Hydrogen-Air Mixture Ignition and Combustion behind the Shock Waves

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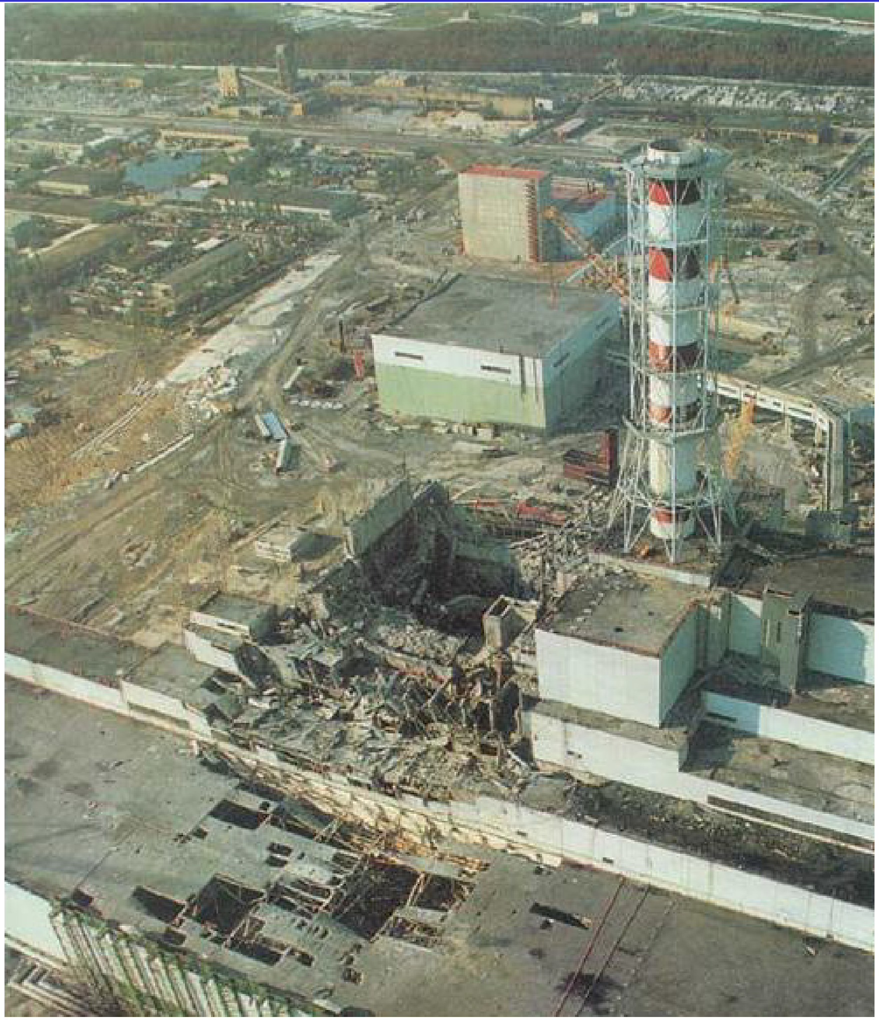
Hydrogen accidents in:

- Nuclear reactors
- Tunnels and urban streets
- Refuelling stations
- Pipelines



Chernobyl reactor number four after the disaster, showing the extensive damage to the main reactor hall (image center) and turbine building (image lower left)

1:23:47 AM. Due to the thermal expansion the cladding of fuel rods opened up.

1:23:49 AM. Thermal deformation of the fuel rods broke the coolant pipes.

1:24:00 AM. Above 1100 °C water reacts with the zirconium alloy of the rod cladding and graphite This reaction lead to the production of carbon monoxide and hydrogen:

