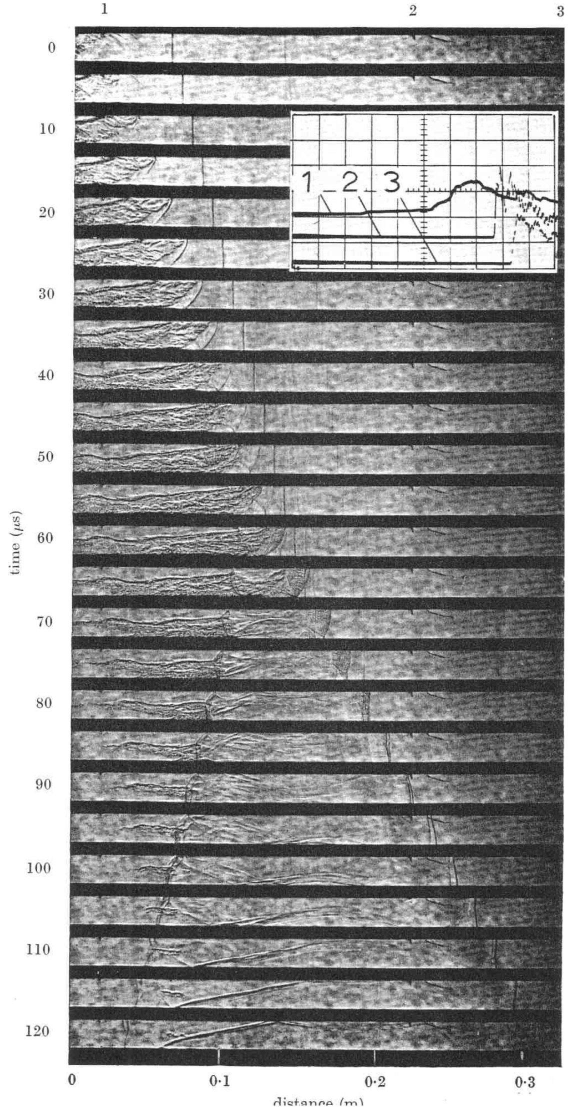


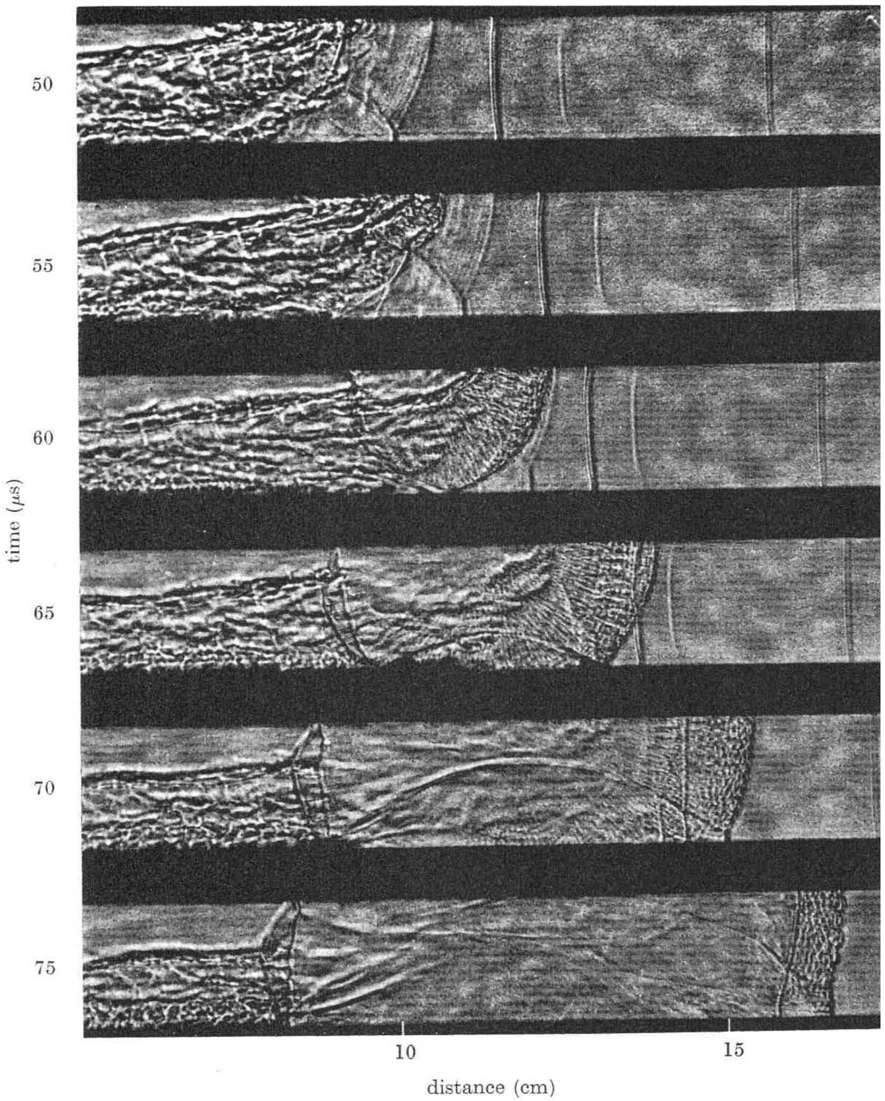


Schlieren framing
photographs
by rotating
mirror camera

(Urtiev&Oppenheim, 1965)

