Fast deflagrations, deflagration to detonation transition (DDT) and direct detonation initiation in hydrogen-air mixtures

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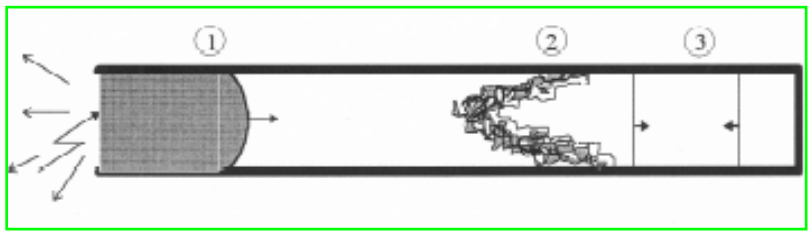
Outline

- Flame acceleration in tubes and channels
- DDT in smooth tubes
- DDT in rough tubes (with obstacles)
- DDT in large scale
- Numerical simulation of DDT
- Direct detonation initiation

Regimes of flame propagation in tubes

Tube opened at ignition end



- Acoustic and pressure waves generated by the turbulent flame interact with the flame after reflection from the tube end
- Further instabilities and increase of the flame surface area

Tube closed at ignition end

- 6/7 of reactants vented outside

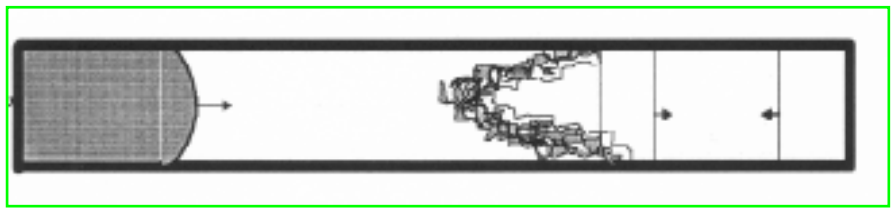
$$V_f = F/f \cdot V_n + V_d$$

V_d – velocity of displacement

- In long tubes: pressure waves ⇒ shock wave ⇒ DDT

Regimes of flame propagation in tubes

Tube closed at both ends

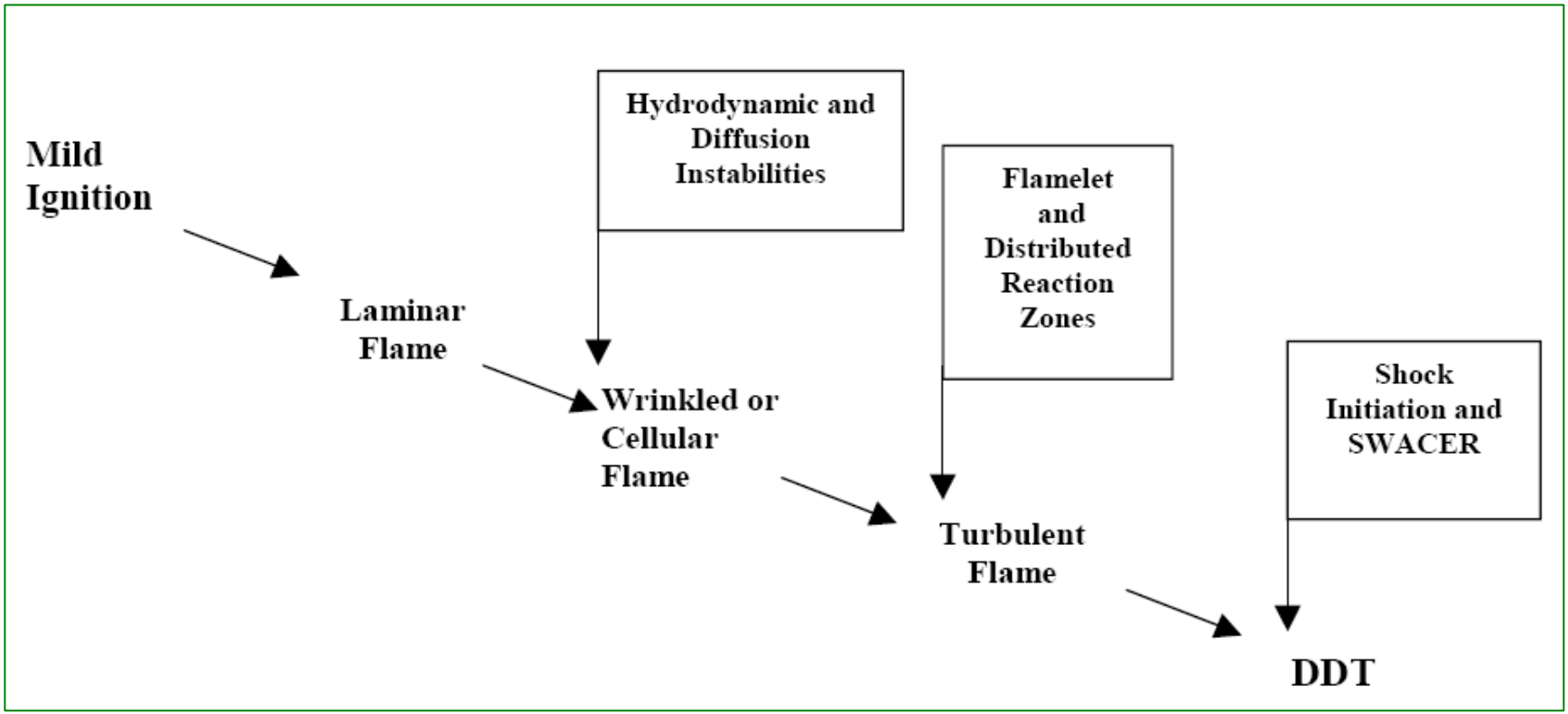


- First stage ⇒ high displacement velocity
- Second stage ⇒ low V_d
- Oscillations and interactions with acoustic and pressure waves reflected from the closed end
- Long tubes ⇒ acceleration ⇒ DDT

Flame propagation in tubes

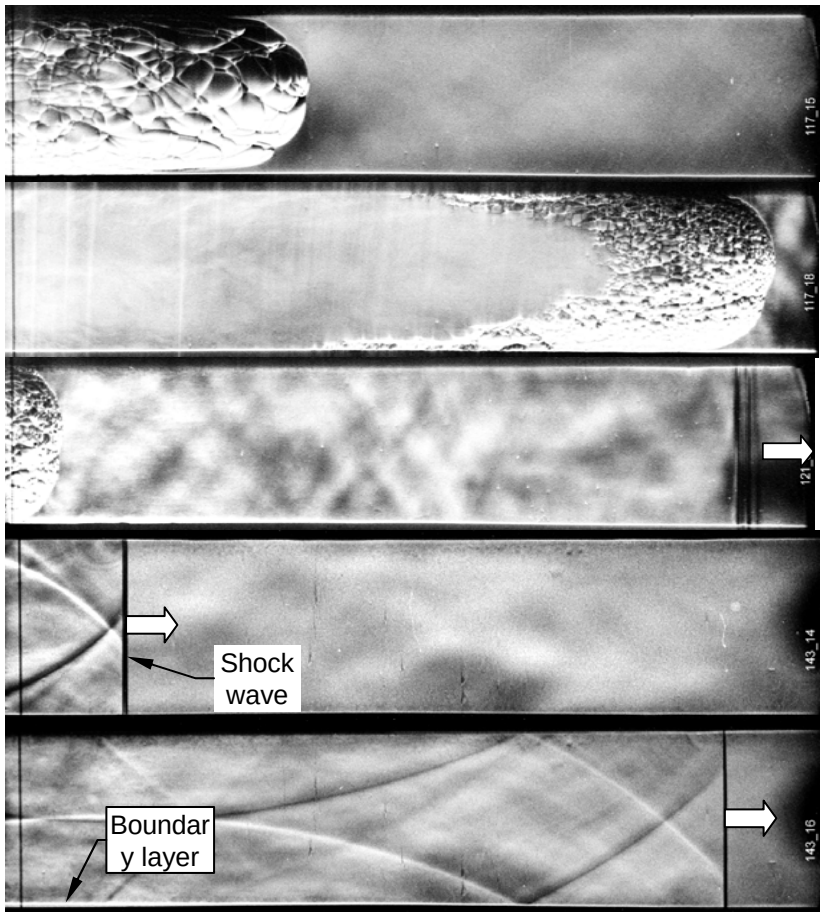
- **Lower limit** ⇒ LAMINAR FLAME (m/s)
- **Upper limit** ⇒ CJ DETONATION (km/s)
- **Between limits** ⇒ spectrum of TURBULENT FLAMES depeneding on:
  - Initial conditions (pressure, temperature, composition)
  - Geometry (size, obstacles, etc.)
- **Smooth tubes** ⇒ continuous flame acceleration and abrupt DDT
- **Rough (obstructed) tubes** ⇒ several distinct regimes of steady flame propagation

Regimes of flame propagation leading to DDT



Effect of boundary layer on the flame acceleration and DDT

Premixed flames in smooth closed tube - stoichiometric hydrogen-oxygen



Shadow photograph of early stage of flame propagation

p_0=0.75 bar

at 210-440 mm from ignition

Ignition by electric spark of 20mJ

(Kuznetsov M., Dorofeev S., 2005)

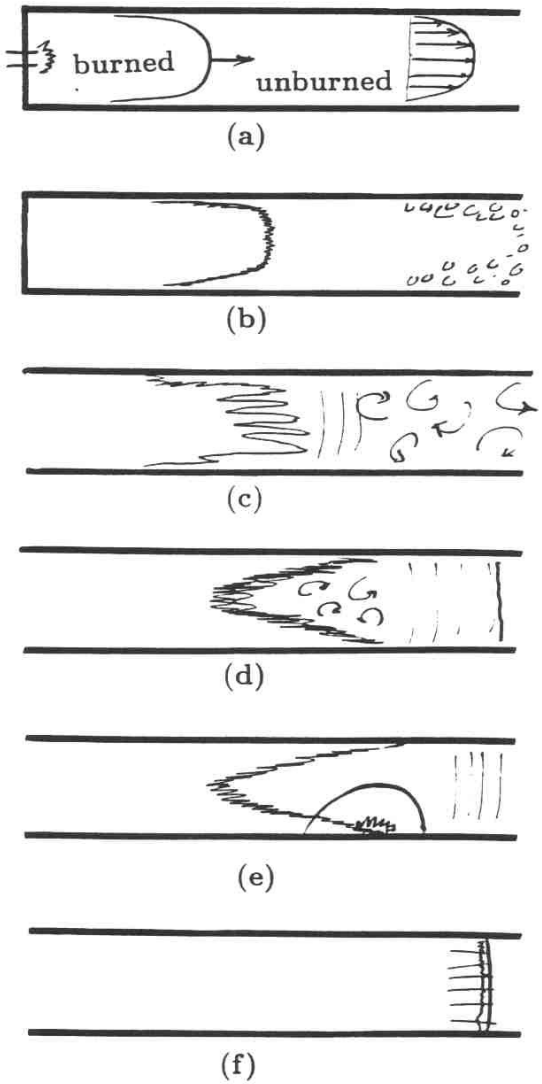
Mechanisms of flame acceleration

- Growth of flame surface area:
  - flame folding
  - velocity gradient in the flow
- Baroclinic vorticity generation
  - Density gradient normal to the pressure gradient
- Hydrodynamic instabilities
  - Rayleigh – Taylor
  - Richtmyer – Meshkov
- Microexplosions of vortices

Mechanisms of turbulence growth

- Initial gas flow turbulence in the mixture
- Gas flow turbulence generated at the shear layer near the wall
- Nonuniform concentration (temperature, pressure) distribution in the flammable mixture
- Interaction of the flame front with an accoustic or pressure wave

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;

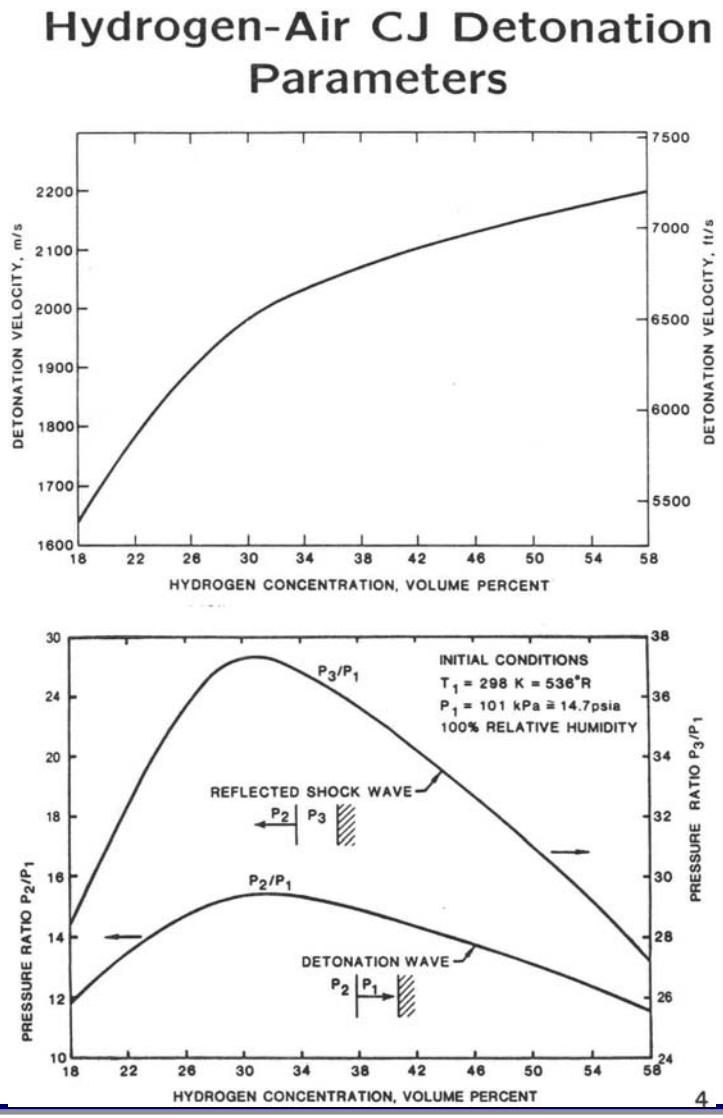
d) production of pressure waves ahead of the turbulent flame;

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

f) transition to detonation.

(Shepherd&Lee, 1992)

CJ Detonation



- Velocity
- Pressure
- Temperature

Are simple to calcutale from equilibrium codes:

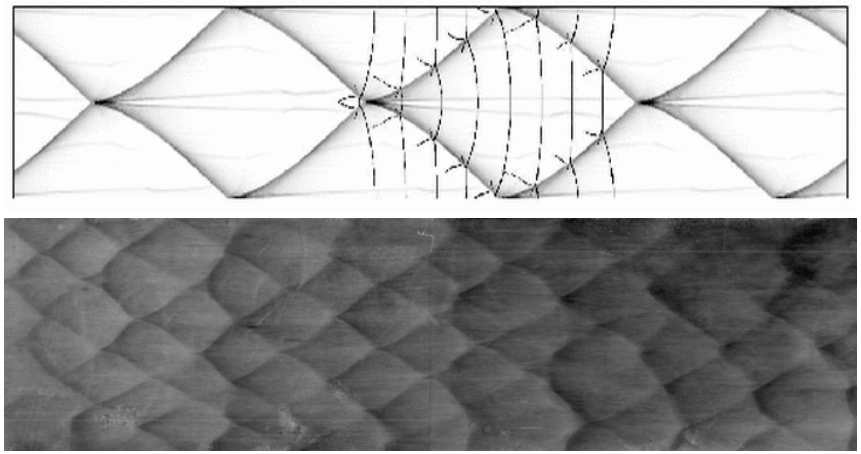
NASA

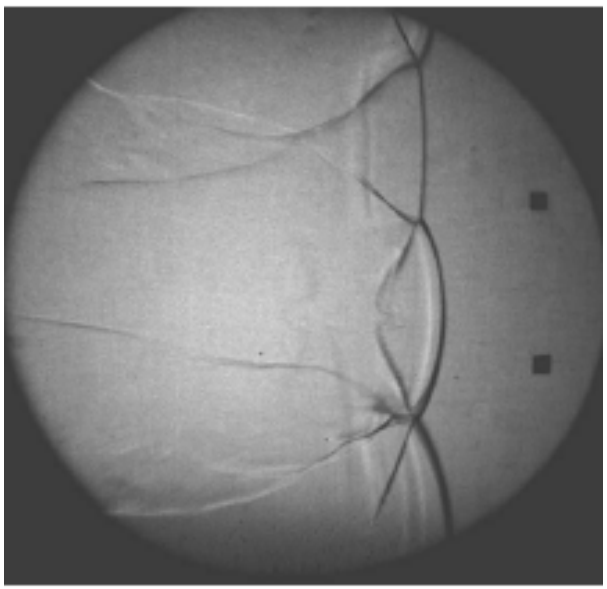
STANJAN

SUPERSTATE

Etc.

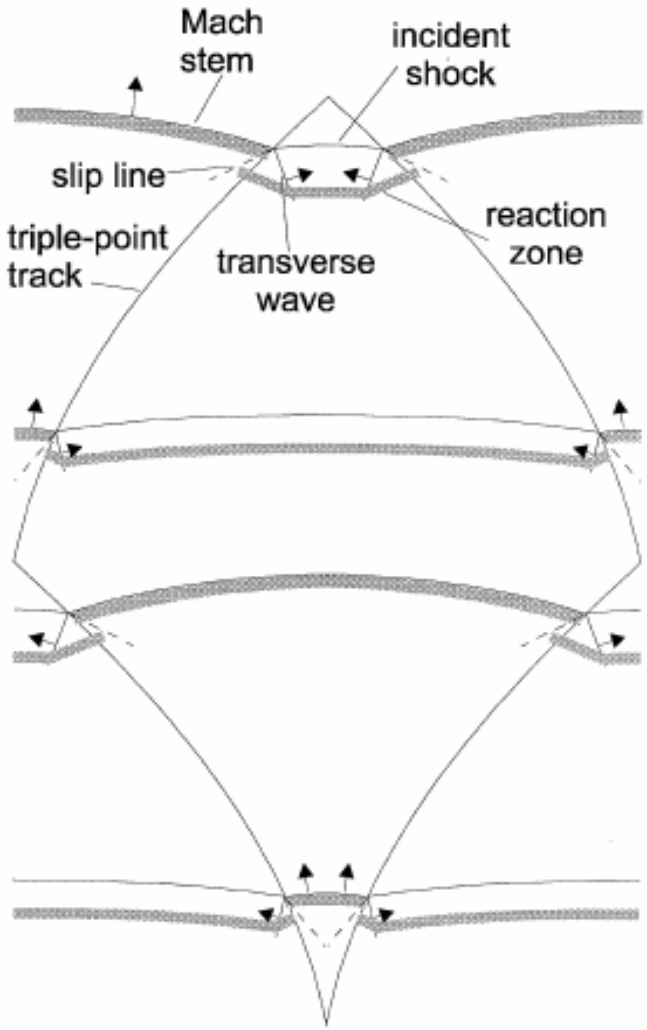
Detonation wave structure





2H2+O2+17Ar at 20kPa

(Austin&Shepherd)