$$Zr + 2\ H_2O = ZrO_2 + 2\ H_2,$$

$$C + H_2O = CO + H_2.$$

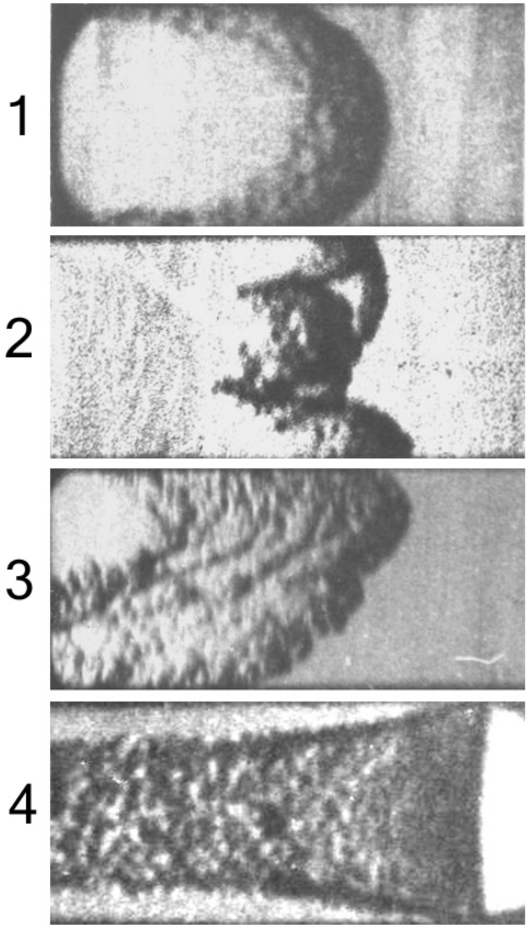
The flammable hydrogen and carbon monoxide mixed with the oxygen of air and exploded. This second, chemical explosion brushed off the roof of the building. Graphite started to burn in air and the smoke contaminated the building and its growing vicinity with radioactivity.

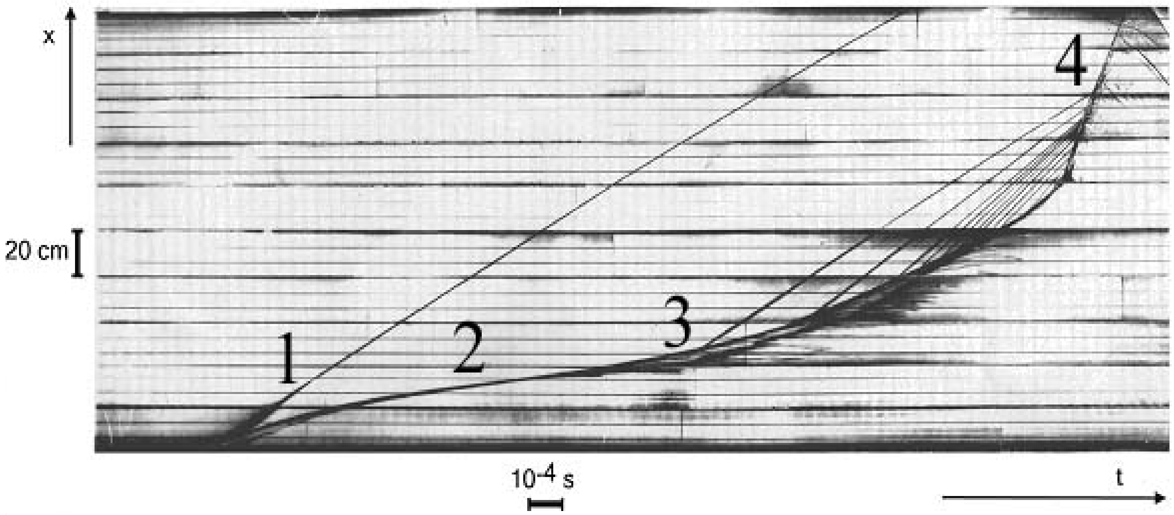
Contents

- Detonation initiation in quiescent mixture
- Detonation diffraction
- Numerical simulations of the detonation formation
- Experimental and numerical research on large-scale combustion and detonation in confined volumes up to 900 m^3 for different conditions.
- Mitigation of hydrogen explosions: chemical, acoustic and thermal
- Conclusions