DDT in smooth tube

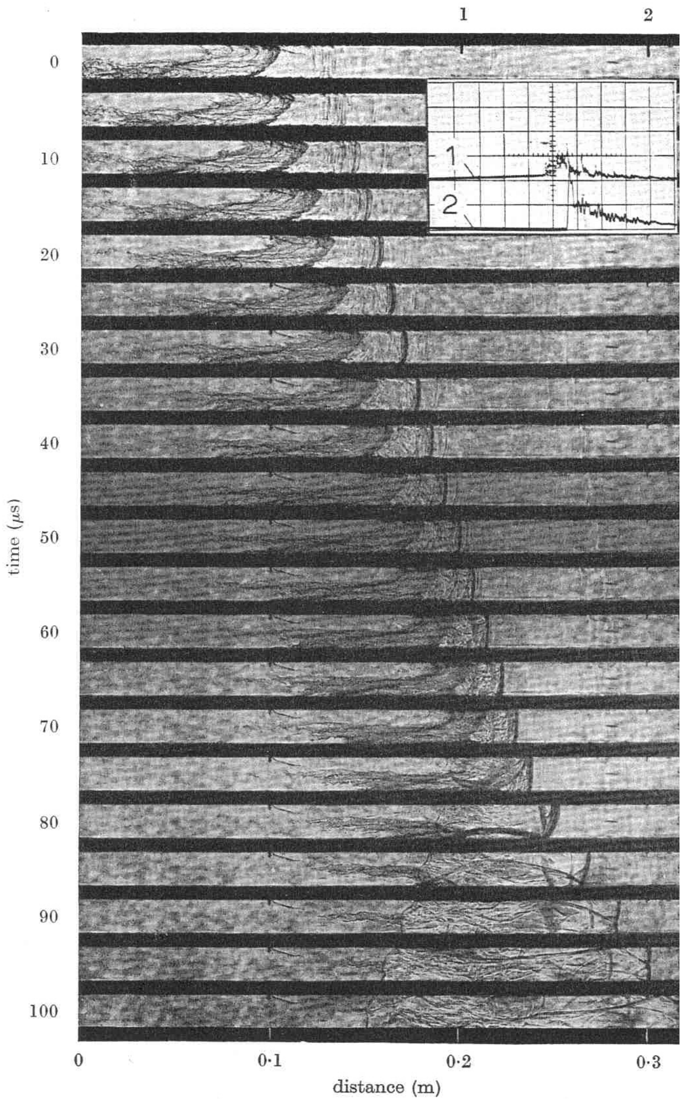


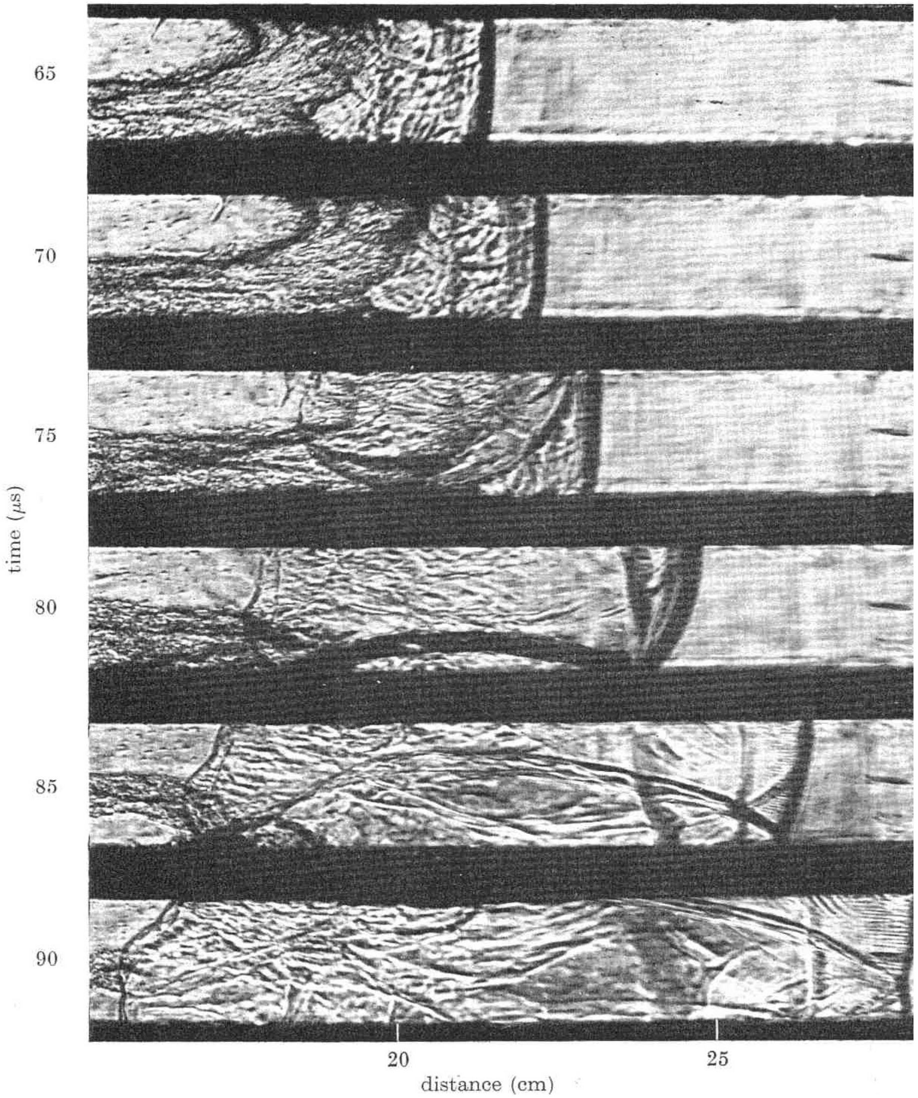


Schlieren framing photographs by rotating mirror camera

(Urtiev&Oppenheim, 1965)