Detonation limits

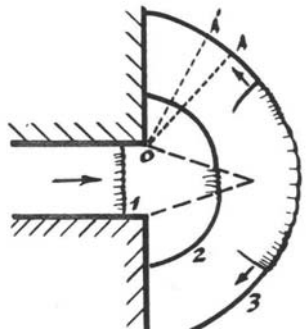
- propagation limit: $d_{tube} > d_f$

$$d_f = \lambda/\pi$$

- critical tube diameter for diffraction: $d_{tube} > d_c$

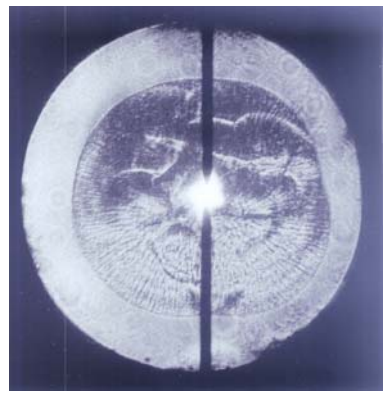
Tube: $d_c = 13\ \lambda$

Square channel: $l_c = 10\ \lambda$



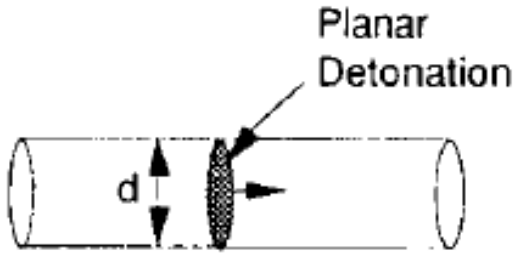
- Critical energy for direct initiation: $E > E_c$

$$E_c = 430 \rho_0 U_{CJ}^2 \lambda^3$$

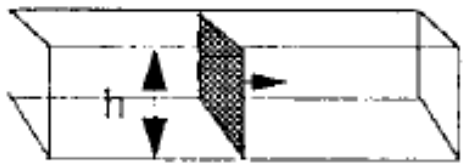


Detonation limits

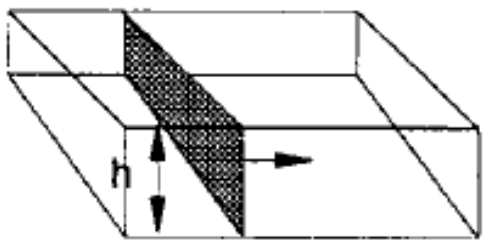
- propagation limit



$d > \lambda/3$



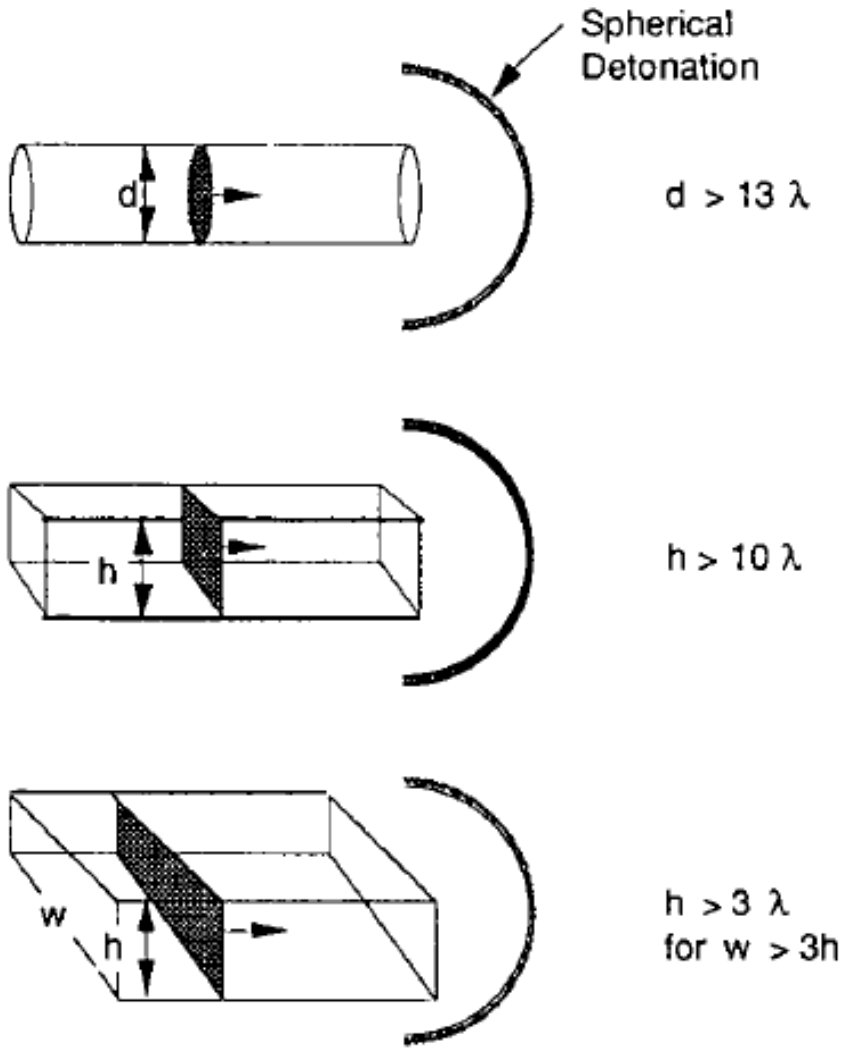
$h > \lambda$



$h > \lambda$

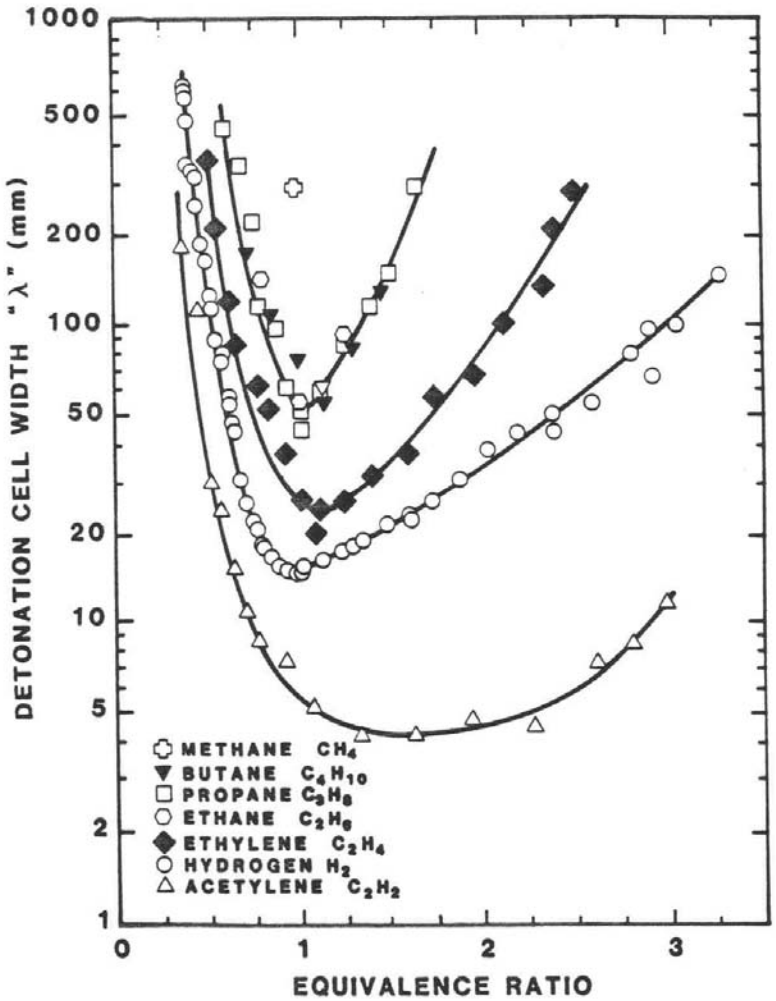
Detonation limits

- critical tube diameter for diffraction



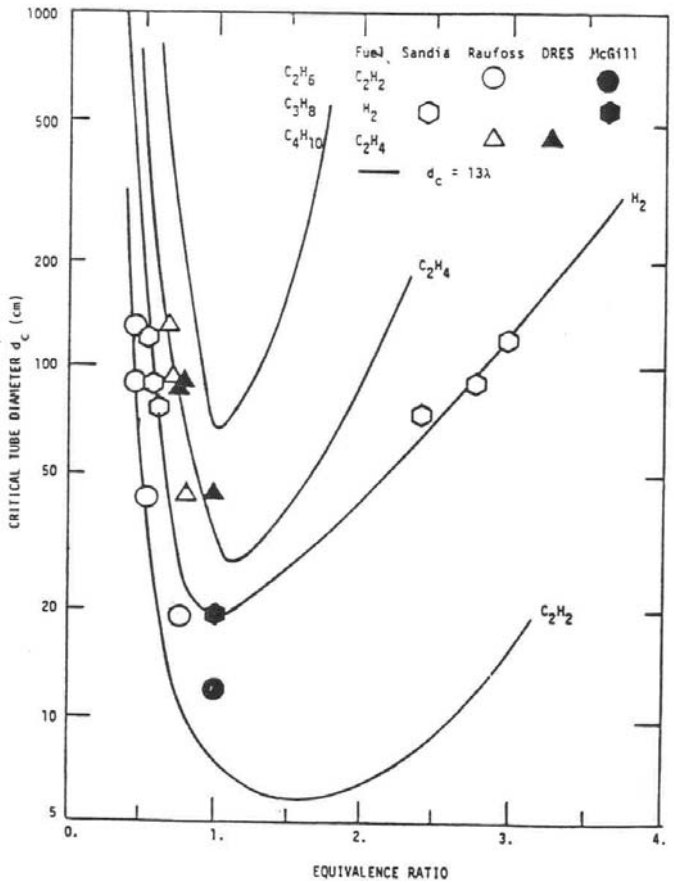
Detonation cell size

Fuel-air mixtures



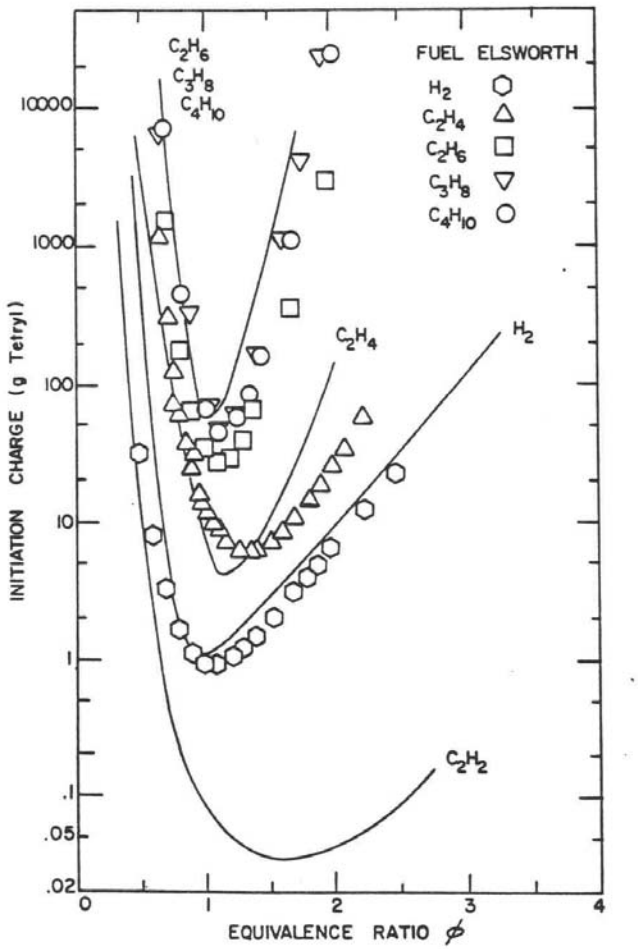
Critical tube diameter

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

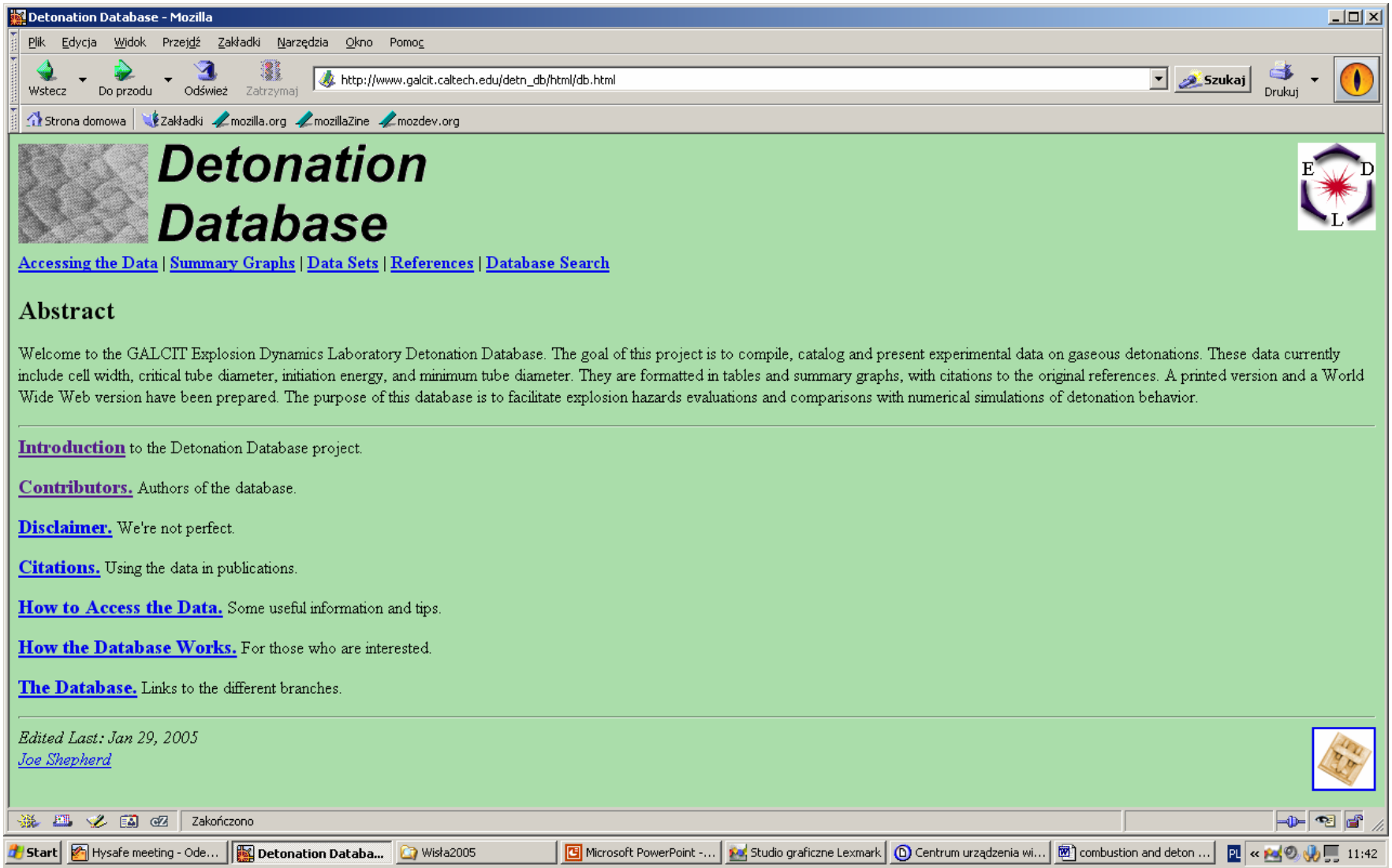


Critical energy for direct initiation

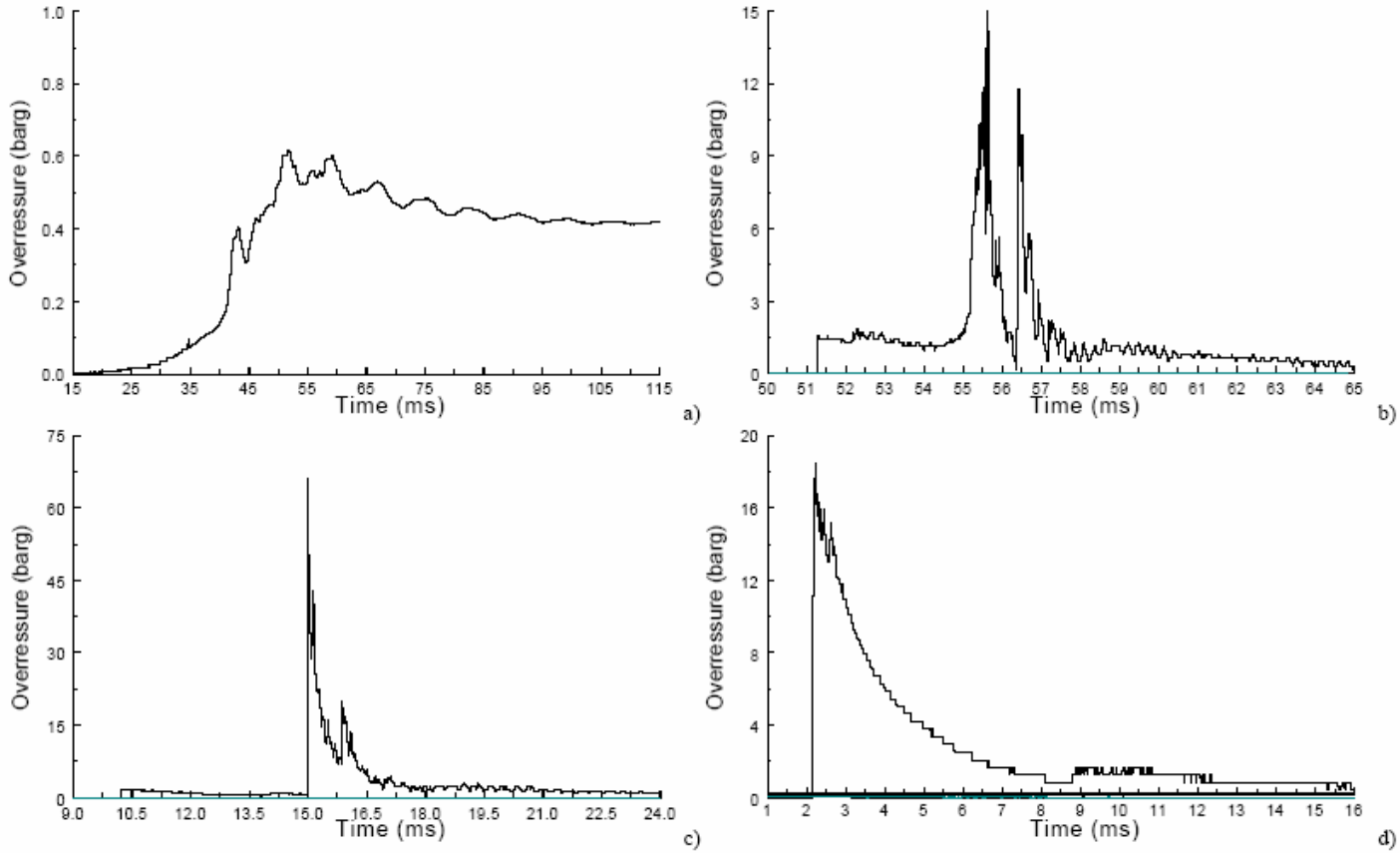
Fuel-Air Mixtures (T_o = 300 K, P_o = 1 atn



Detonation database

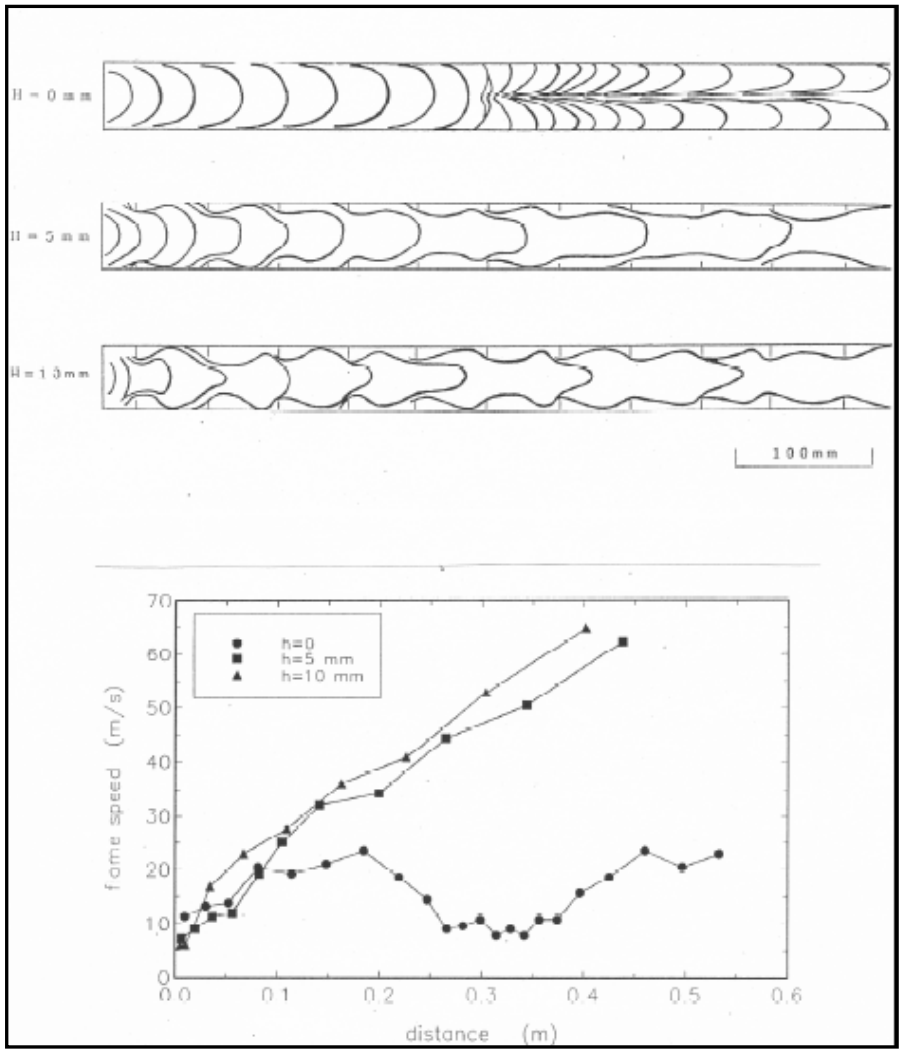


Deflagration and detonation pressure



a) Slow deflagration; b) fast deflagration; c) overdriven detonation DDT; d) CJ detonation

Flame acceleration in tube



Open end channel;

Stoichiometric propane-air at 1 bar

(Teodorczyk et al., 1992)