Detonation initiation in quiescent mixture

Detonation onset at deflagration-to-detonation transition in quiescent mixture

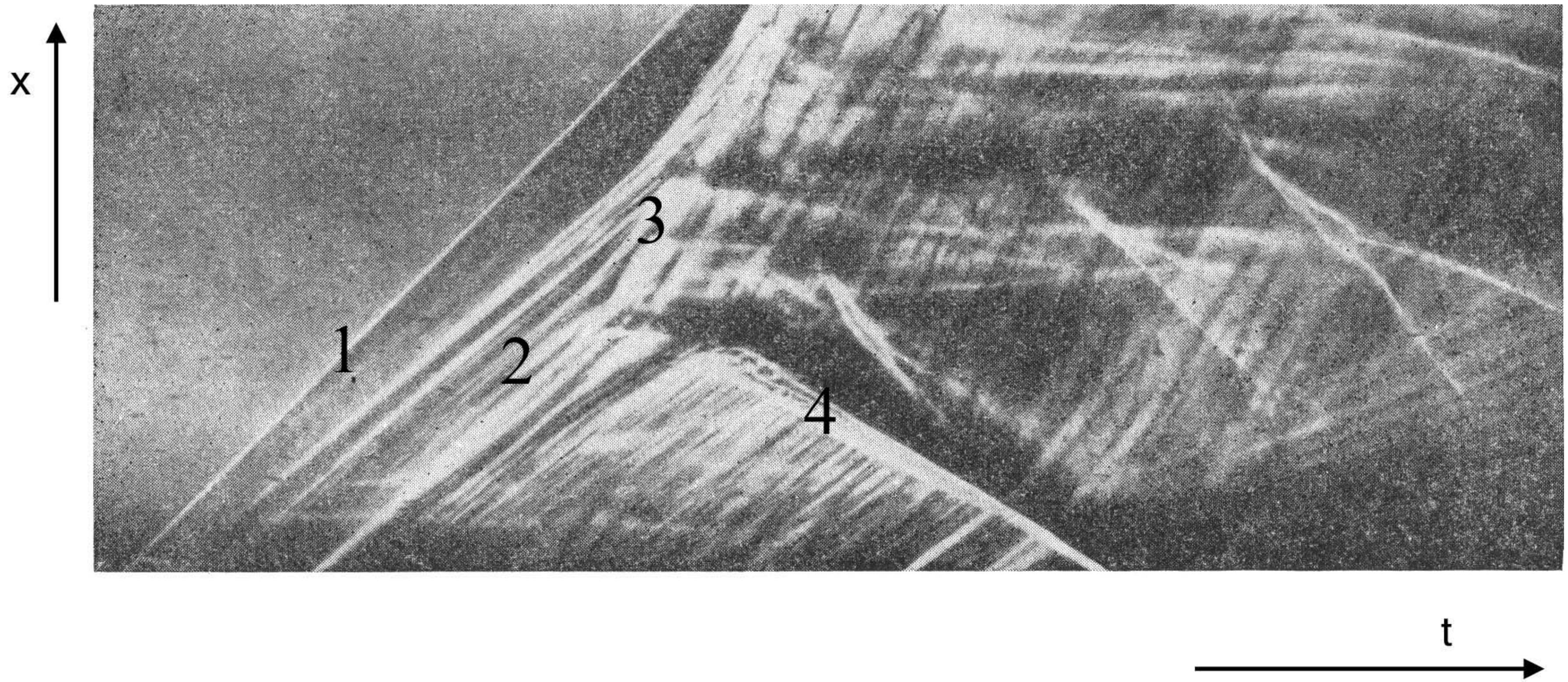




Streak record of flame front and shock waves propagation at detonation formation in the tube

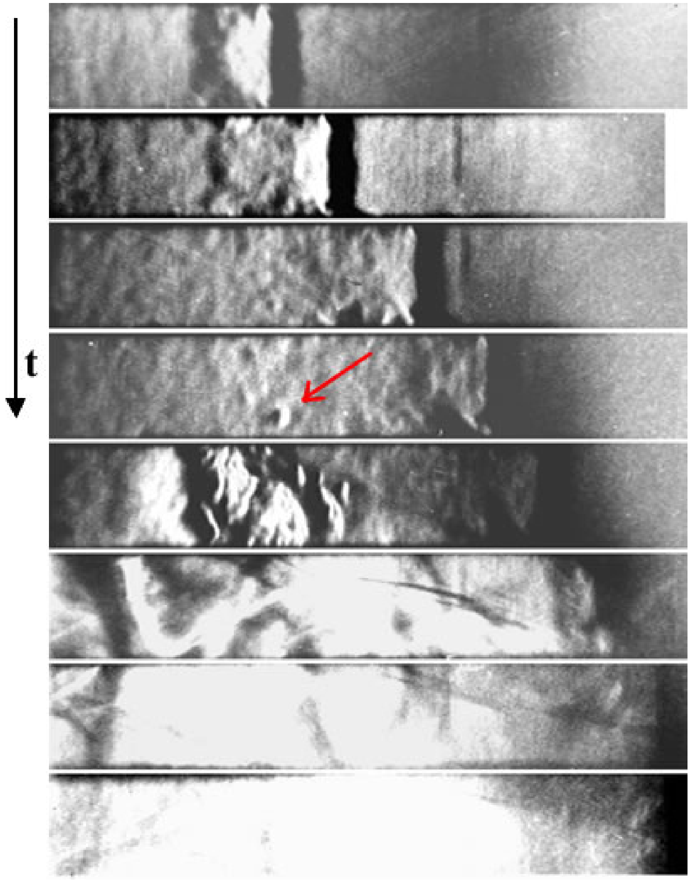
Sequence of schlieren photographs selected from movie showing the flame front propagation. 1, 2, 3, 4 – photo numbers, obtained in different moments from the process beginning