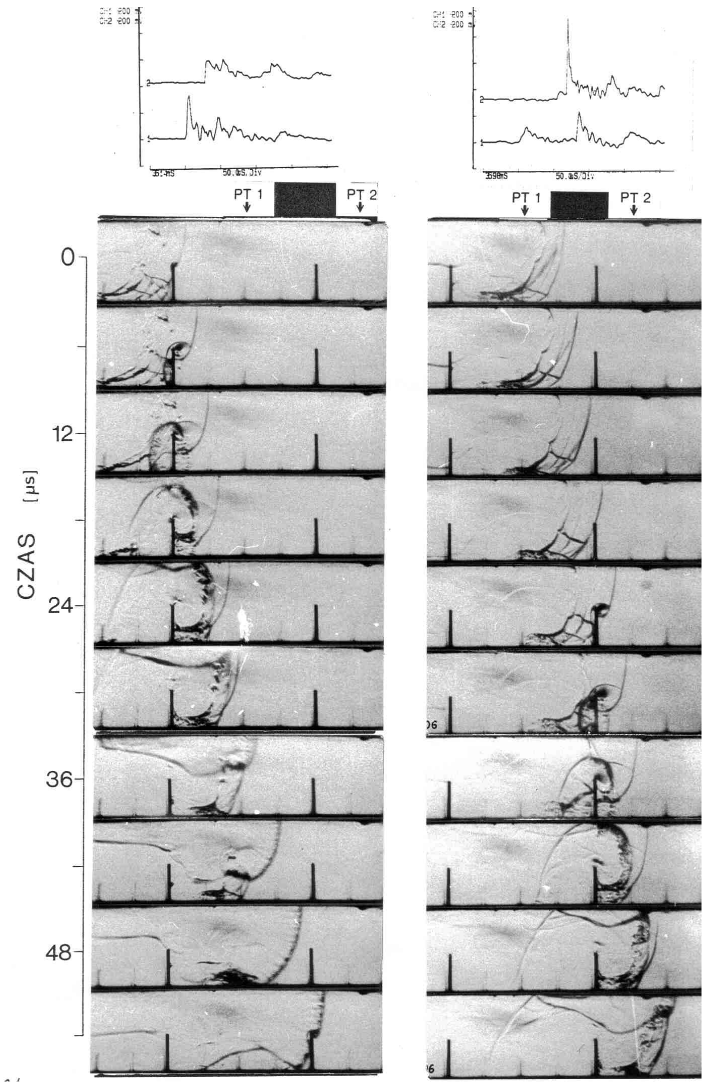
DDT in smooth tube

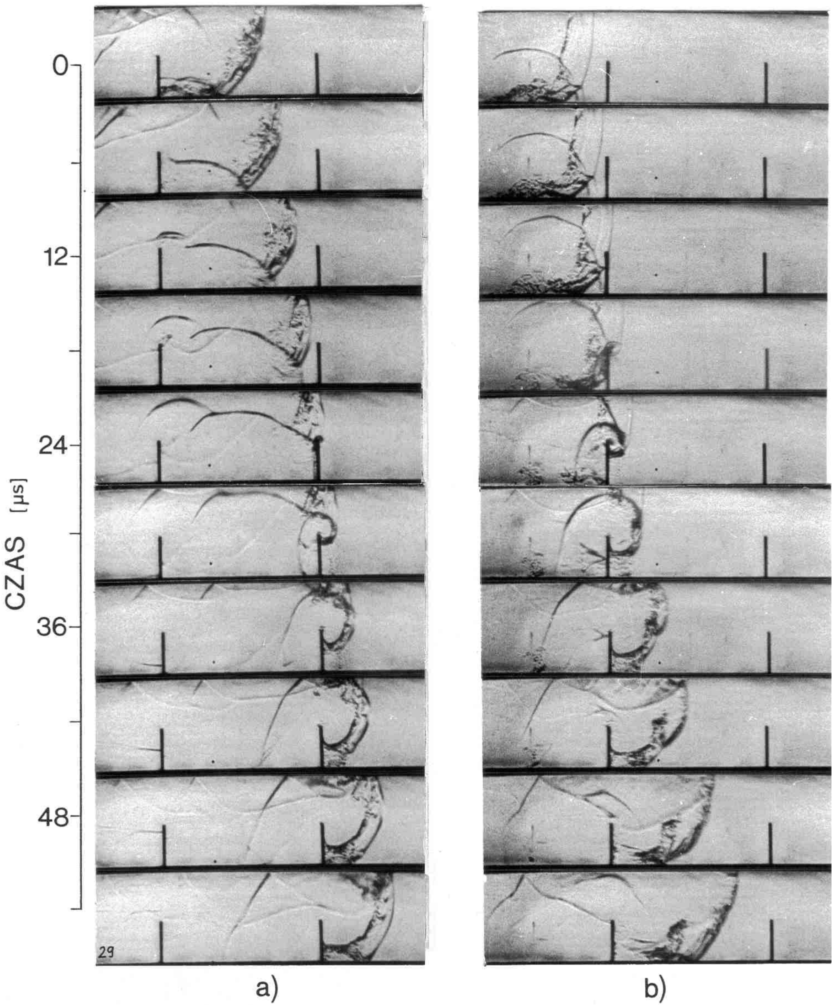




(Urtiev&Oppenheim, 1965)