Early accelarating flame

Phil. Trans. R. Soc. Lond. A, volume 315 *Oppenheim, plate* 3

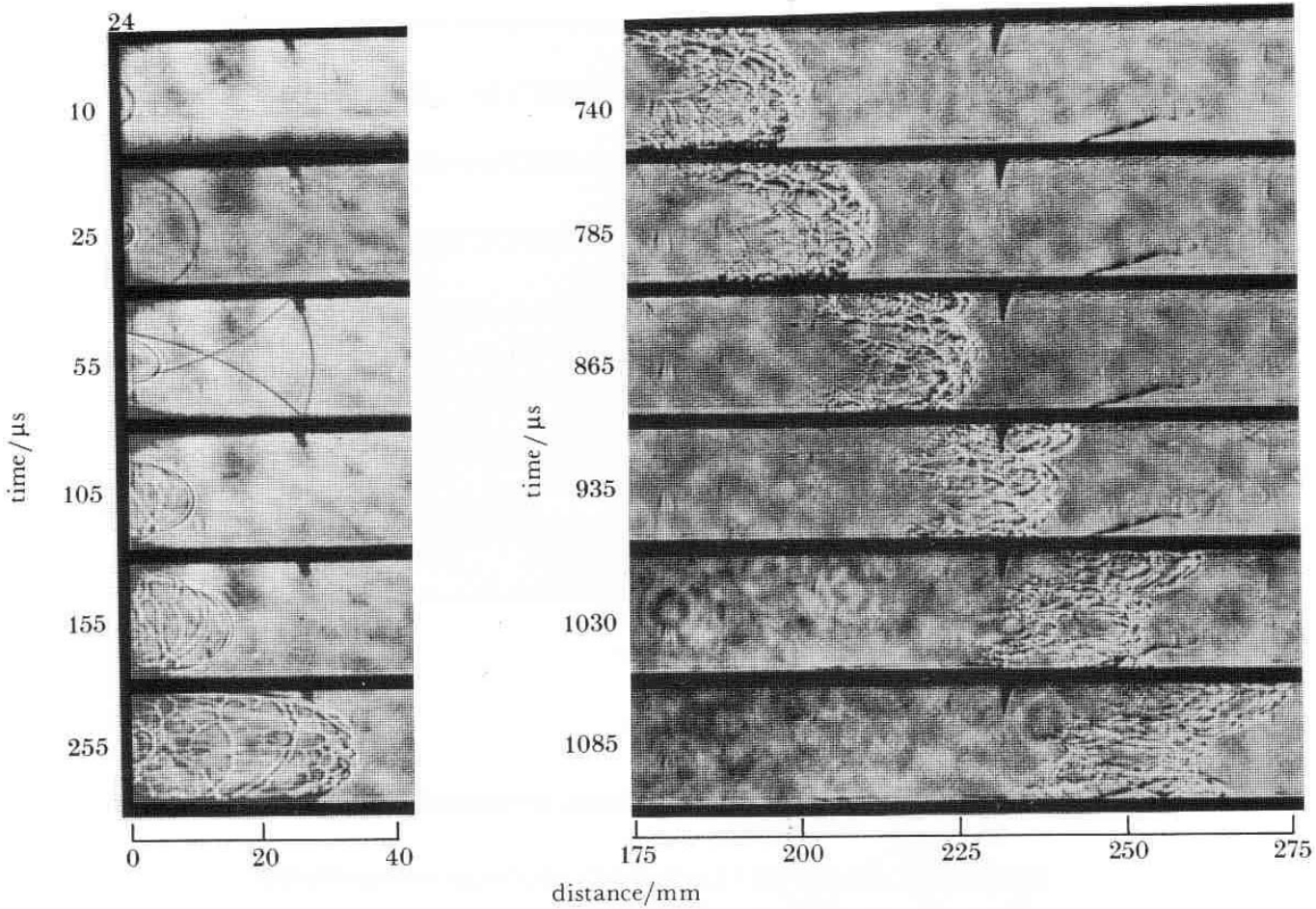
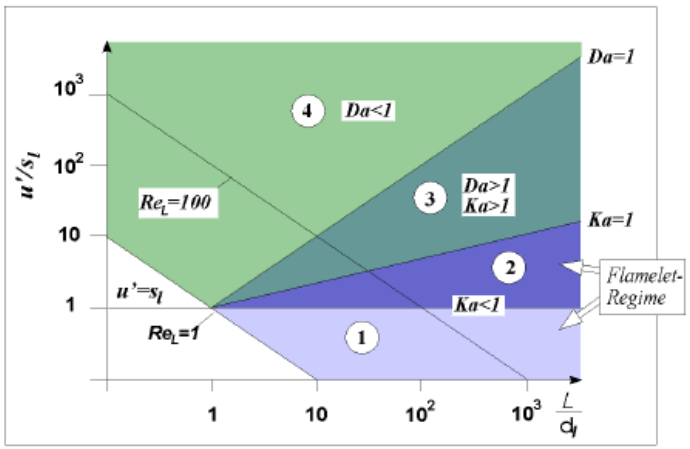
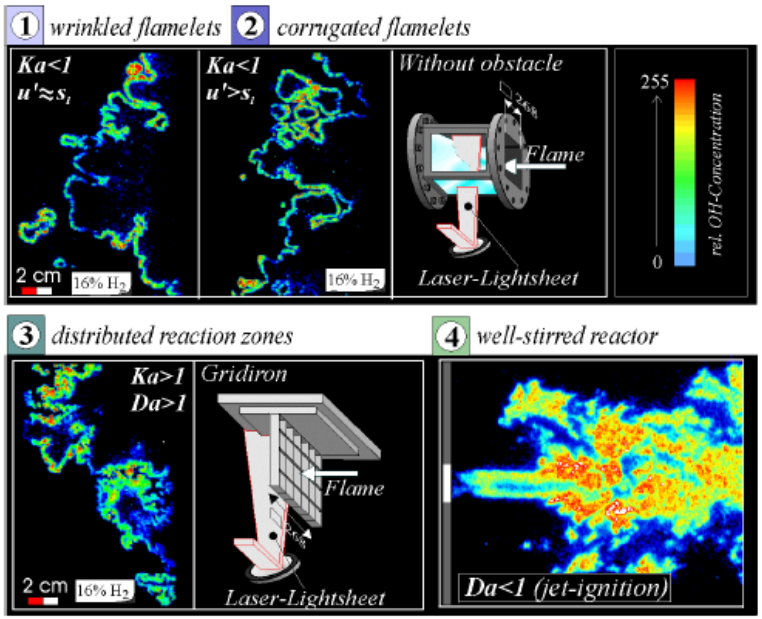


FIGURE 24. Cinematographic schlieren records of ignition, and initial stages of inflammation in a stoichiometric hydrogen–oxygen mixture.

Borghi Diagram





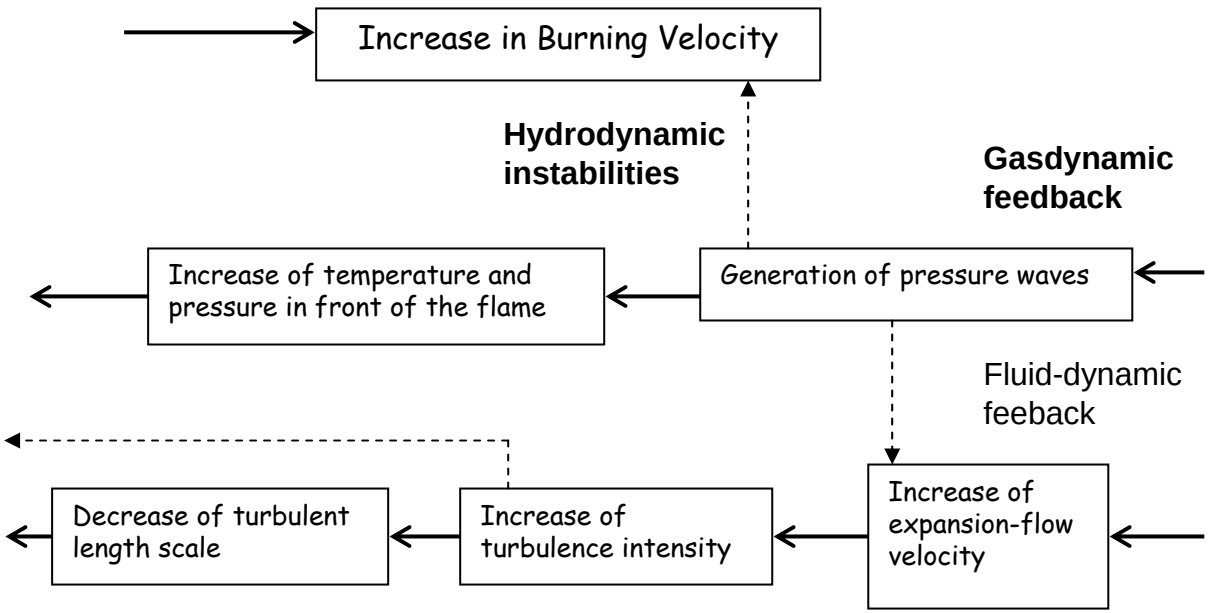
Flame propagation regimes in terms of:

- turbulence intensity, u',
- laminar burning velocity, s_l,
- integral length scale, L,
- laminar flame thickness, d_l,
- Damköhler number, Da ,
- Karlowitz number, Ka,
- turbulent Reynolds number, Re_L.

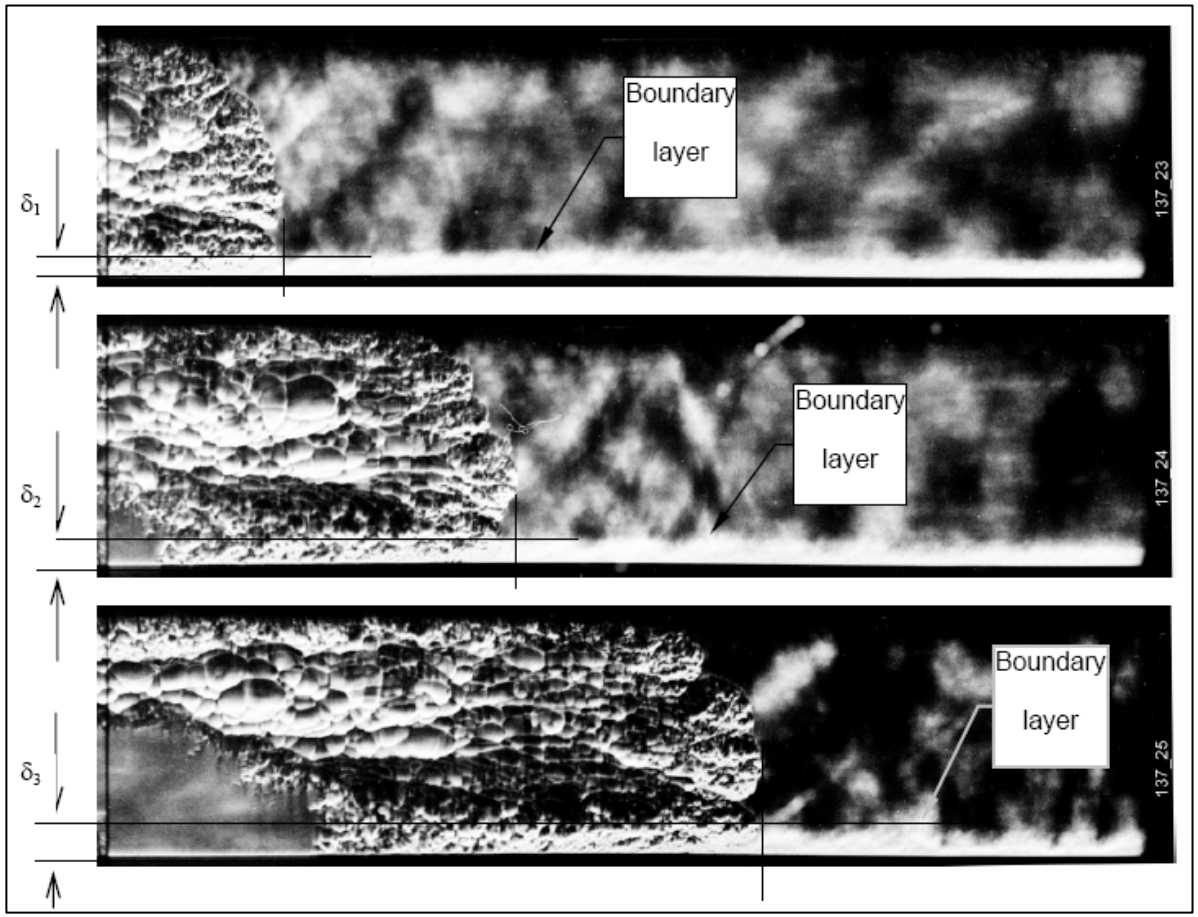
LIPF images (bottom) of flame structure for the various regimes.

(Peters, 1986)

Feedback mechanism of flame acceleration



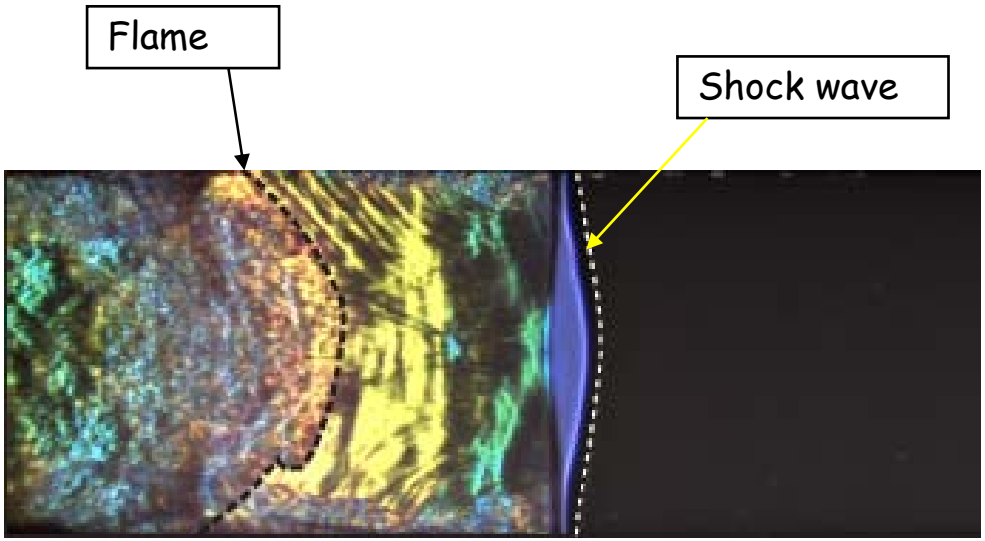
Feedback mechanism of flame acceleration



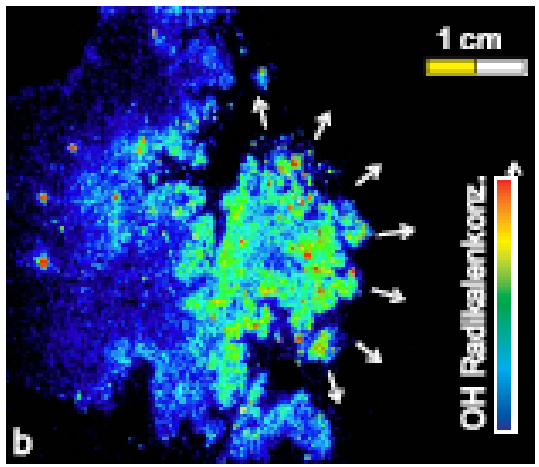
Shadow photographs of later stages of turbulent flame propagation

(Kuznetsov et al., 2005)

Fast deflagration



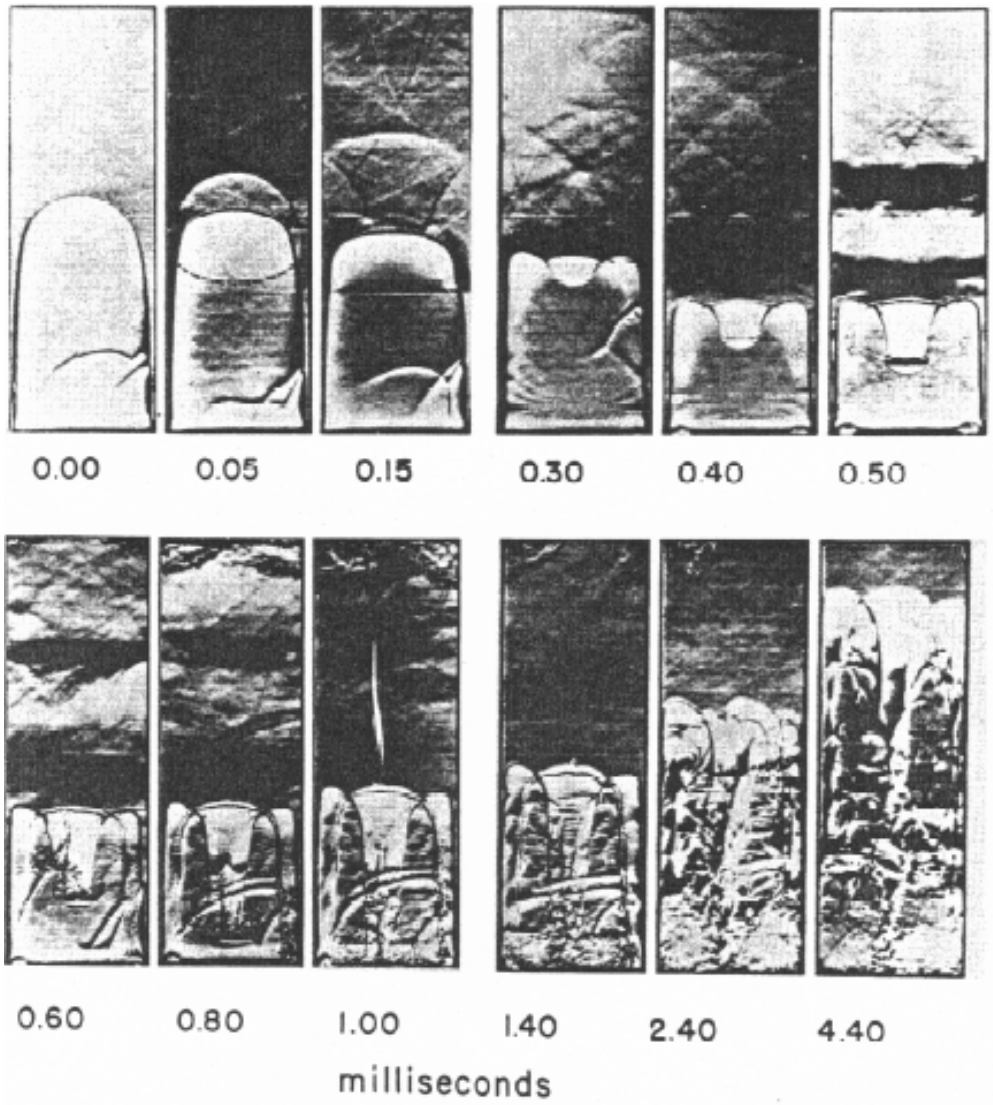
Schlieren image of a fast deflagration wave (22% H2 in air), flame velocity 1200 m/s;



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

(Eder, 2001)

Flame interaction with shock wave

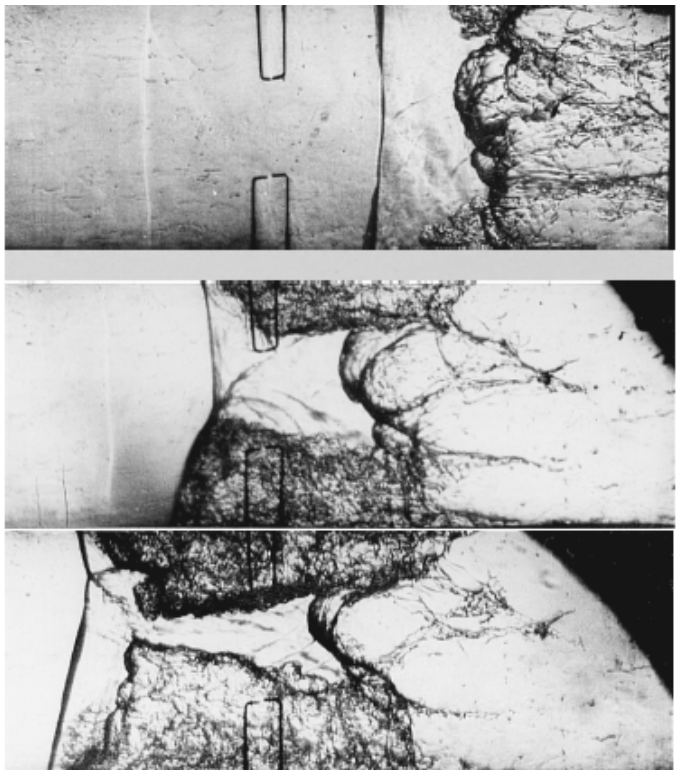


Butane-air flame;

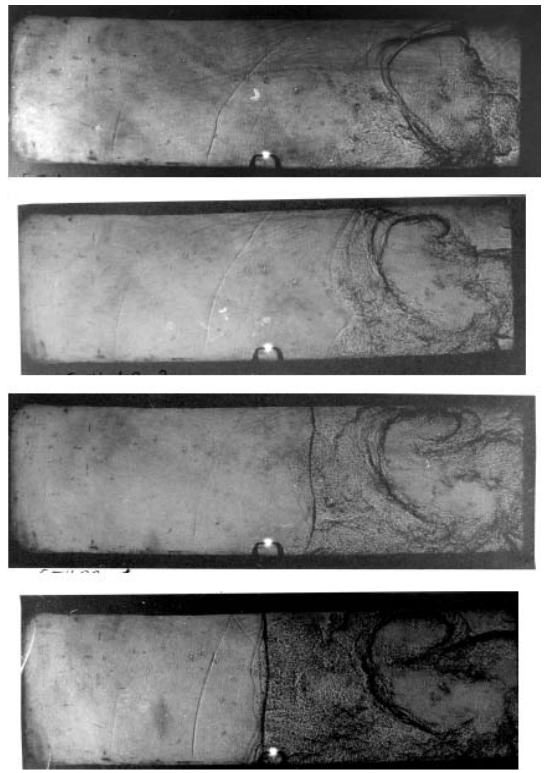
Shock wave of pressure ratio of 1.3

(Markstein, 1968)

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 C2H4 + 3O2 + 4N2, initial pressure 13.2 kPa, Δt 50 µs



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

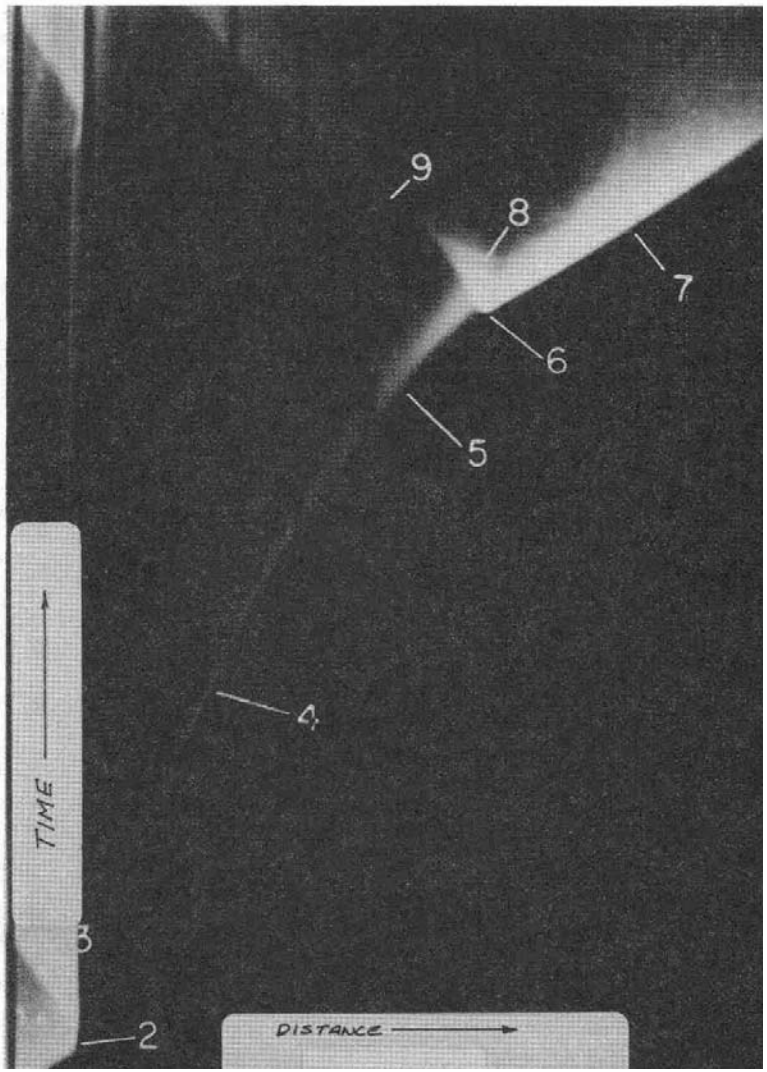
(Bombrey&Thomas, 2002)