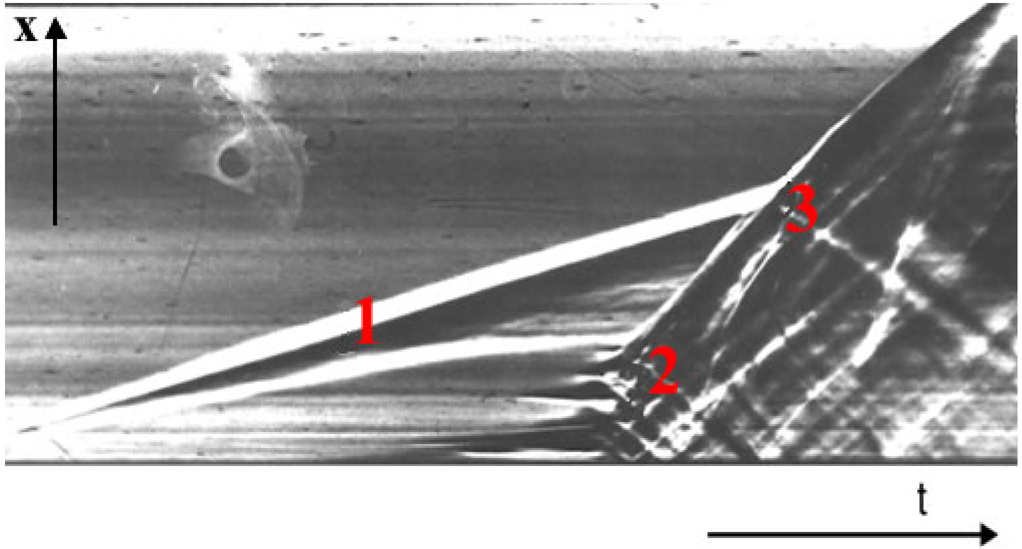
Detonation initiation behind the weak shock waves



Streak record of detonation onset behind the igniting shock wave front ($H_2 + O_2$, $p_0 = 0.1$ bar, $M_0 = 3.8$) 1 – shock wave, 2 – flame spots, 3 – detonation wave, 4 – retonation wave