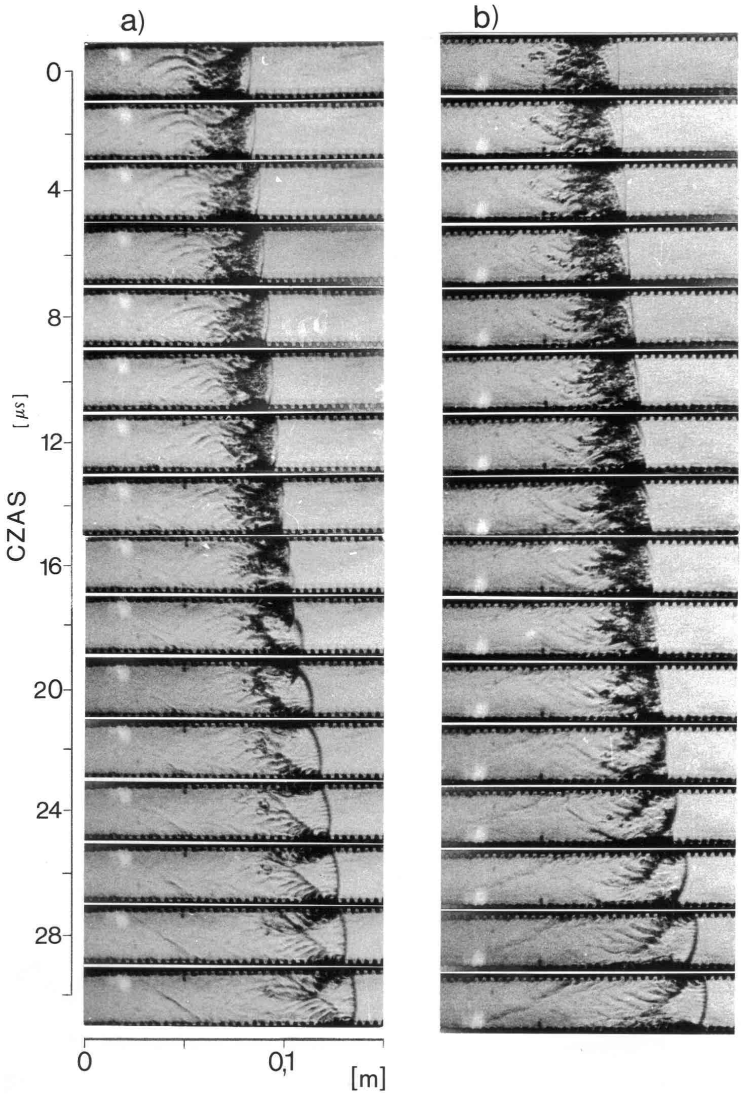
DDT in tube with obstacles





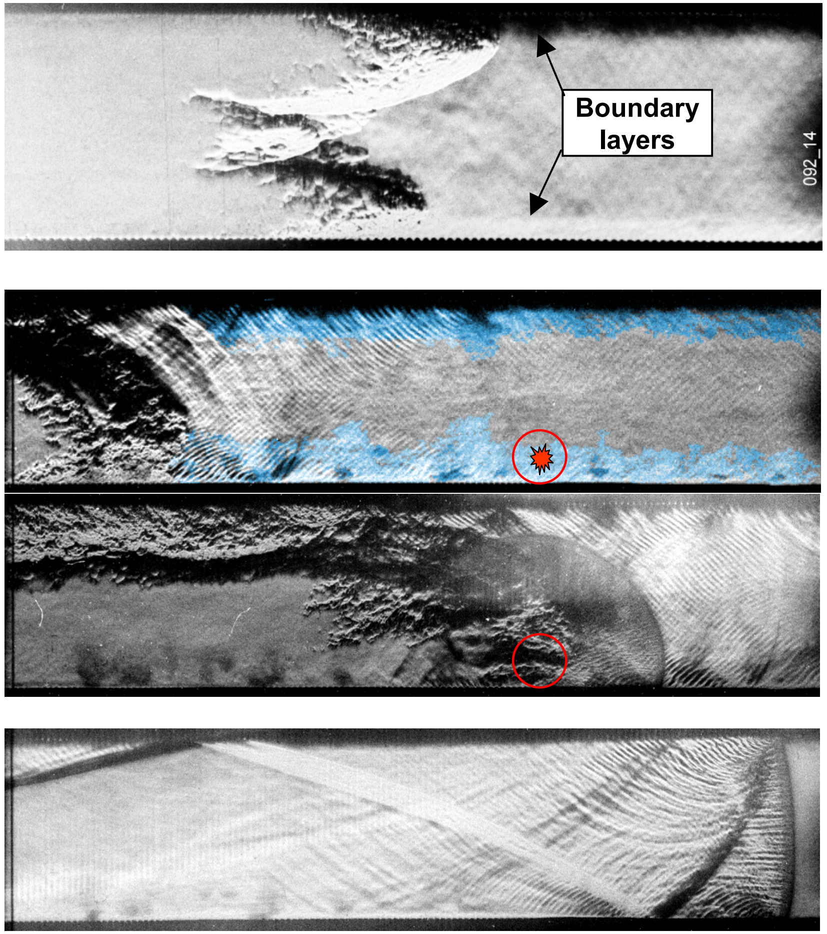
(Teodorczyk, et al..1988)