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

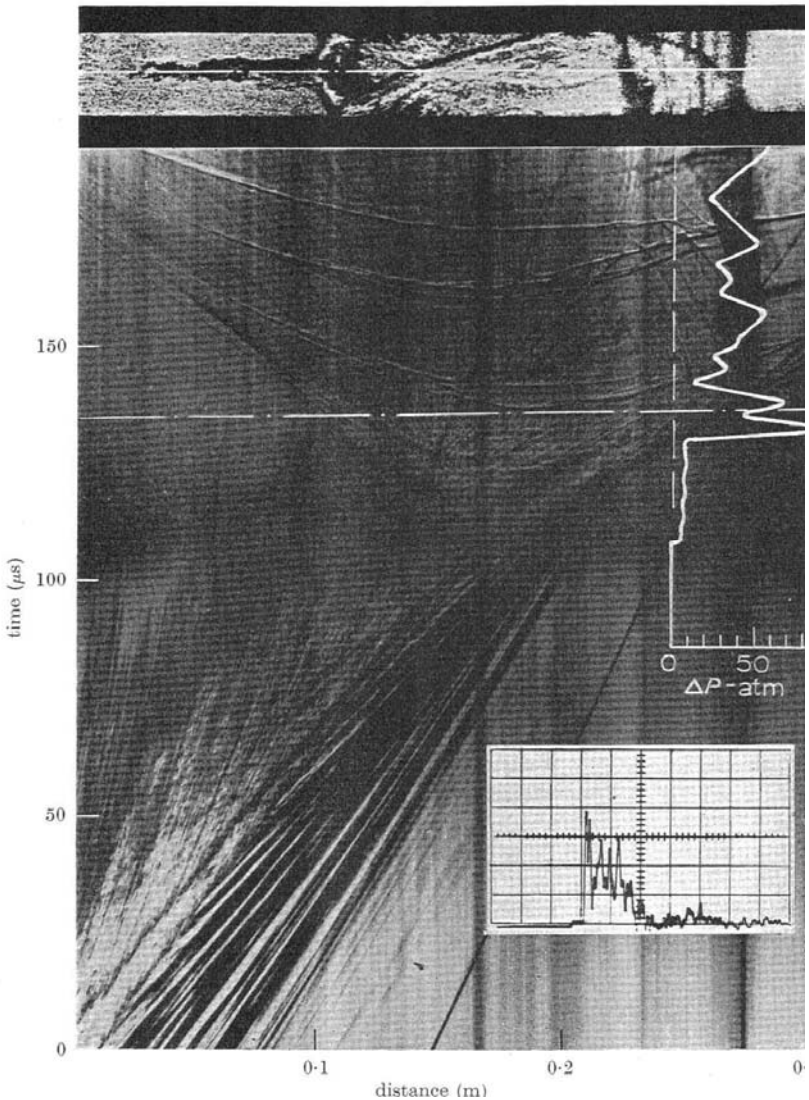
6 – explosion ahead of the flame

7 – detonation

8, 9 – retonation wave

(Lee, 1978)

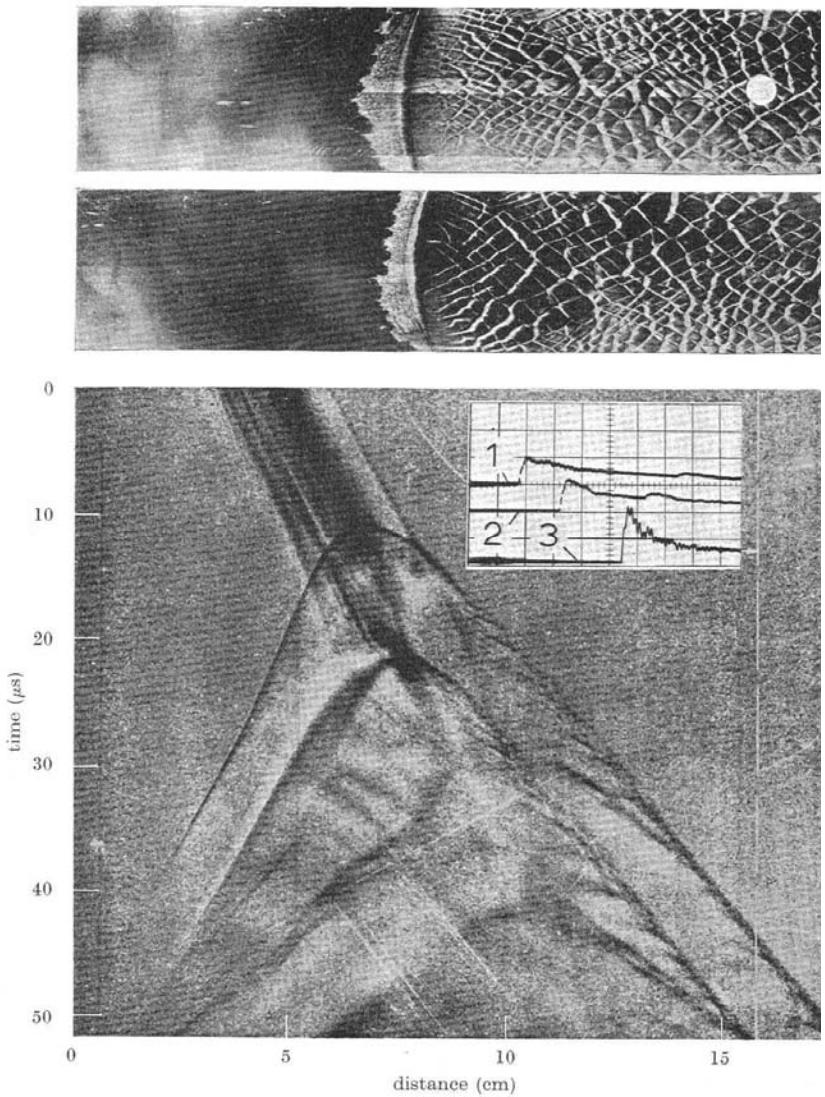
DDT in smooth tube



Streak schlieren photograph

(Myer&Oppenheim, 1965)

DDT in smooth tube



Streak schlieren photograph

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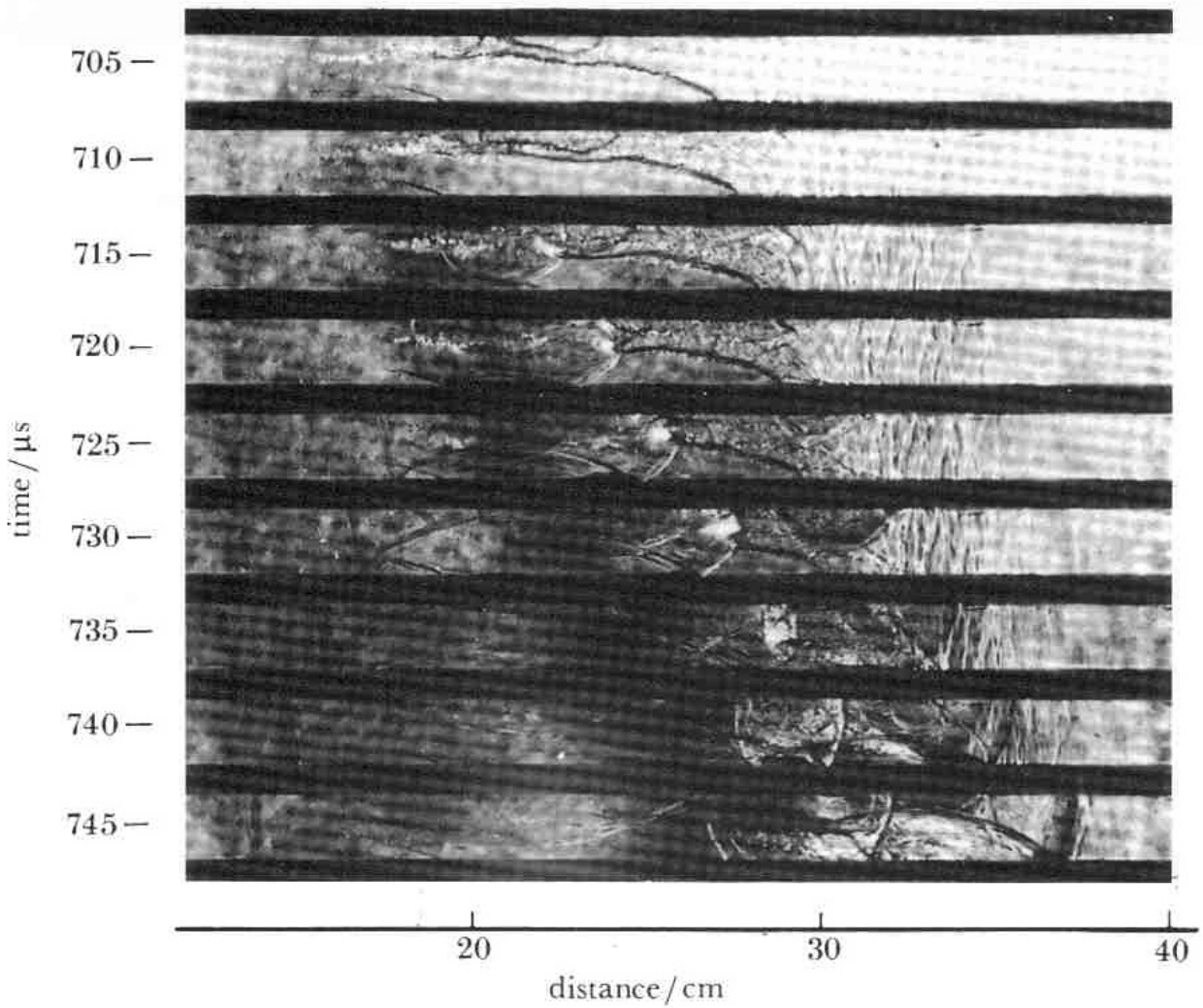
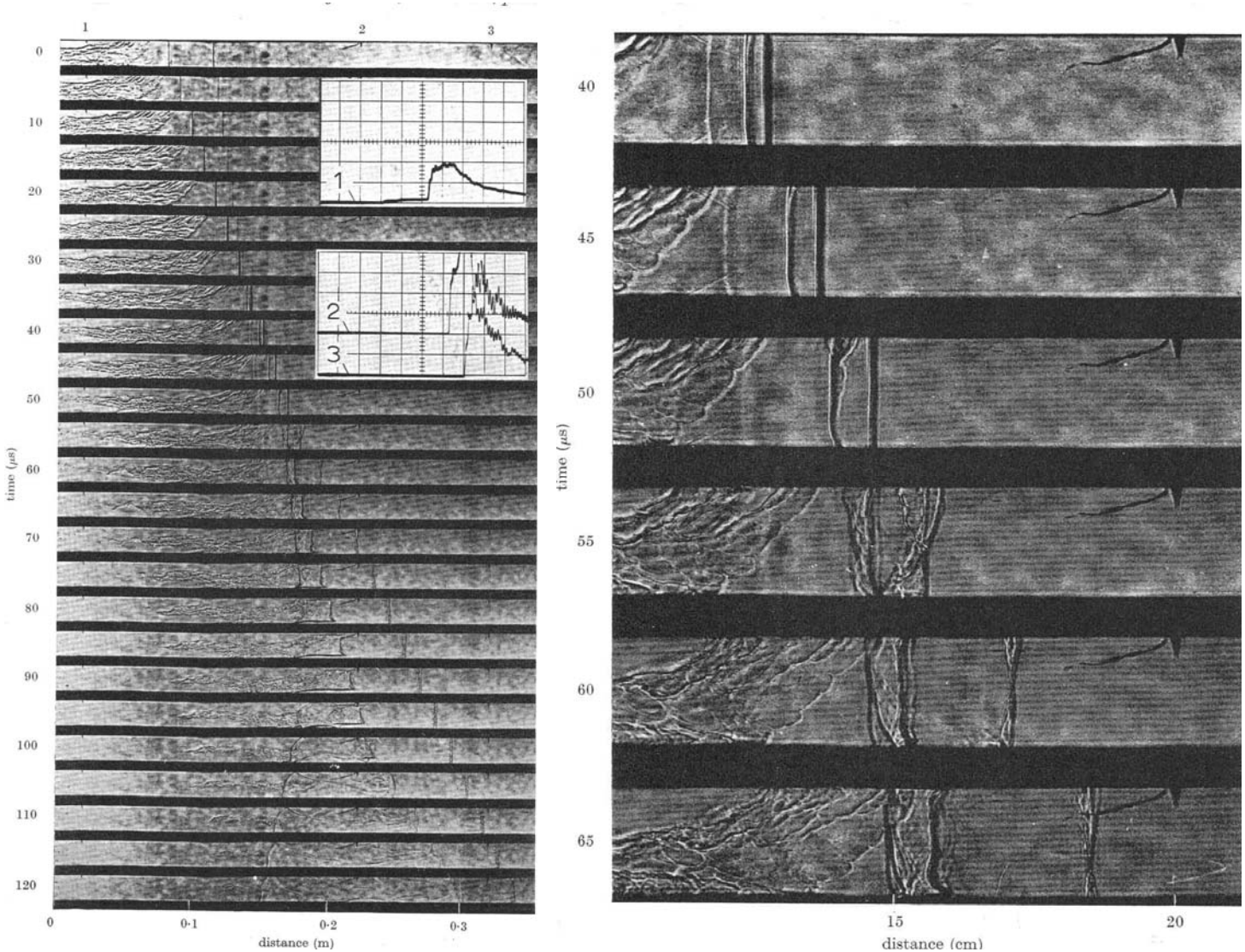
DDT in smooth tube



Schlieren framing photographs by rotating mirror camera

(Myer&Oppenheim, 1965)

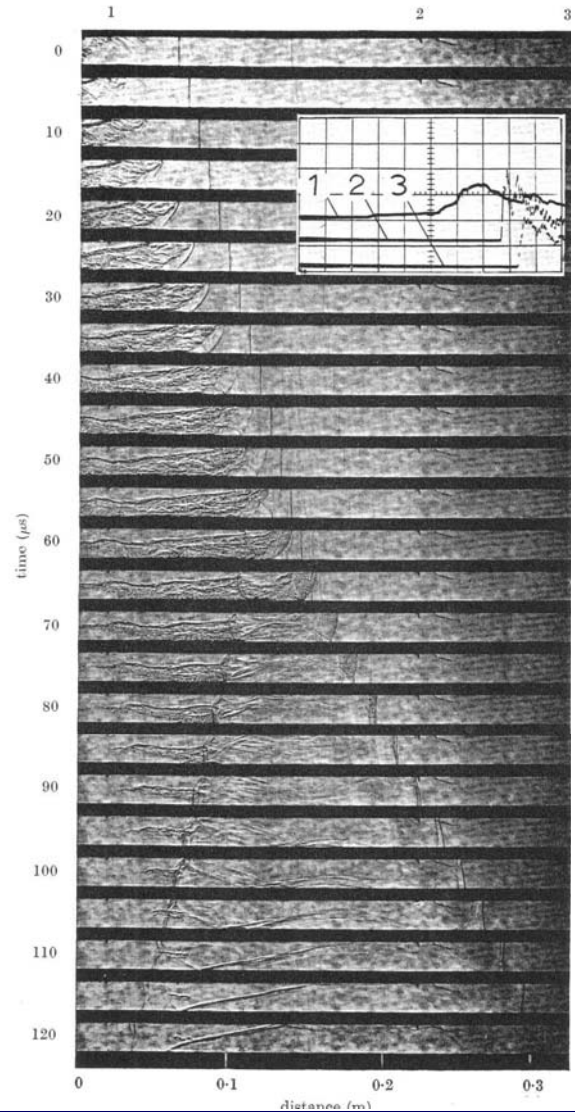
DDT in smooth tube

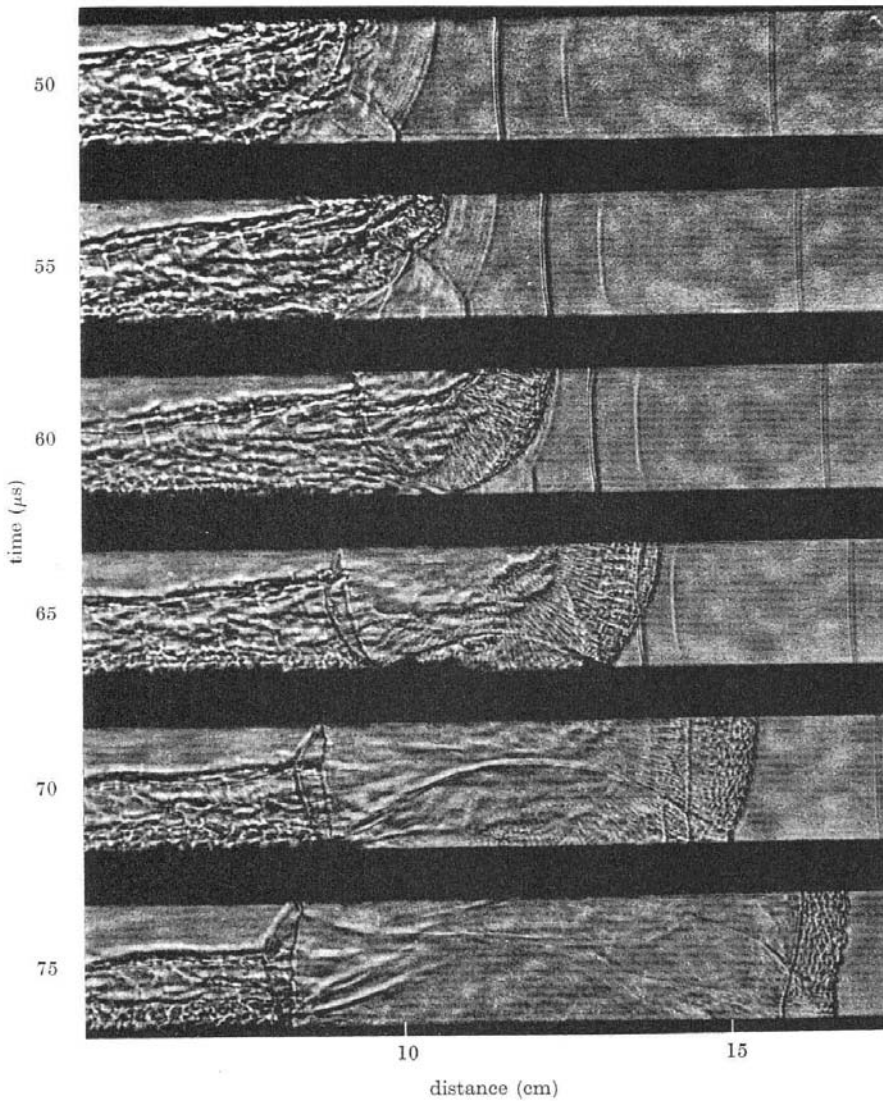


Schlieren framing photographs by rotating mirror camera

(Urtiev&Oppenheim, 1965)