DDT in rough channel



(Teodorczyk, 1990)

DDT in rough channel

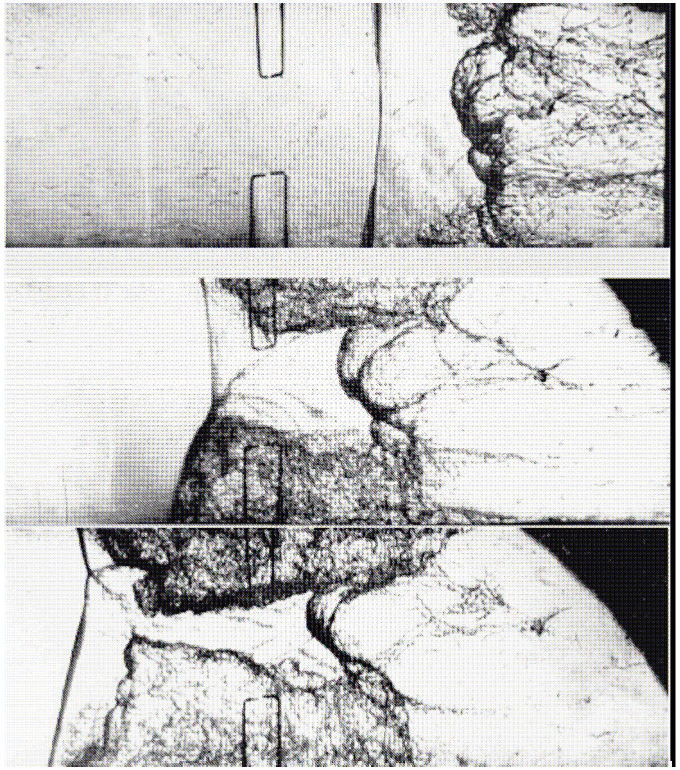


Flame speed 320 m/s

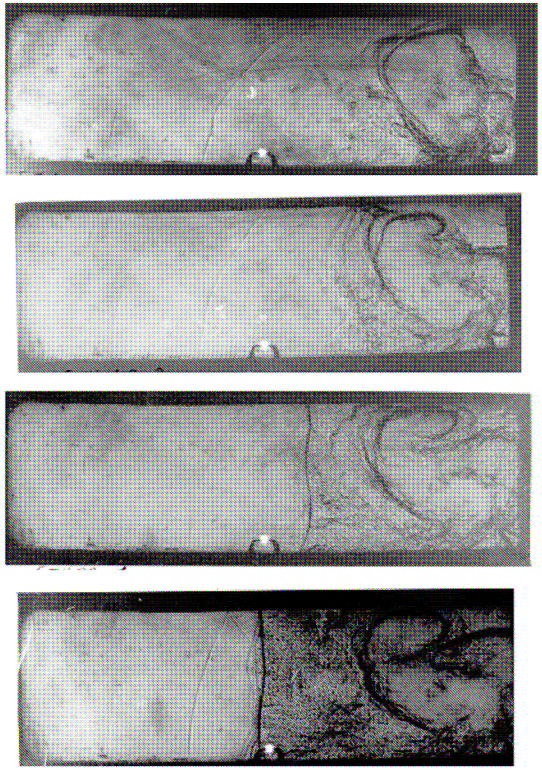
p_0=0.55 bar, 1090-1320 mm from ignition

(Kuznetsov M., Dorofeev S., 2005)

Flame interaction with shock wave



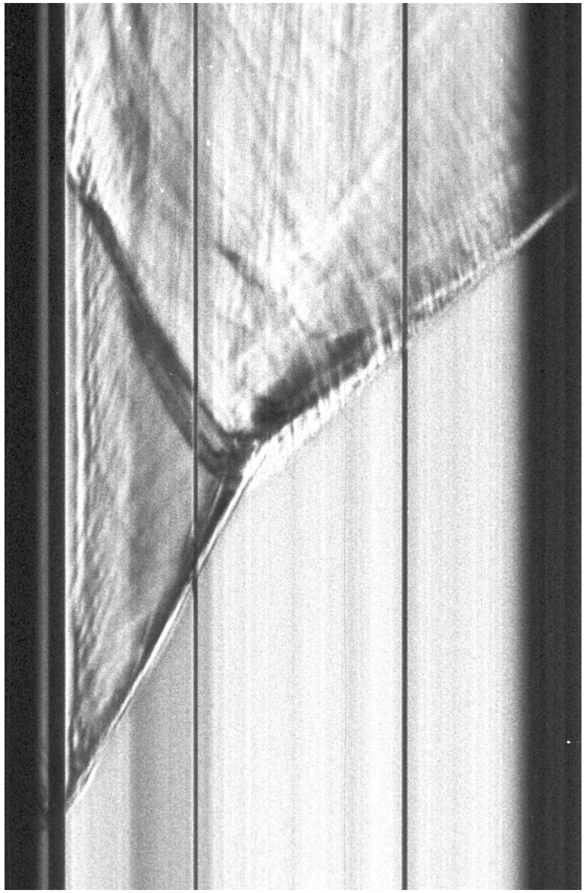
Reflected shock (*moving right to left*) emerging following multiple-shock flame interaction. Original incident shock Mach No. 1.7 (incident not shown). Mixture $C_2H_4 + 3O_2 + 4N_2$, initial pressure 13.2 kPa, *Δ*t 50 μs