DDT in smooth tube





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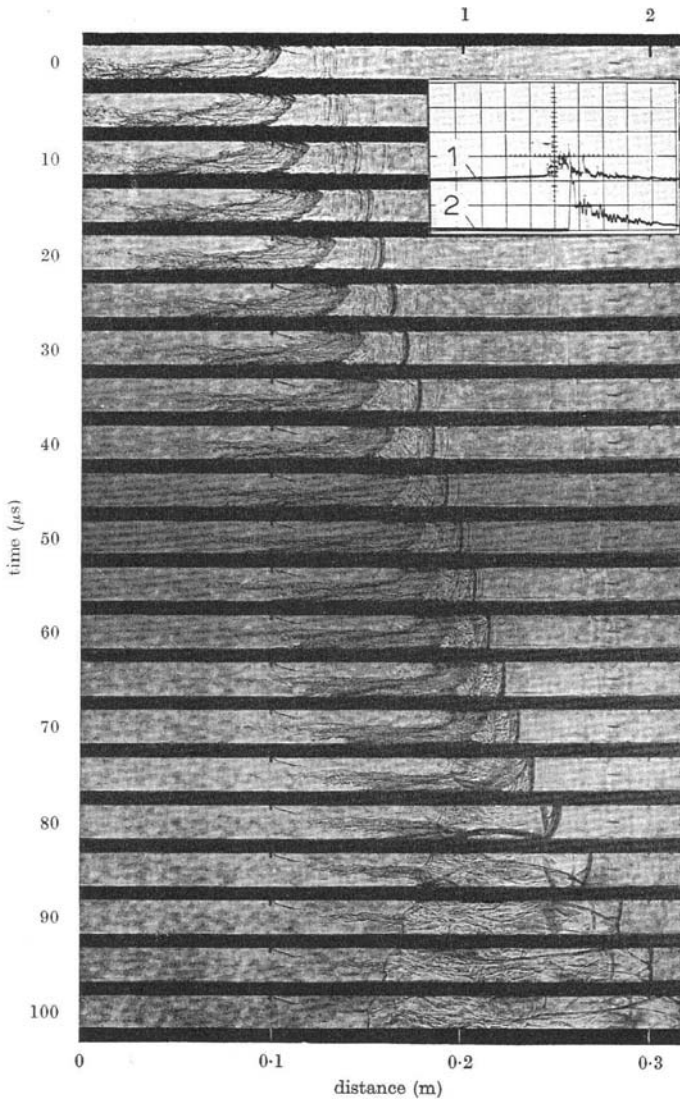
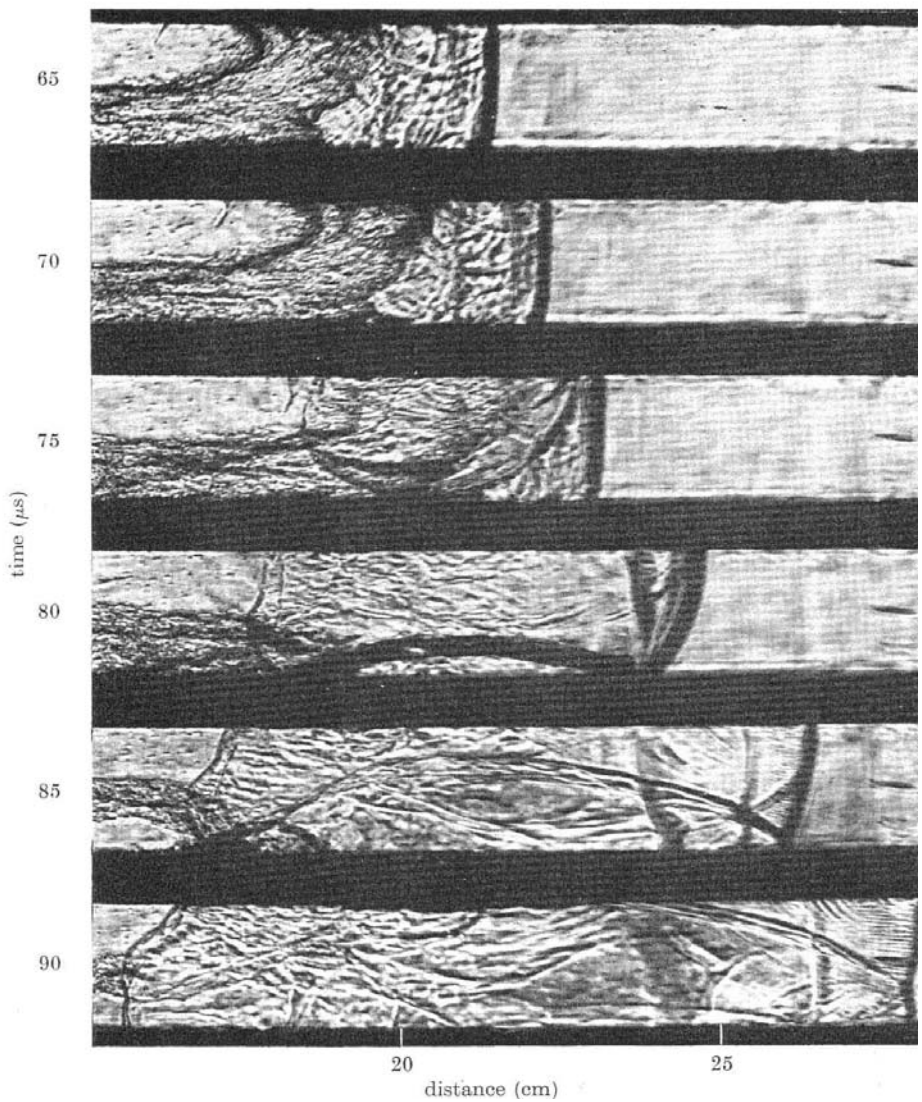
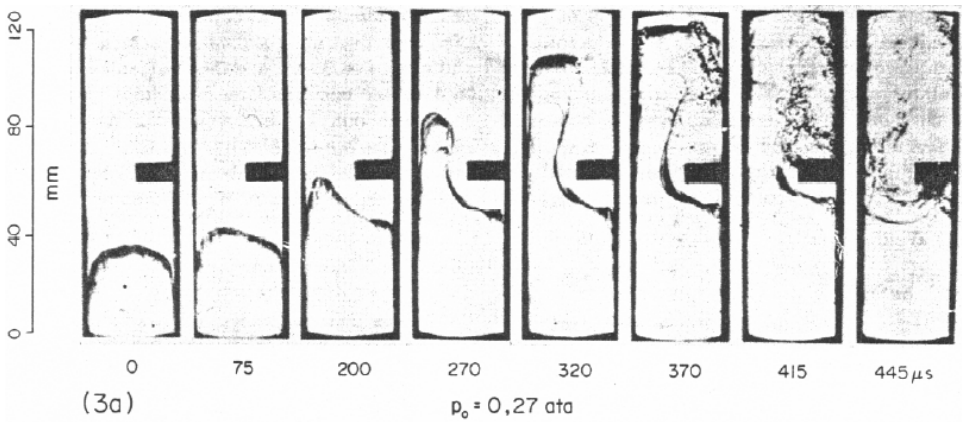
DDT in smooth tube

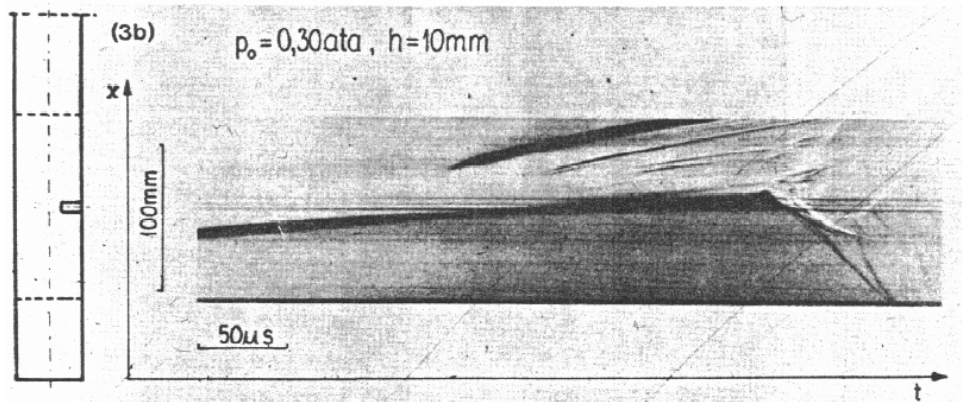




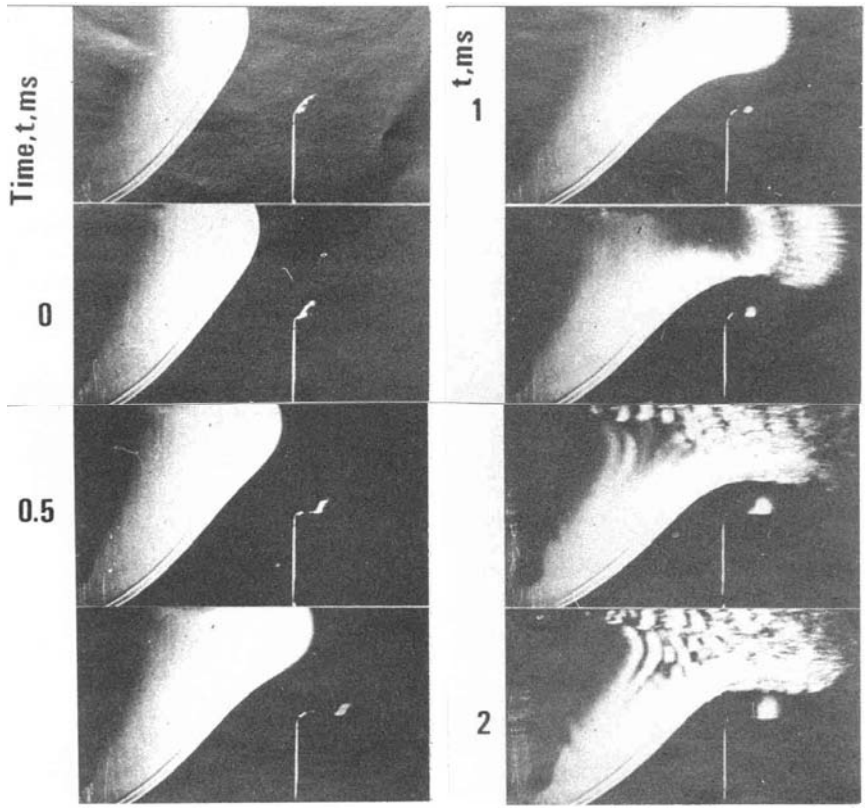
(Urtiev&Oppenheim, 1965)

Flame acceleration over the obstacle



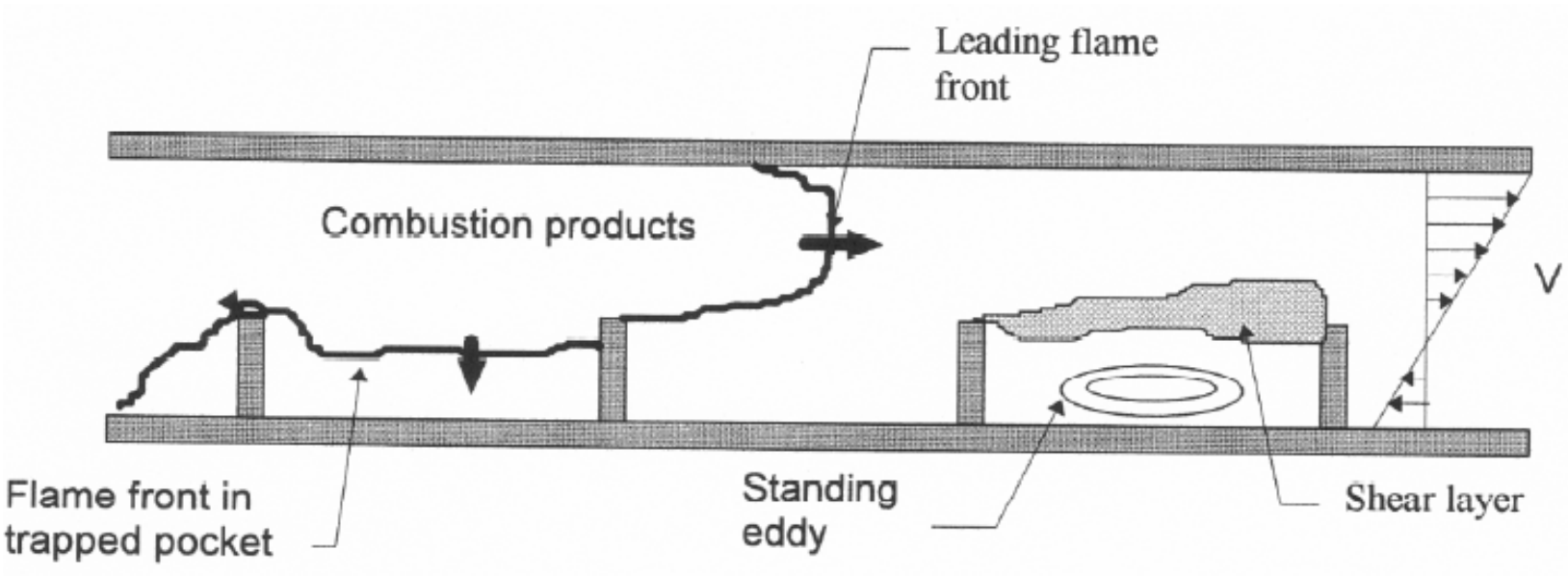


(Wolanski, 1983)

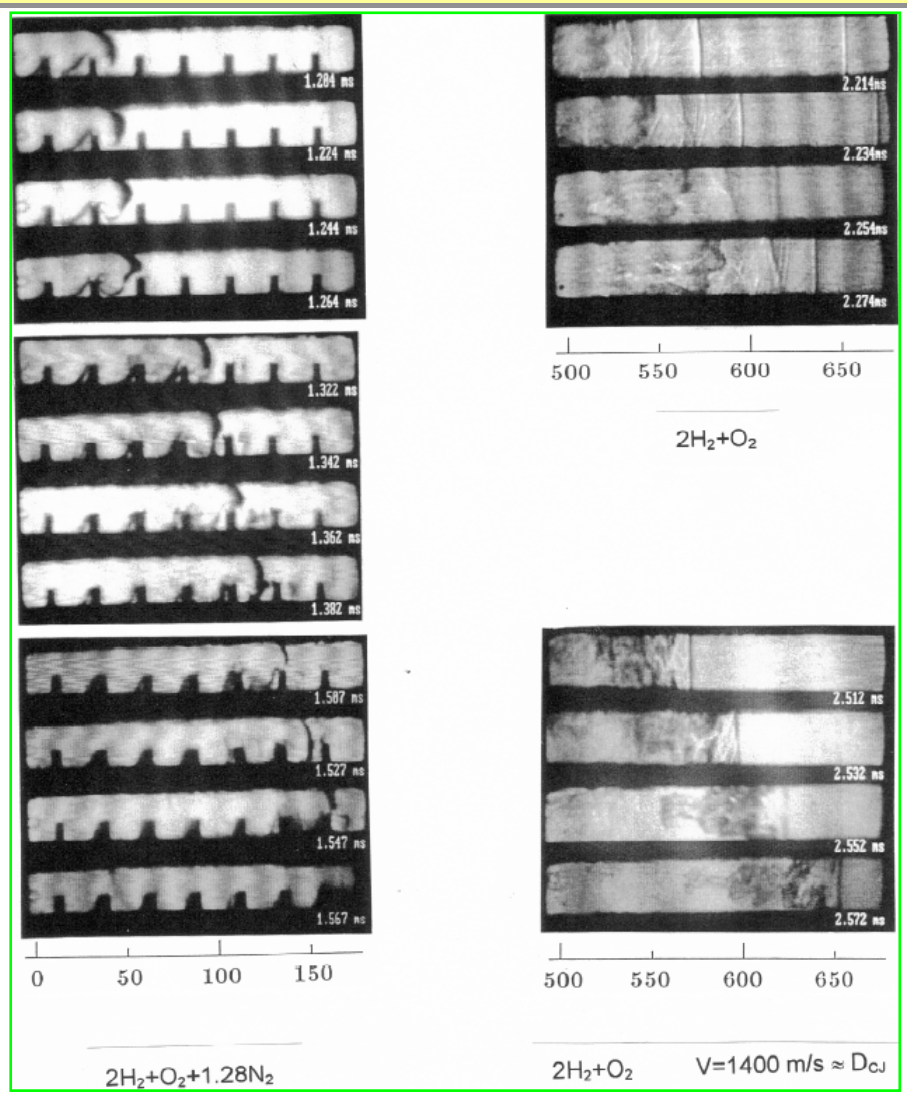


(Hirano, 1987)

Flame acceleration over the obstacle



Flame acceleration in tube



Schlieren CCD camera pictures;

Closed channel

0.5 bar

(Ohyagi et al., 1993)

DDT in tube with obstacles

Flame velocity versus fuel concentration for H2-air mixtures

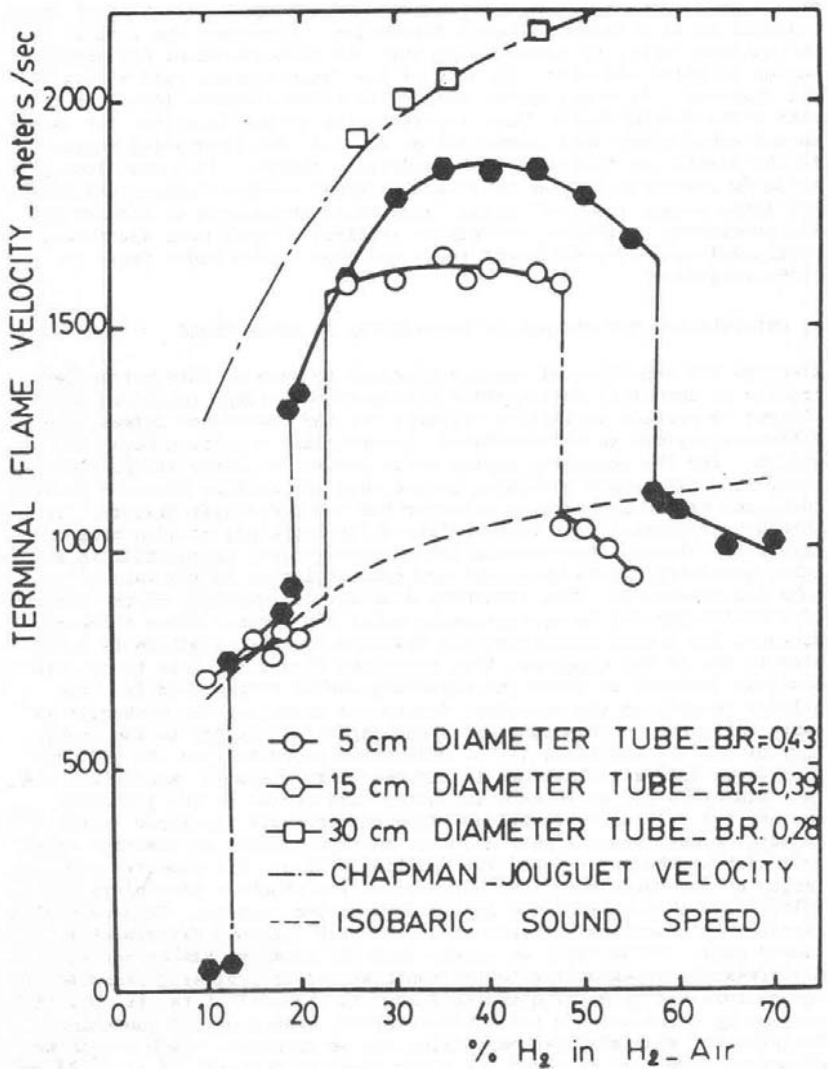
10 m long tubes of 5 cm, 15 cm and 30 cm in internal diameter with obstacles (orifice plates).

BR = 1 - d2/D2 – blockage ratio

d - orifice diameter

D - tube diameter

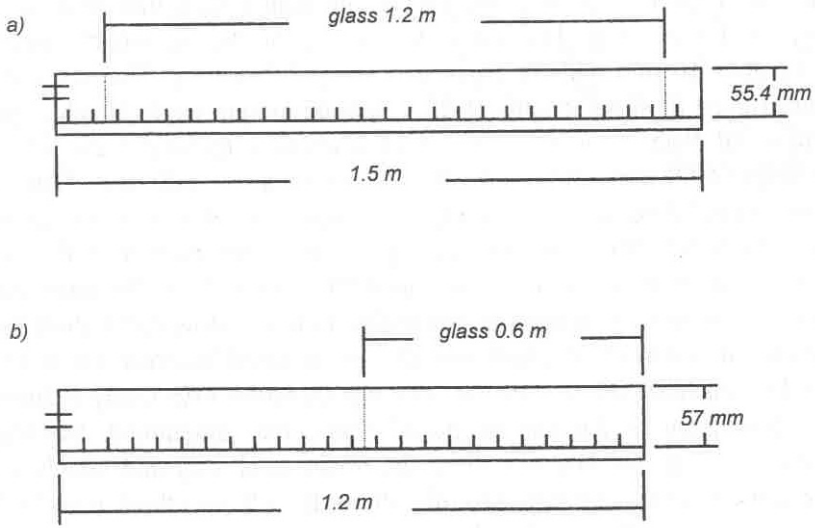
(Lee, 1986)

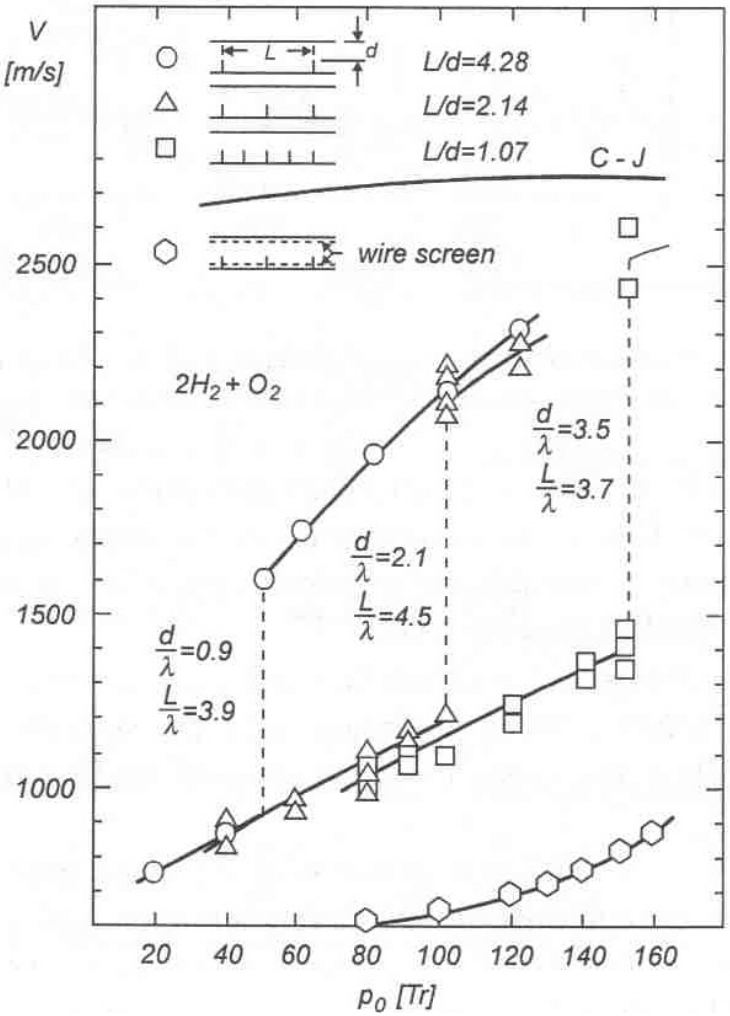


Regimes of flame propagation in tubes with obstacles

- **quenching regime** - flame fails to propagate,
- **subsonic regime** - flame is traveling at a speed that is slower than the sound speed of the combustion products,
- **choked regime (CJ Deflagration)** - flame speed is comparable with the sound speed of the combustion products,
- **quasi-detonation regime** - velocity between the sonic and Chapman-Jouguet (CJ) velocity,
- **CJ detonation regime** - velocity is equal to the CJ detonation velocity