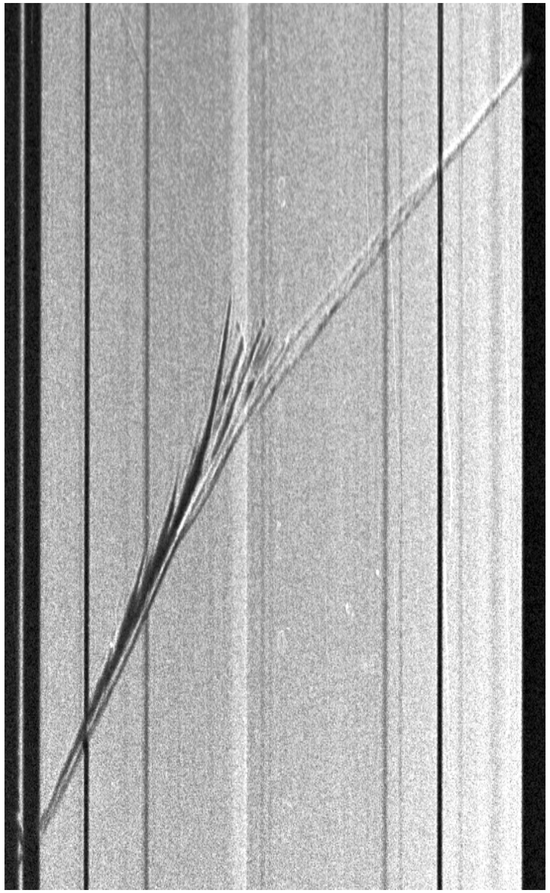
DDT resulting from the interaction of a reflected shock with a flame kernel

(Bombrey&Thomas, 2002)

Two modes of DDT



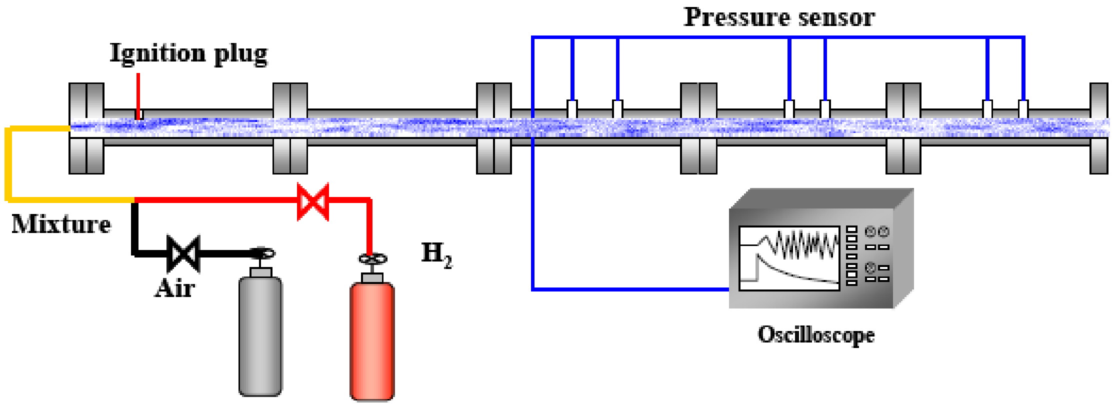
DDT via local explosion

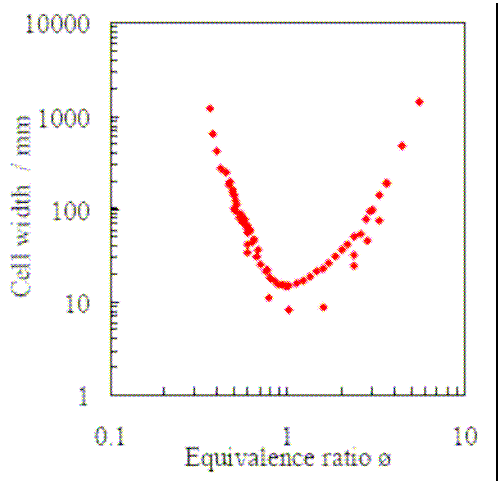


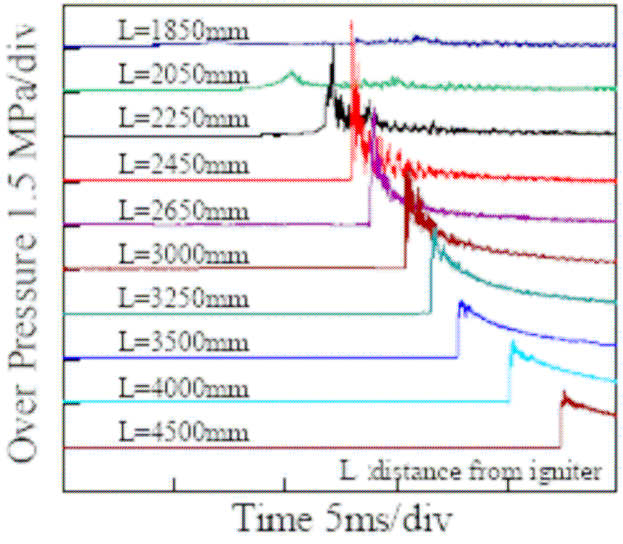
DDT via gradual amplification of transverse waves

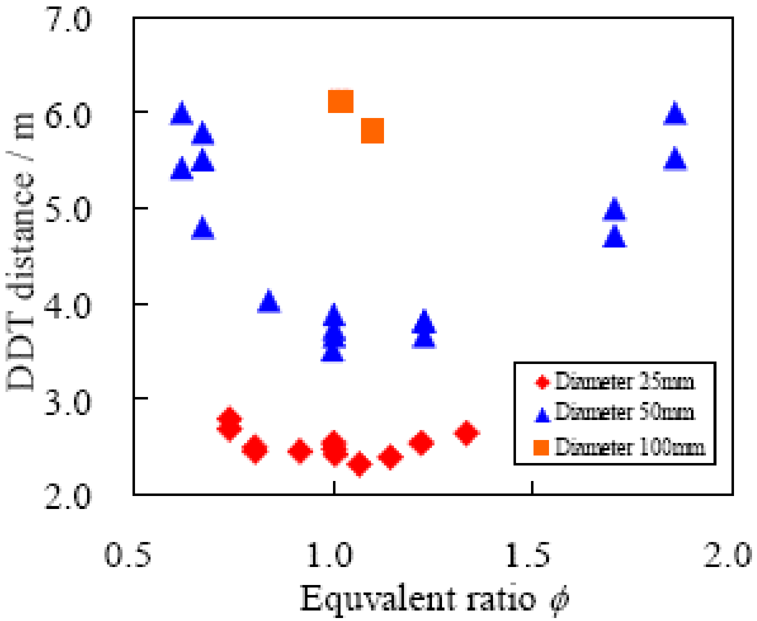
(Chao et al., 2002)

DDT of hydrogen-air in smooth tube



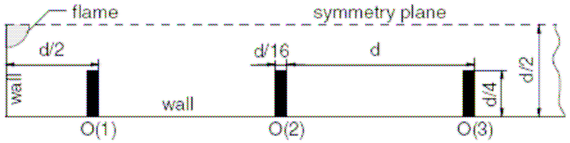






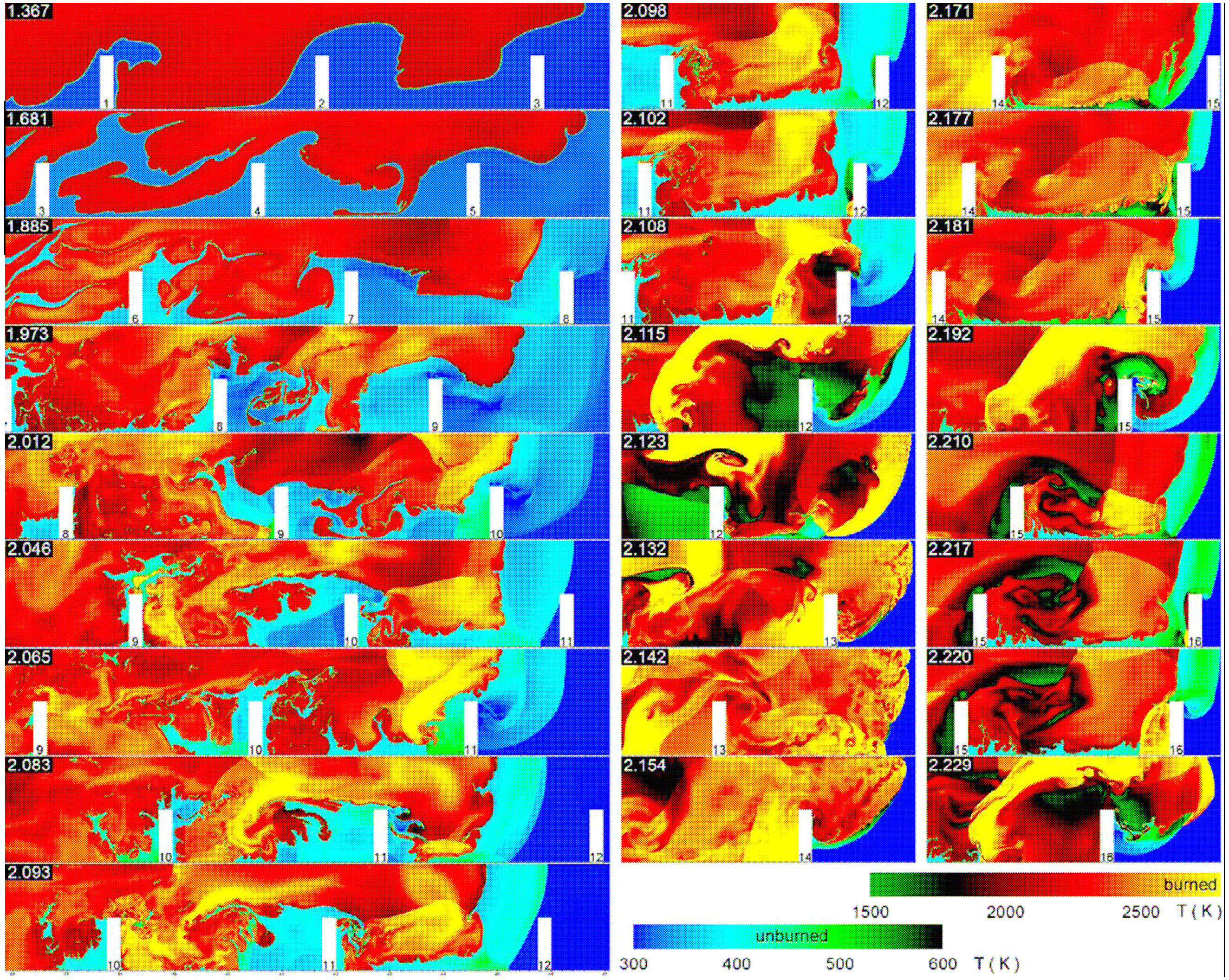
Source:
Aizawa et al..
21st ICDERS, July 23-27, 2007, Poitiers