DDT in tube with obstacles





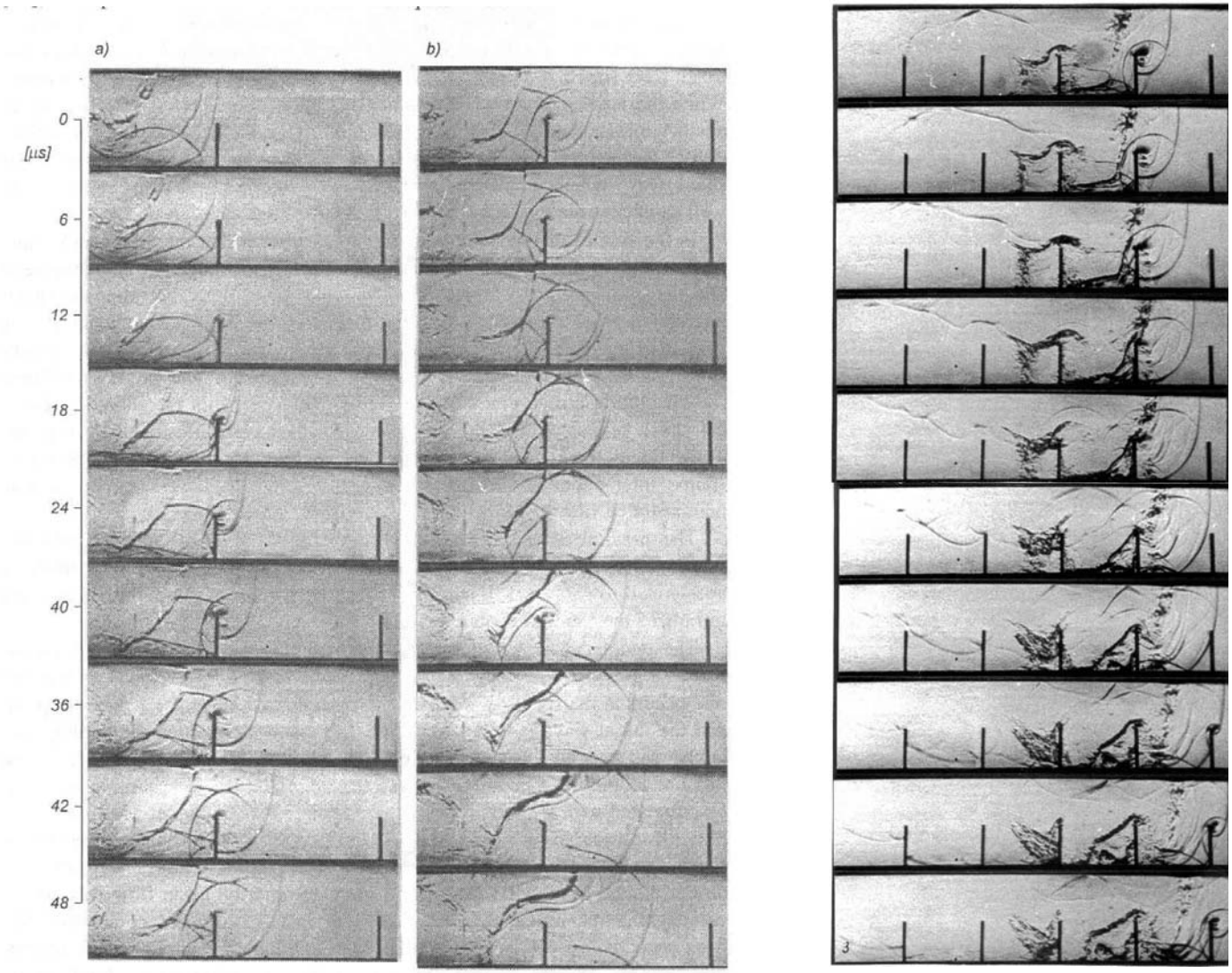
Stoichiometric hydrogen-oxygen

Pressure 20-150 torr

Ignition by exploding wire

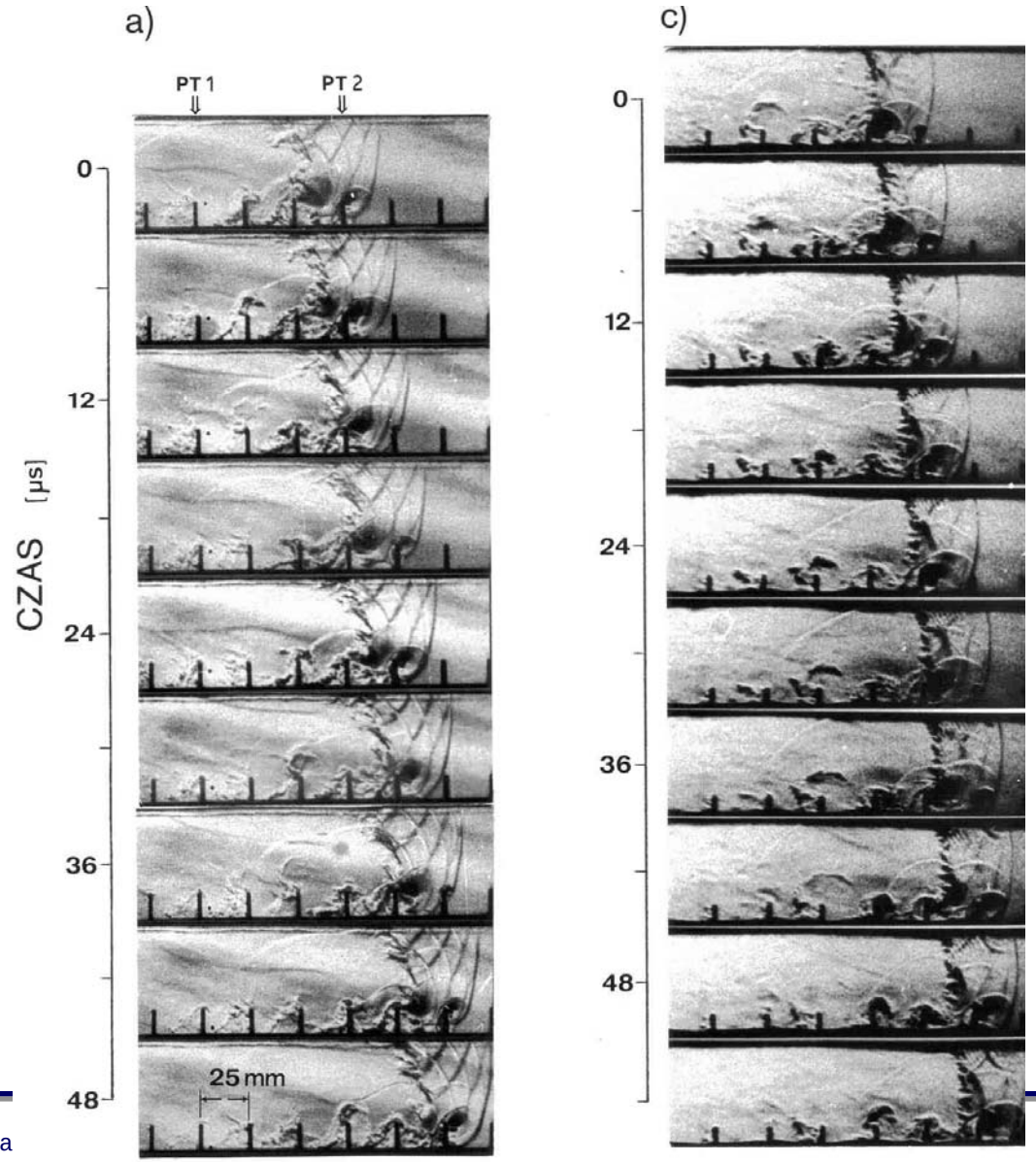
(Teodorczyk, et al..1988)

Fast deflagration in a channel with obstacles



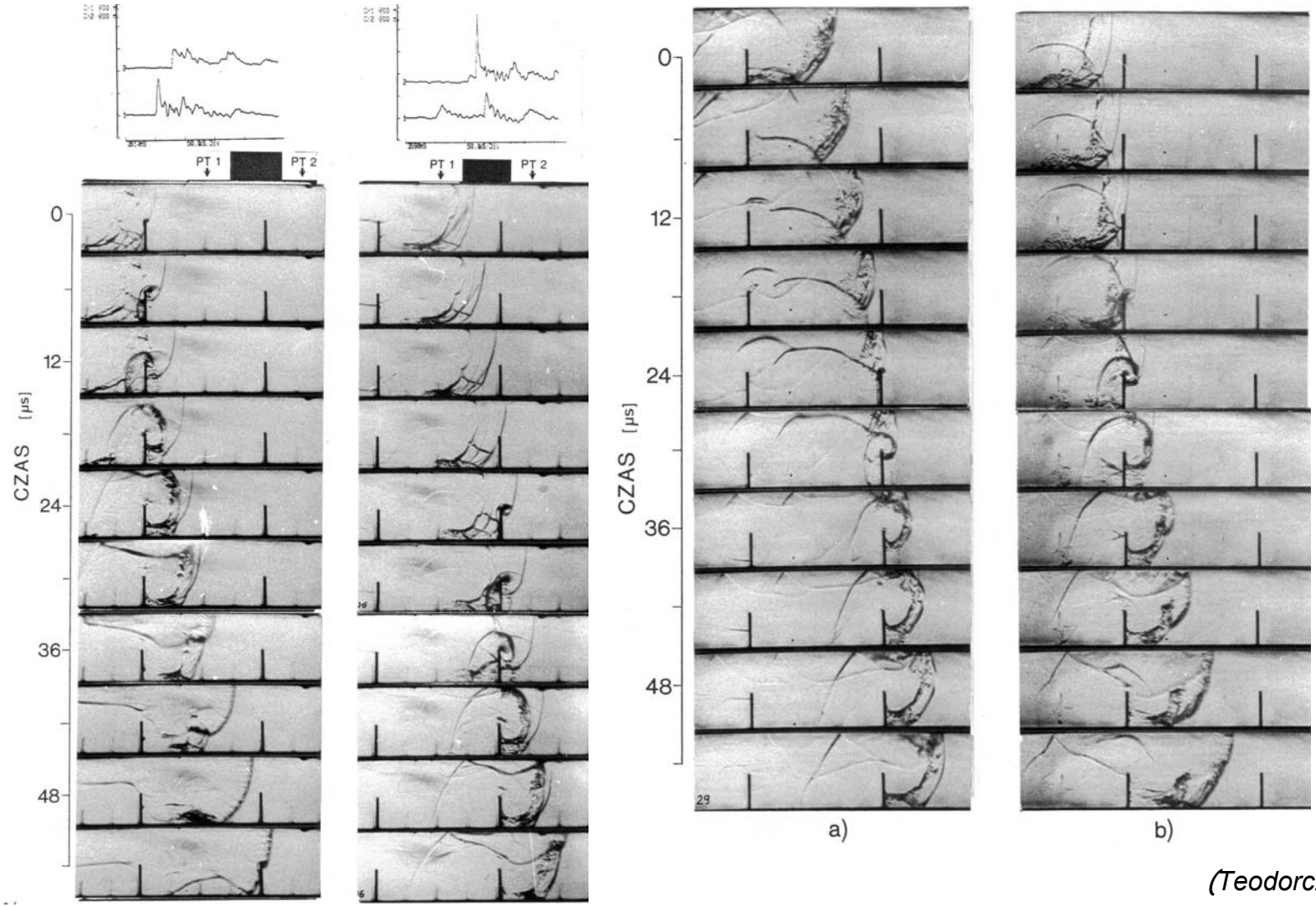
(Teodorczyk, et al..1988)

Fast deflagration in a channel with obstacles



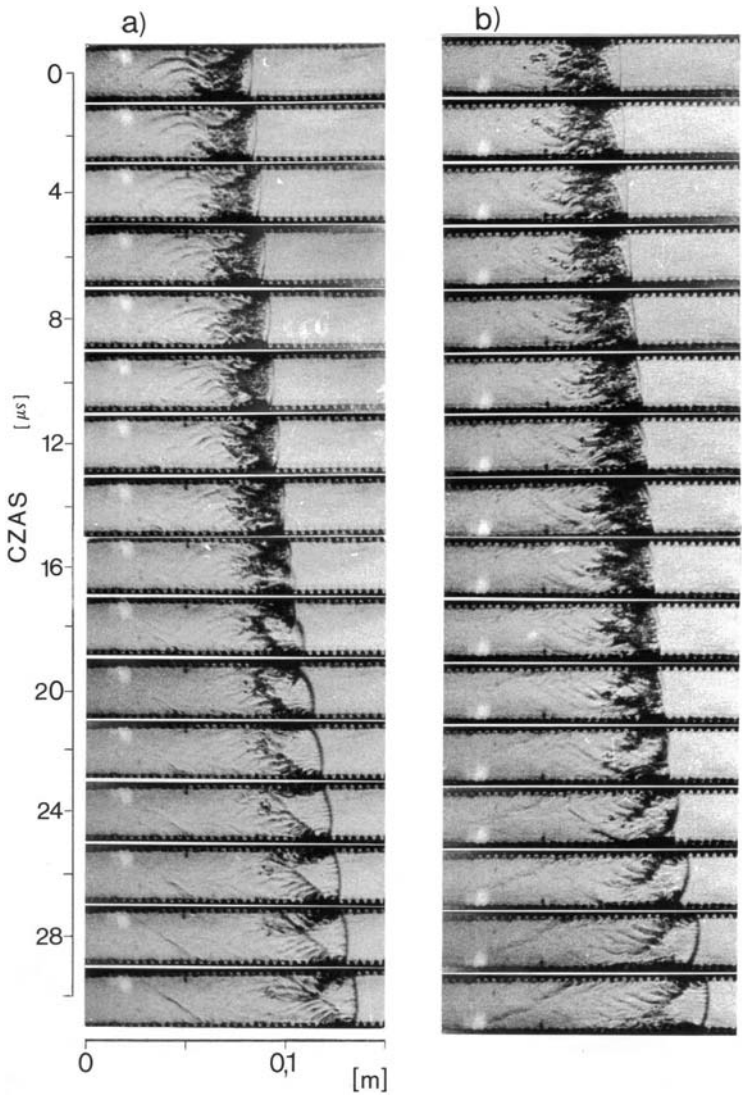
(Teodorczyk, et al..1988)

DDT in tube with obstacles



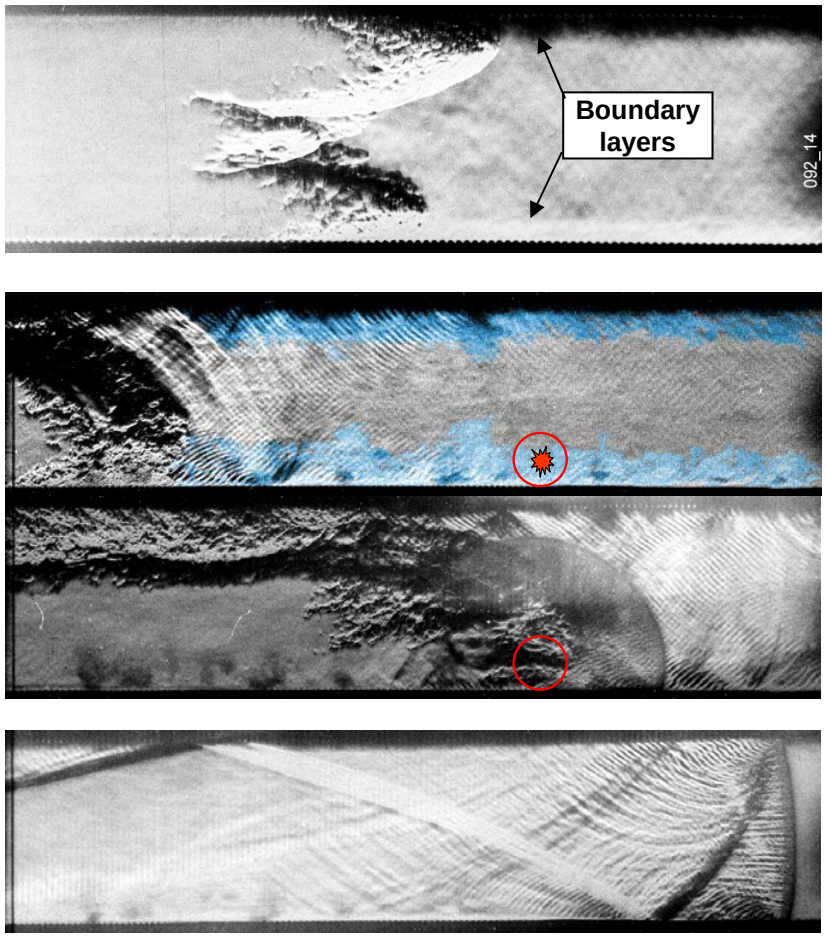
(Teodorczyk, et al..1988)

DDT in rough channel



(Teodorczyk, 1990)

DDT in rough channel

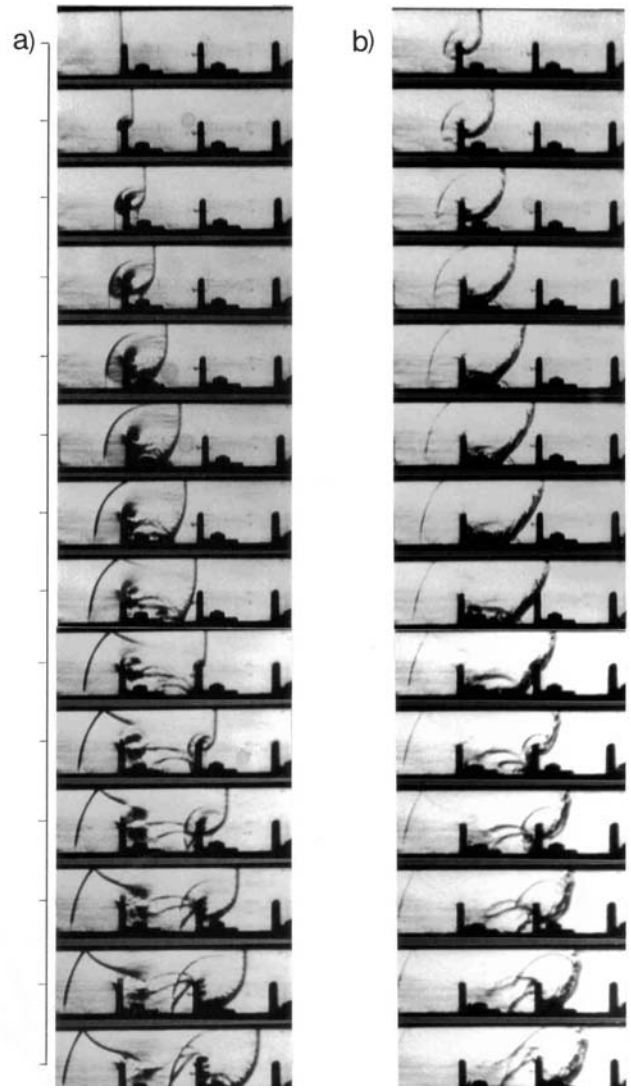


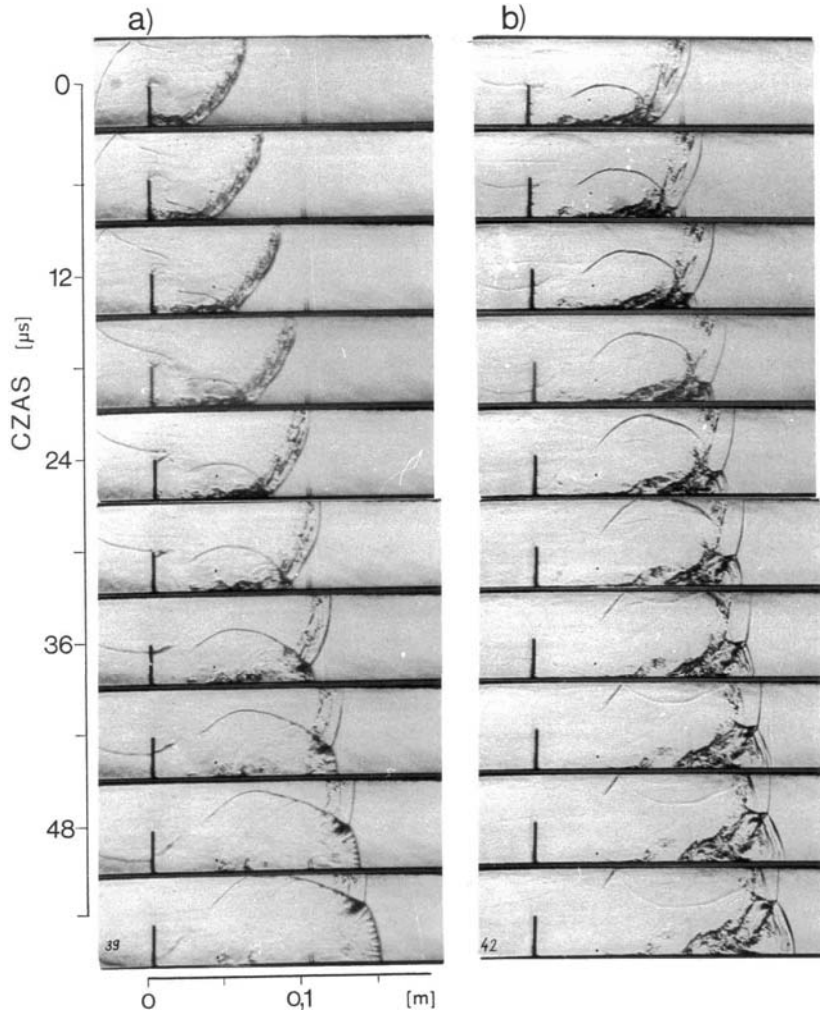
Flame speed 320 m/s

p_0=0.55 bar, 1090-1320 mm from ignition

(Kuznetsov M., Dorofeev S., 2005)

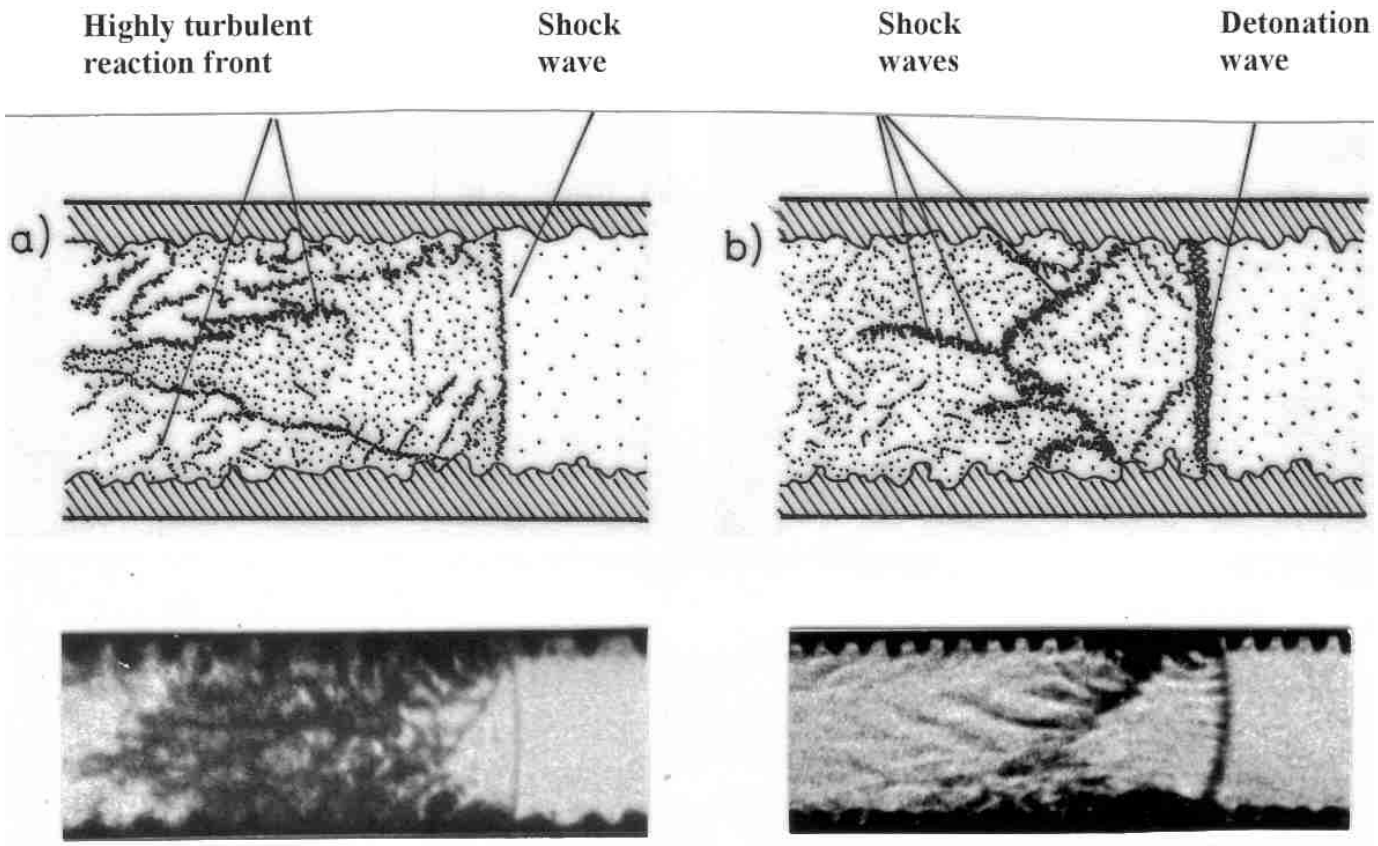
Detonation in a channel with obstacles





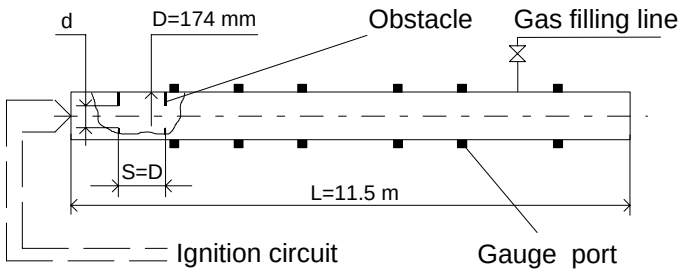
(Teodorczyk, et al..1988)

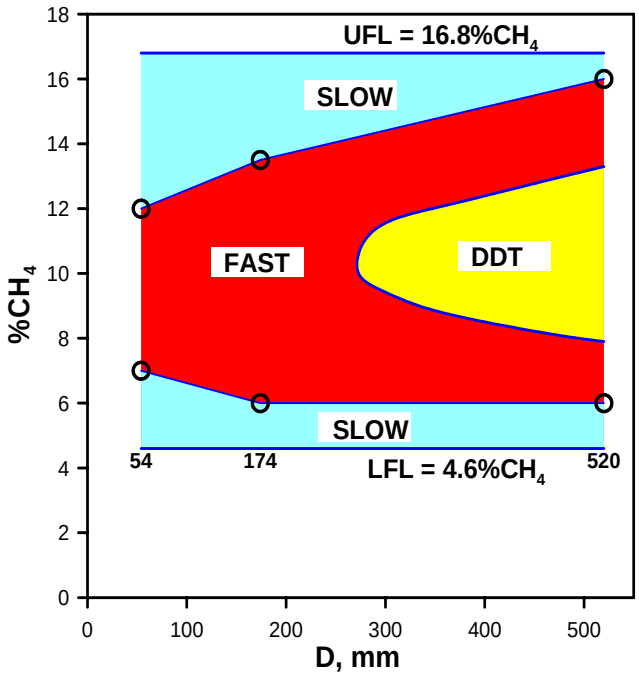
Fast deflagration vs detonation in a very rough channel

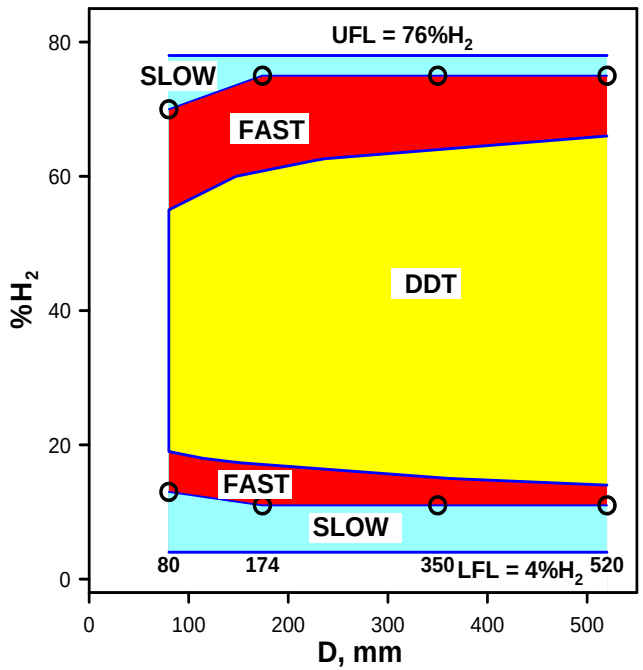


(Teodorczyk, 1990)

Flame acceleration and DDT in obstructed channels



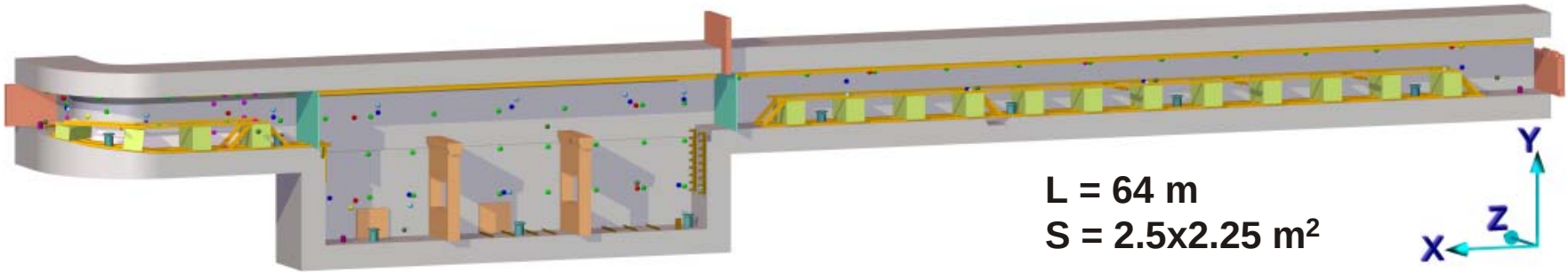




(Courtesy of M.Kuznetzov)

RUT experiments on the premixed H2 combustion

Flame acceleration and DDT experiments in complex channel geometry with hydrogen-air mixtures

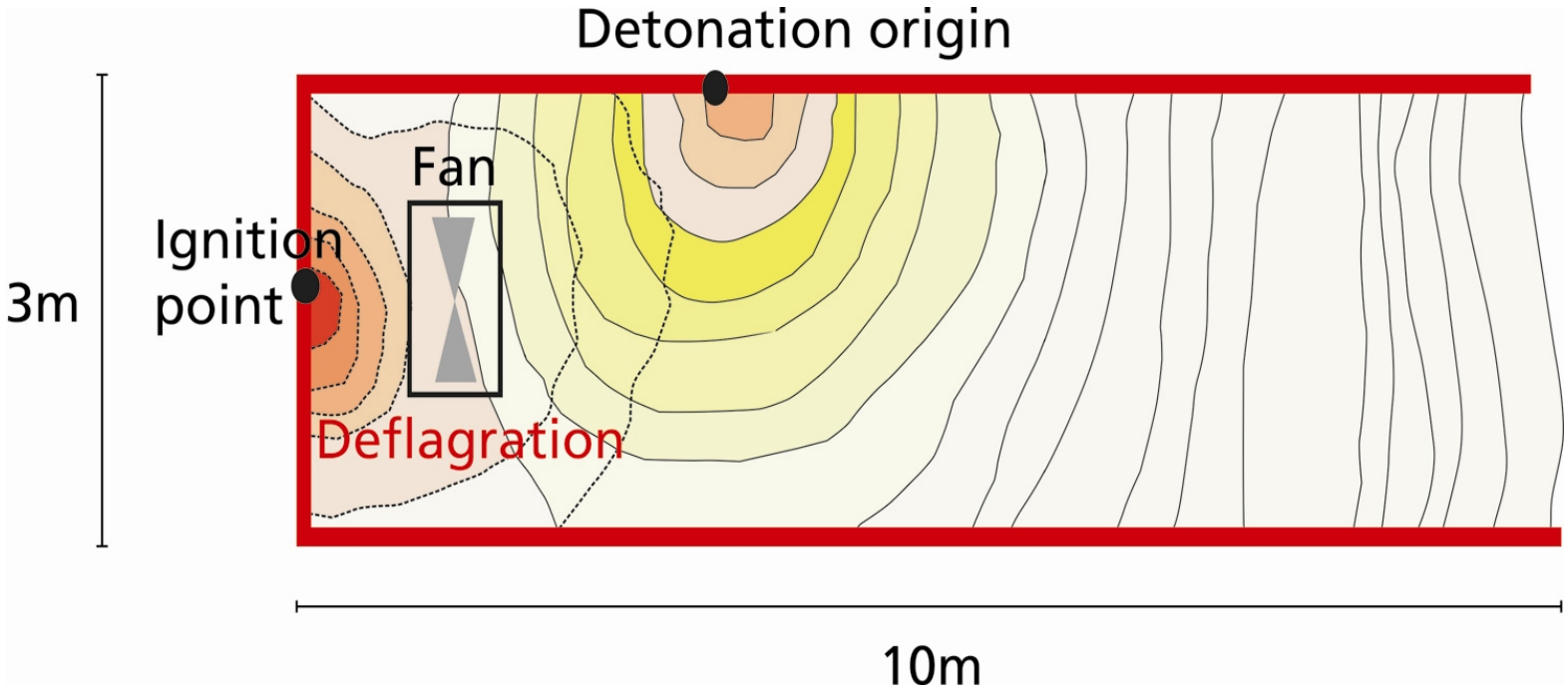


- 11% H2/air –slow flame: p=3-4 bar v = 150-200 m/s
- 12.5% H2/air – sonic flame: p=5-7 bar v = 550-600 m/s
- 14% H2/air – detonation: p=9-12 bar v = 1400 m/s

(Courtesy of M.Kuznetzov)

DDT in large scale

DDT of a hydrogen/air mixture within a "lane", simulated by two parallel walls (top view)



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

DDT in large scale

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

12 ms

30 ms

18 ms

36 ms

24 ms

42 ms

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

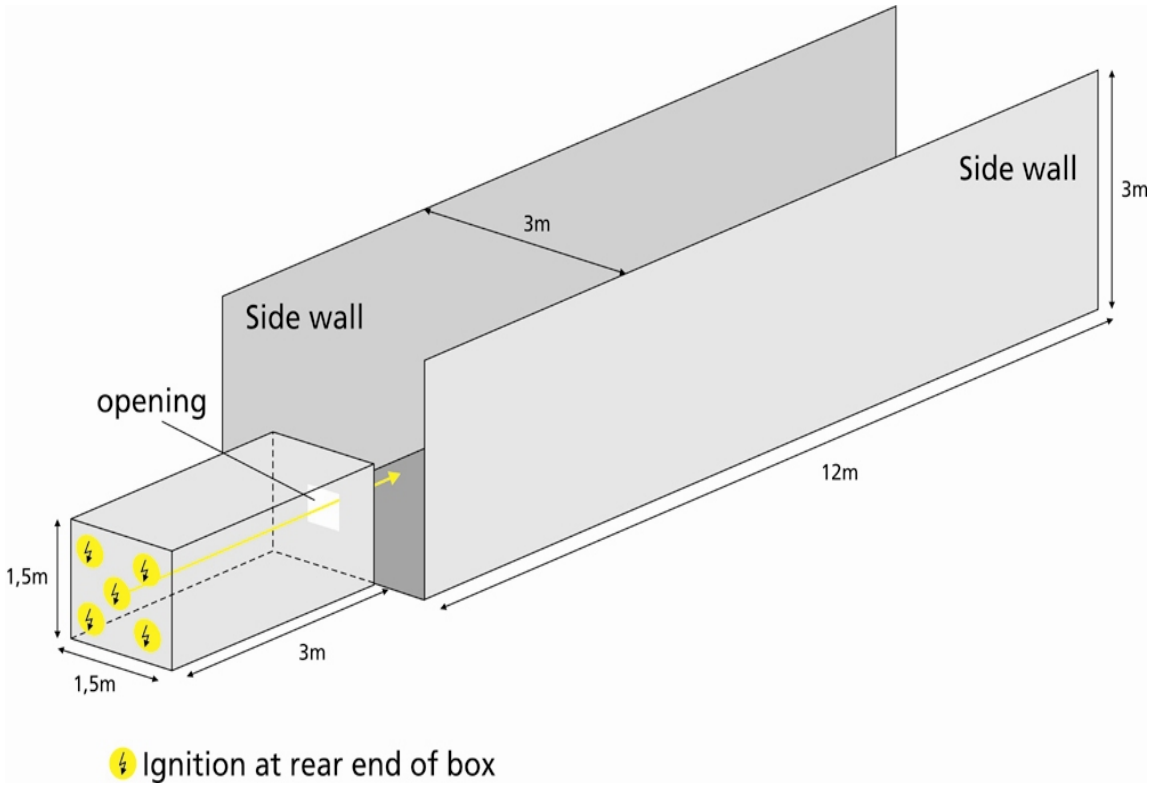
DDT in large scale

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

(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

DDT in large scale

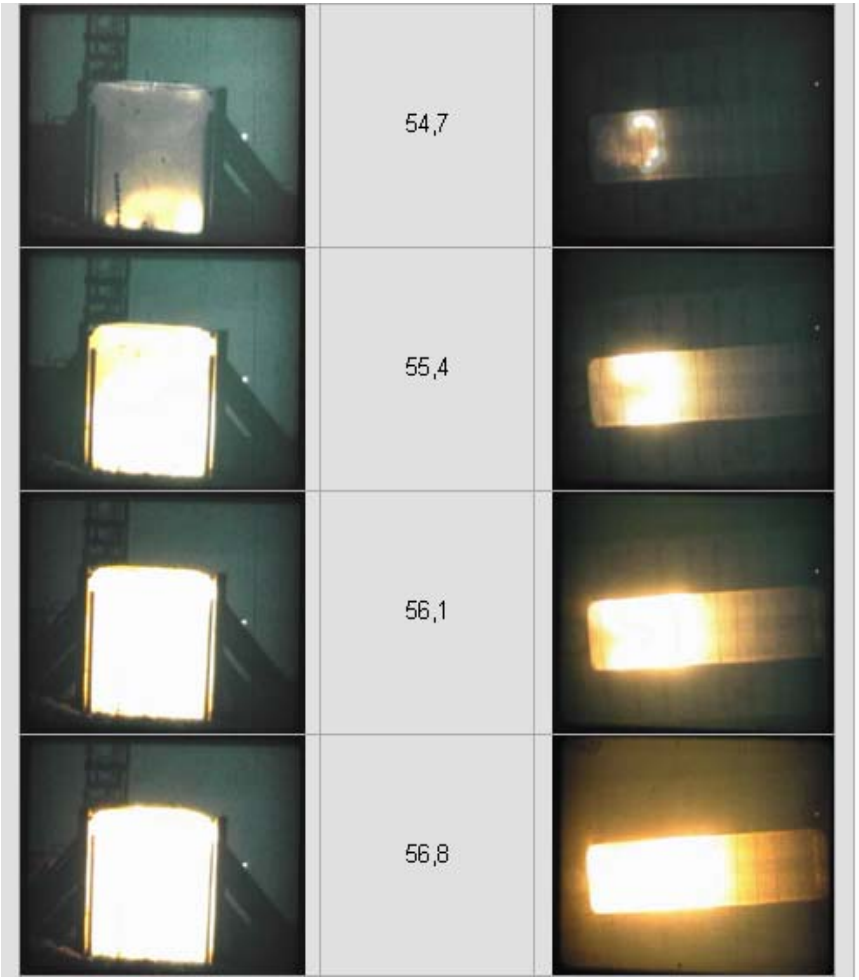
Test set up for igniting a hydrogen/air mixture by means of a flame jet within a “lane“, simulated by two parallel walls