DDT simulation



V.Gamezo et al., 31st Symposium International on Combustion, Heidelberg 2006

- stoichiometric hydrogen-air mixture at 0.1 MPa
- Channel with obstacles 1m × 11cm × 2cm



DDT simulation

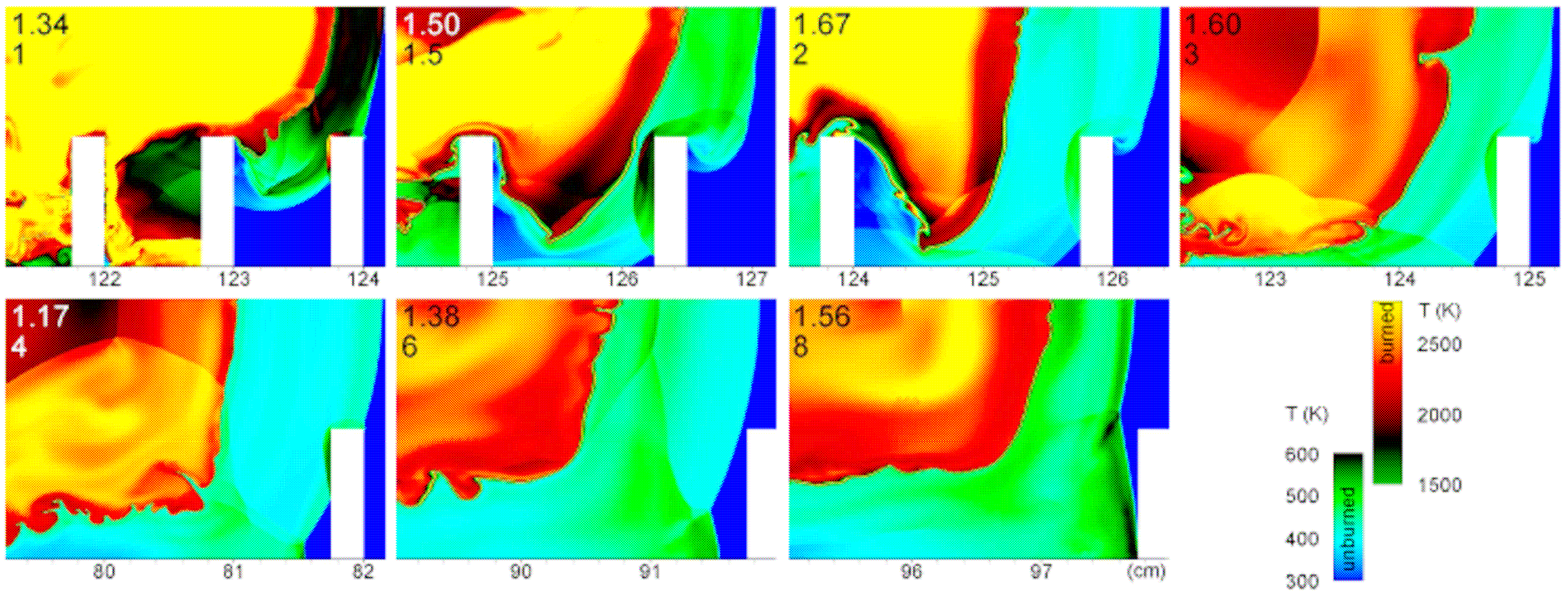


Fig. 2. Flame and shock configurations just before the detonation initiation (S=1, 4, 6, 8) or at the end of the channel (S=1.5, 2, 3). Time in milliseconds and S in centimeters are shown in frame corners. dx_{min}=1/512 cm (S=1, 4) or 1/128 cm (S=1.5, 2, 3, 6, 8).

Source:
Gamezo et al..
21st ICDERS, July 23-27, 2007, Poitiers