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

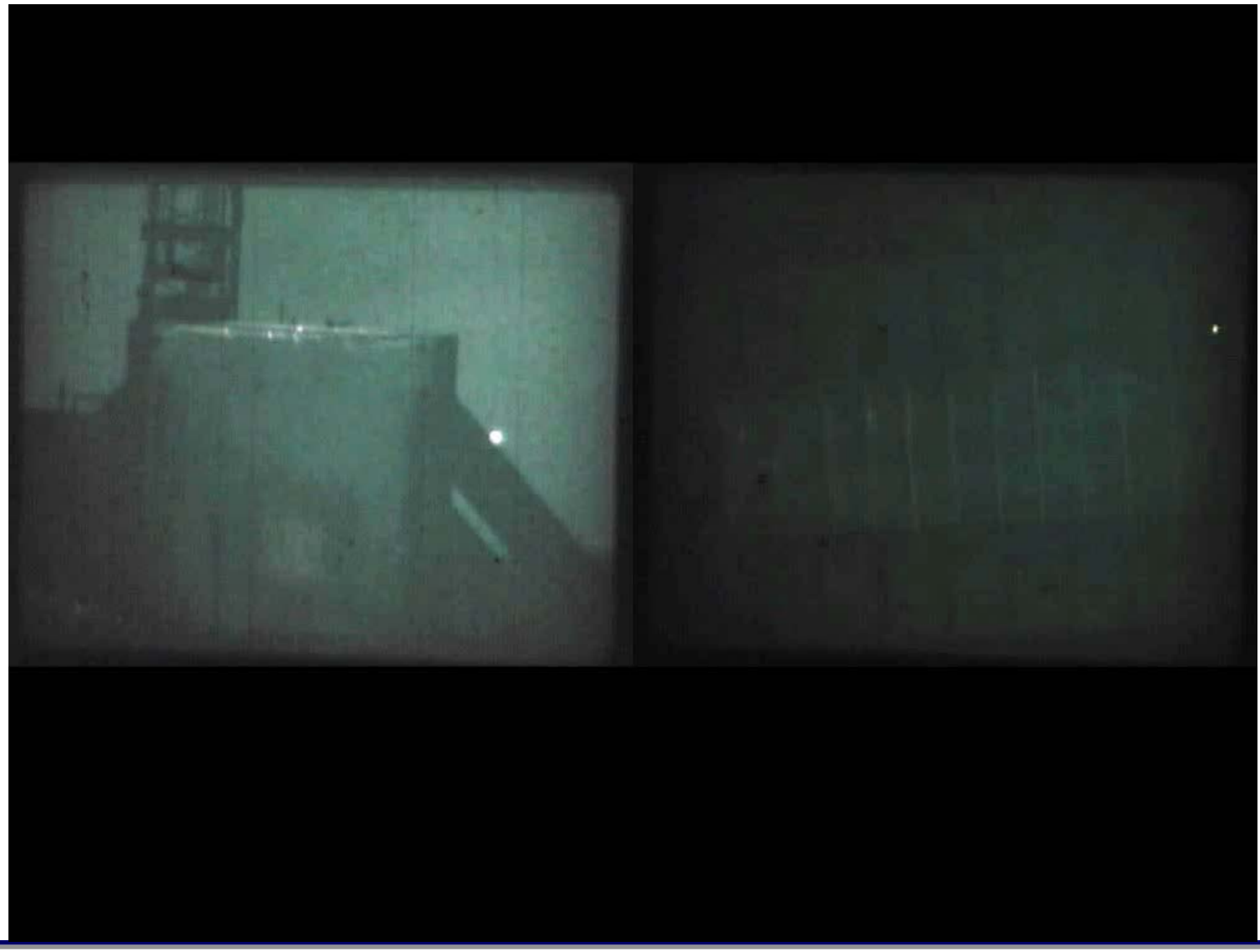
DDT in large scale

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



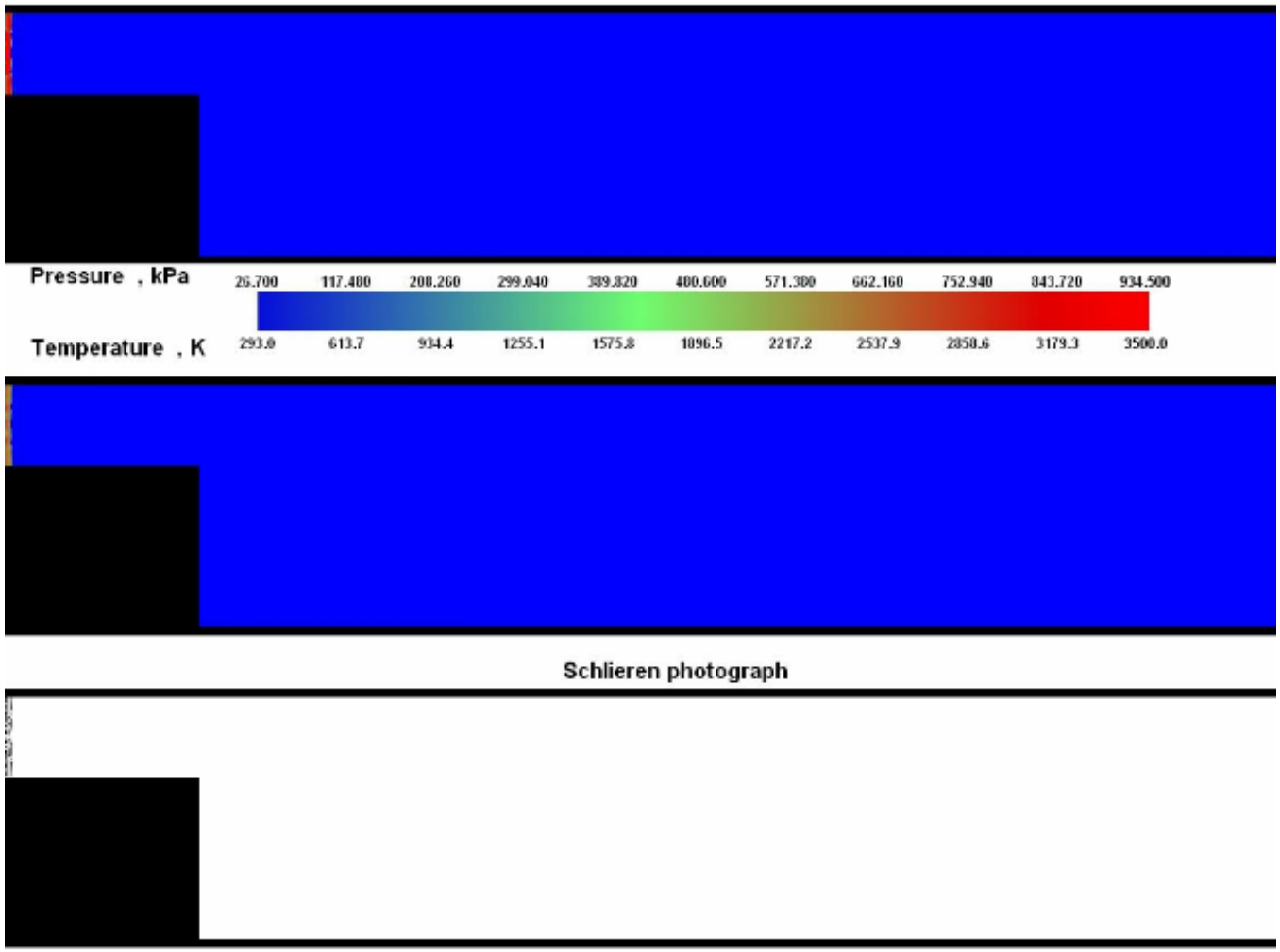
(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

DDT in large scale



(Courtesy of dr Schneider from Fraunhofer Institute Chemische Technologie)

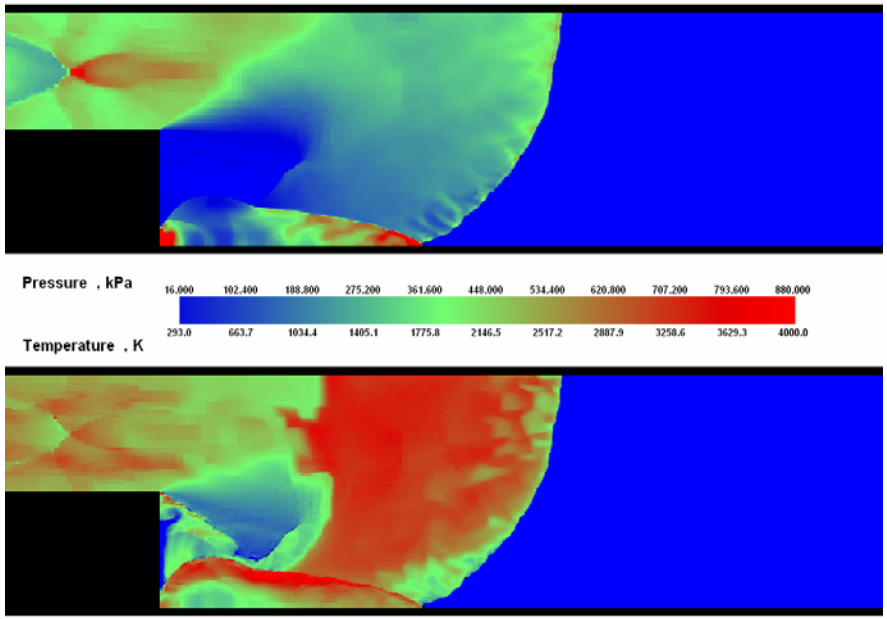
Detonation simulation

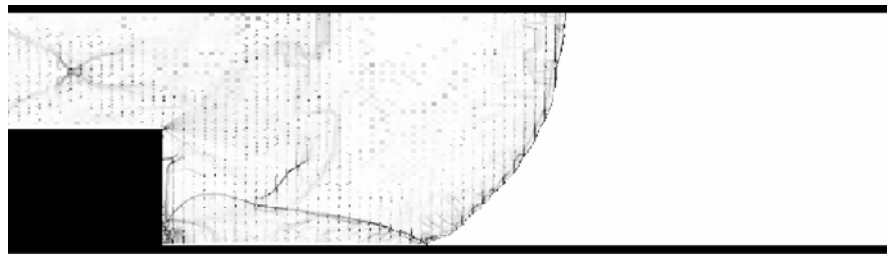


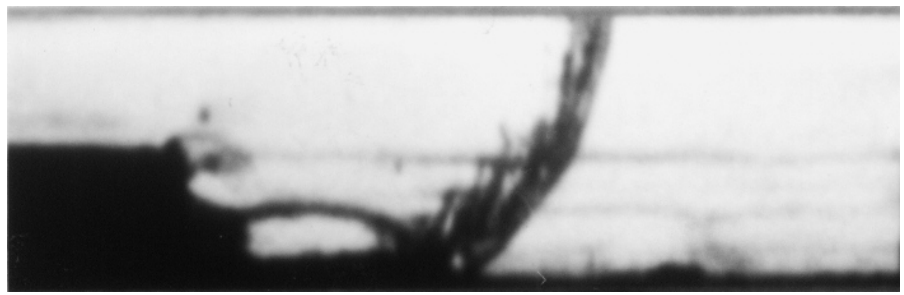
DETO2D code

Piela K., Teodorczyk A.: *Detonation simulation with adaptive grid,* Journal of Technical Physics 2006

Detonation simulation







Simulation: DETO2D

Experiment: Teodorczyk A., Lee J.H.S. and Knystautas R.: *Propagation Mechanism of Quasi-Detonations*, Twenty-Second Symposium (Int.) on Combustion, The Combustion Institute 1988, pp. 1723-1731

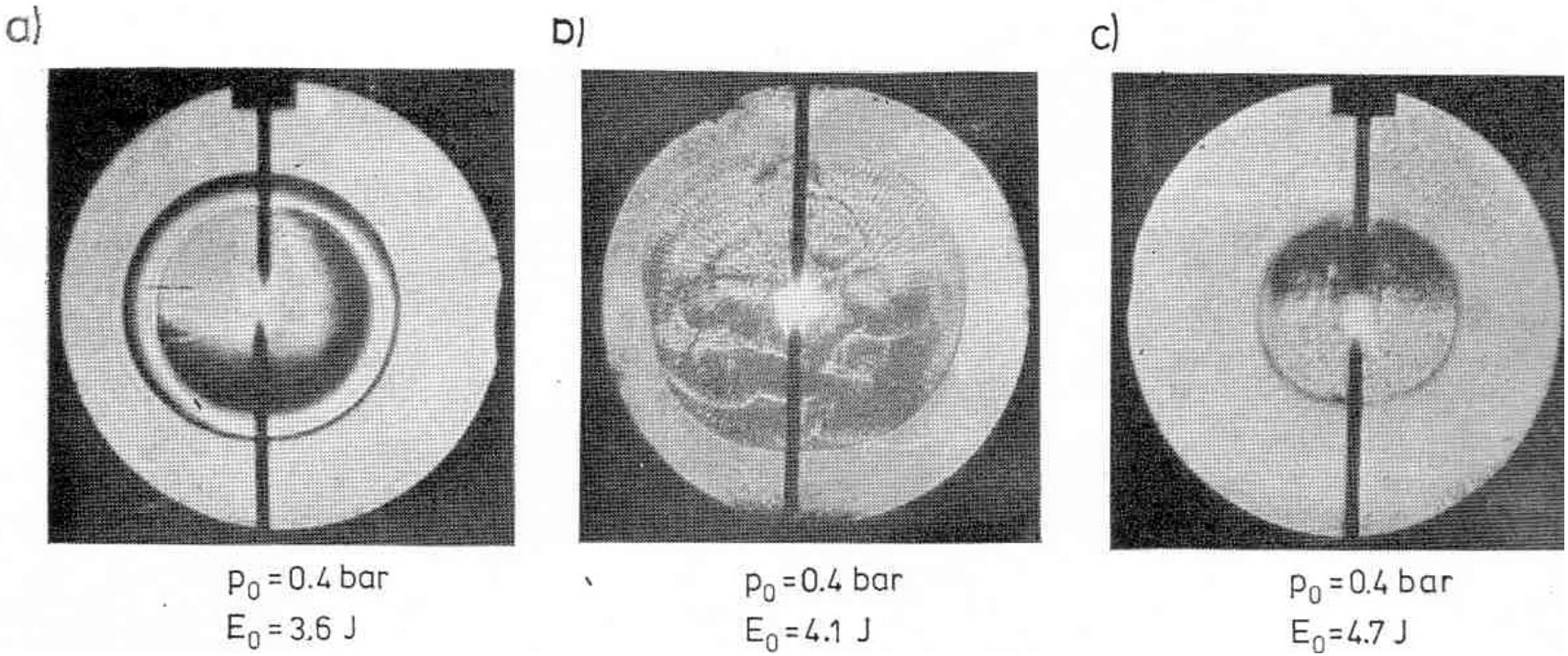
DDT simulation

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

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

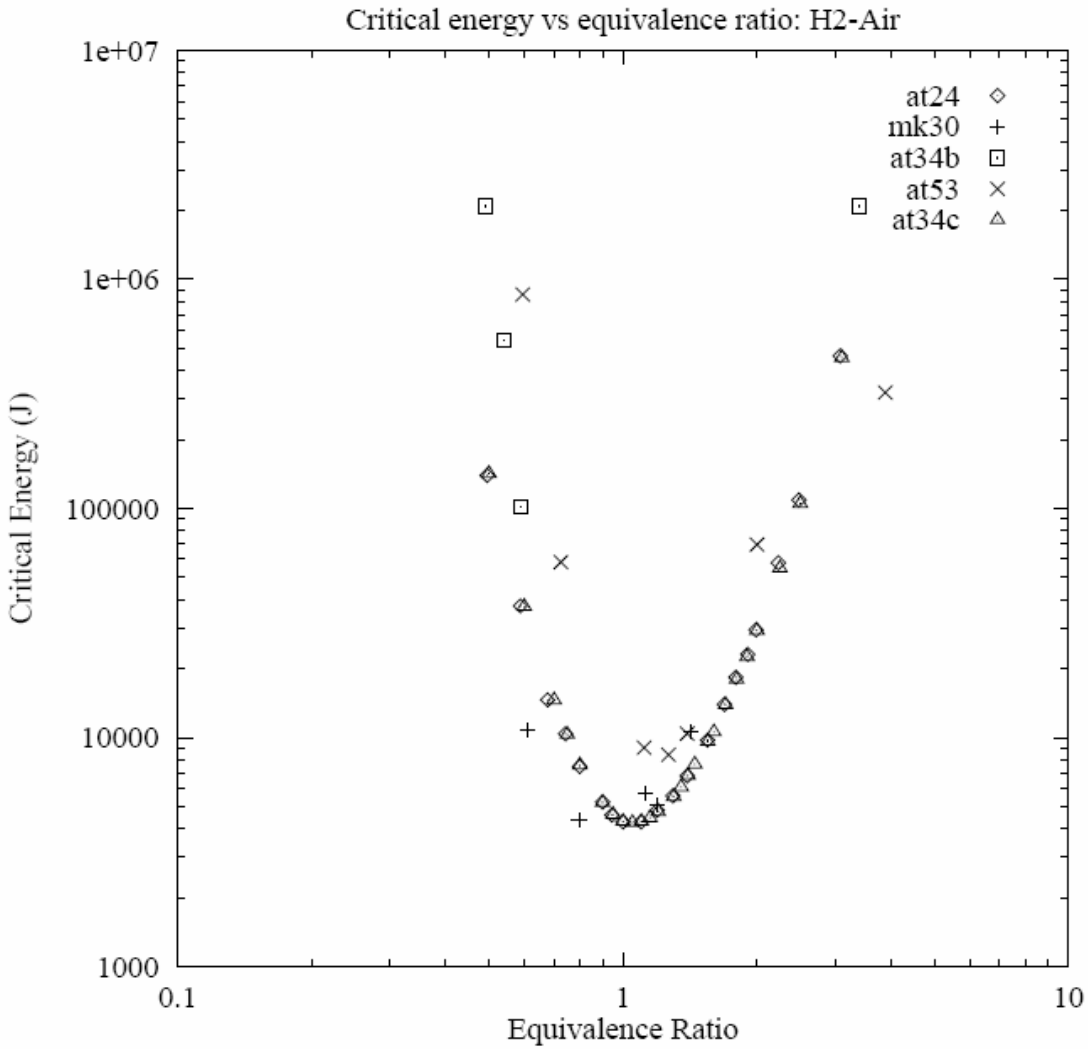
Direct initiation of detonation

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



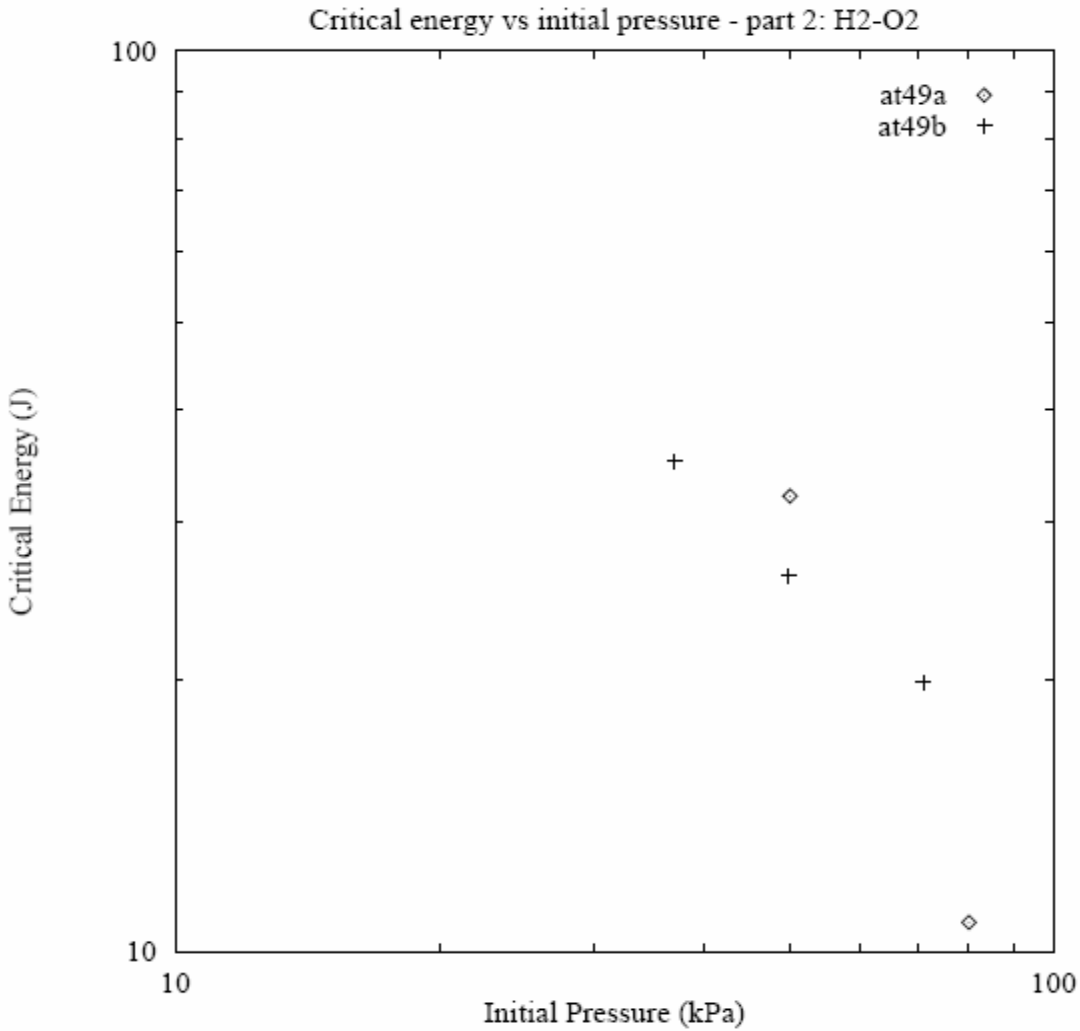
(Levin et al. 1978)

Direct initiation of detonation



From detonation database

Direct initiation of detonation



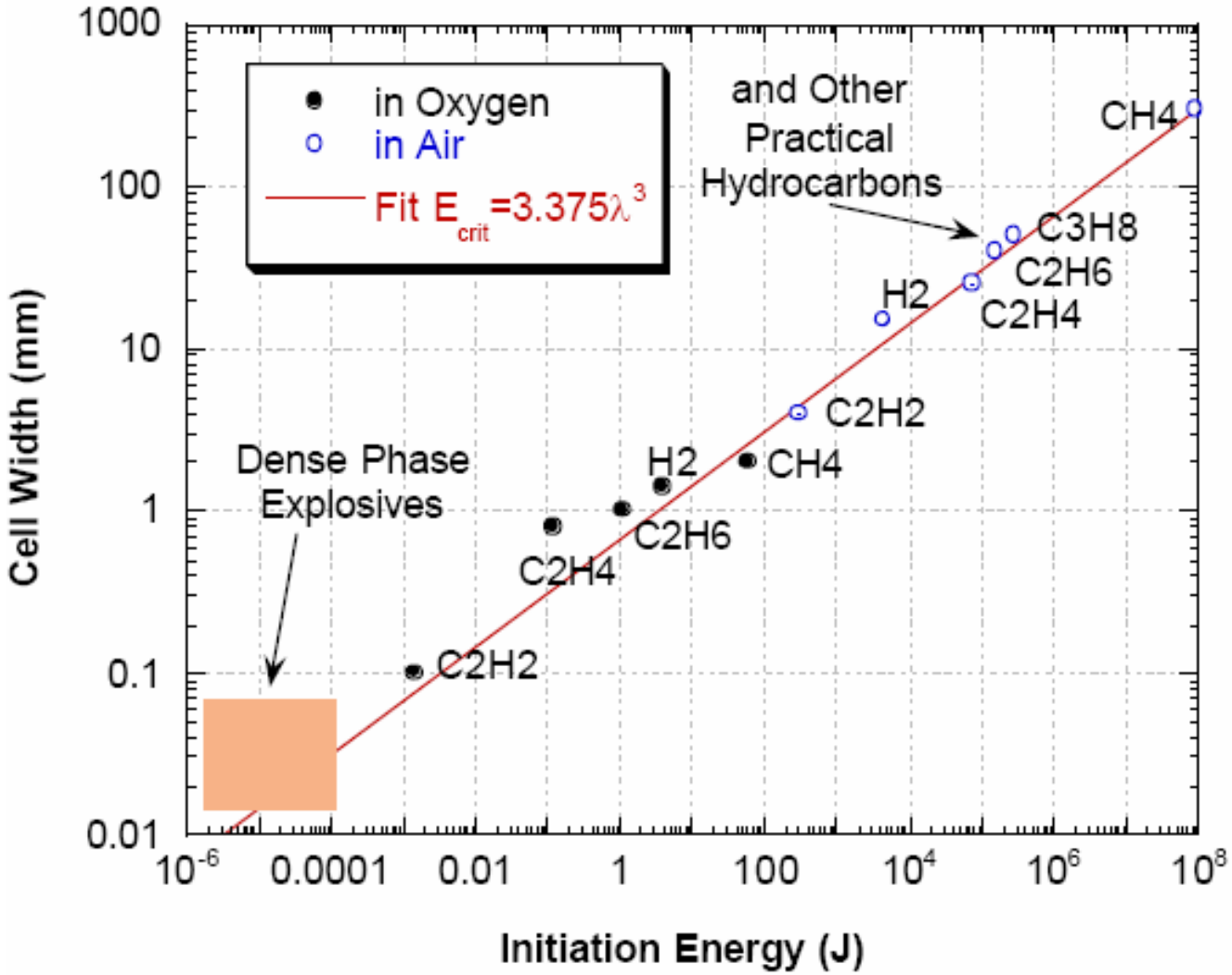
From detonation database

stoichiometric H2-O2 mixture;

at49a: T=293 K;

at49b: T=123 K;

Direct initiation of detonation



(Schauer et al. 2005)