Detonation formation at shock wave reflection from the tube end

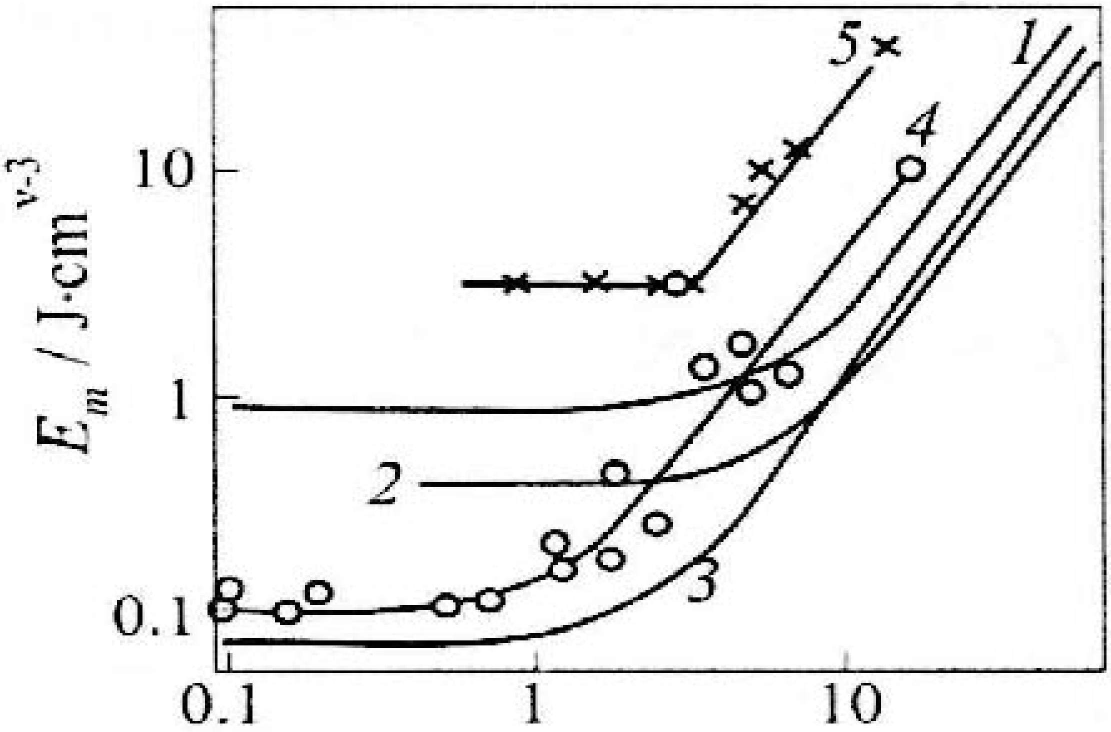




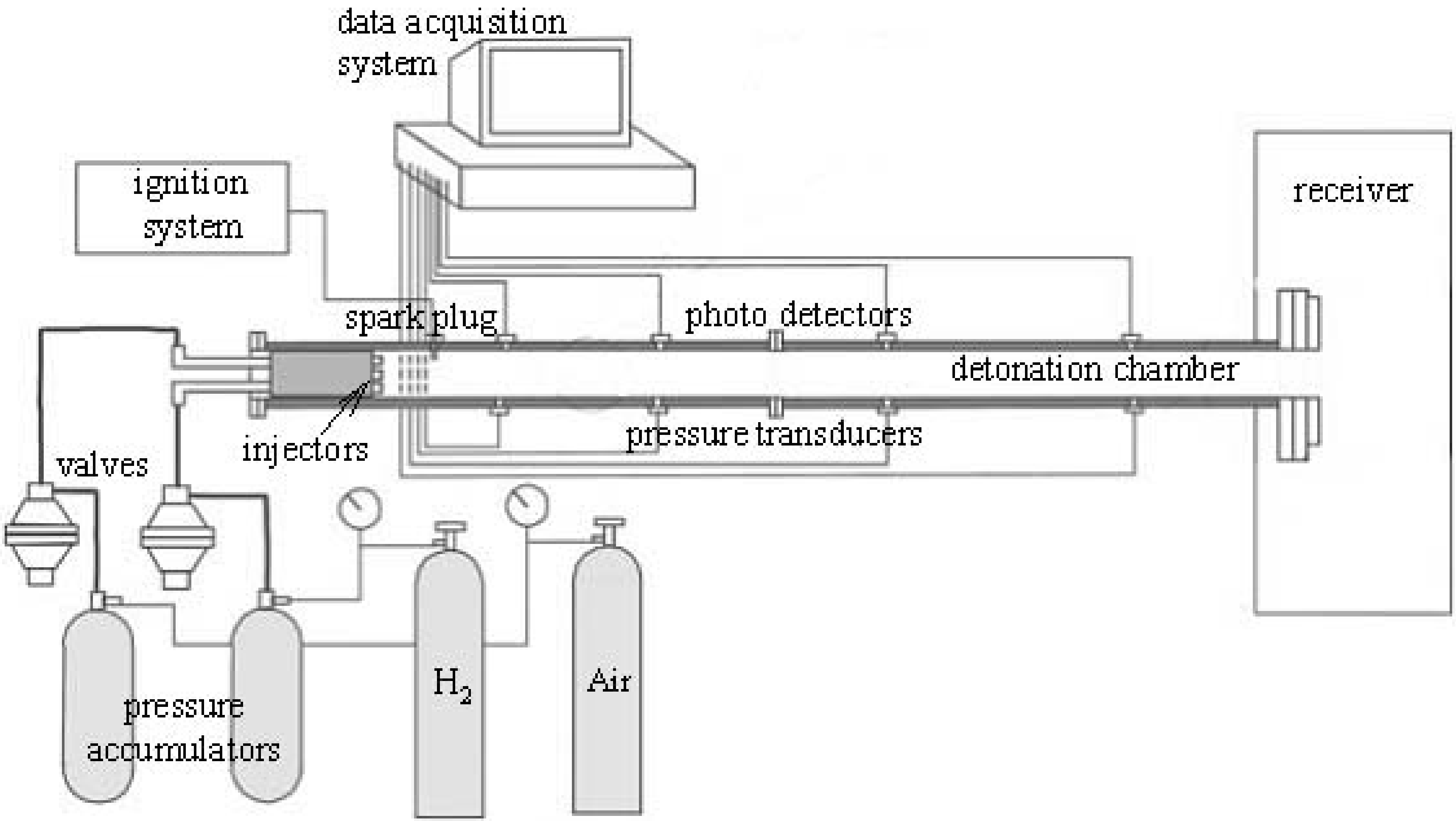
Streak record 1 – reflected shock wave, 2 – ignition spots, 3 – detonation wave, (H_2+O_2, mixture temperature behind the shock wave is equal to 900 K)

Schlieren photographs selected from a movie

Direct detonation initiation behind the strong shock waves

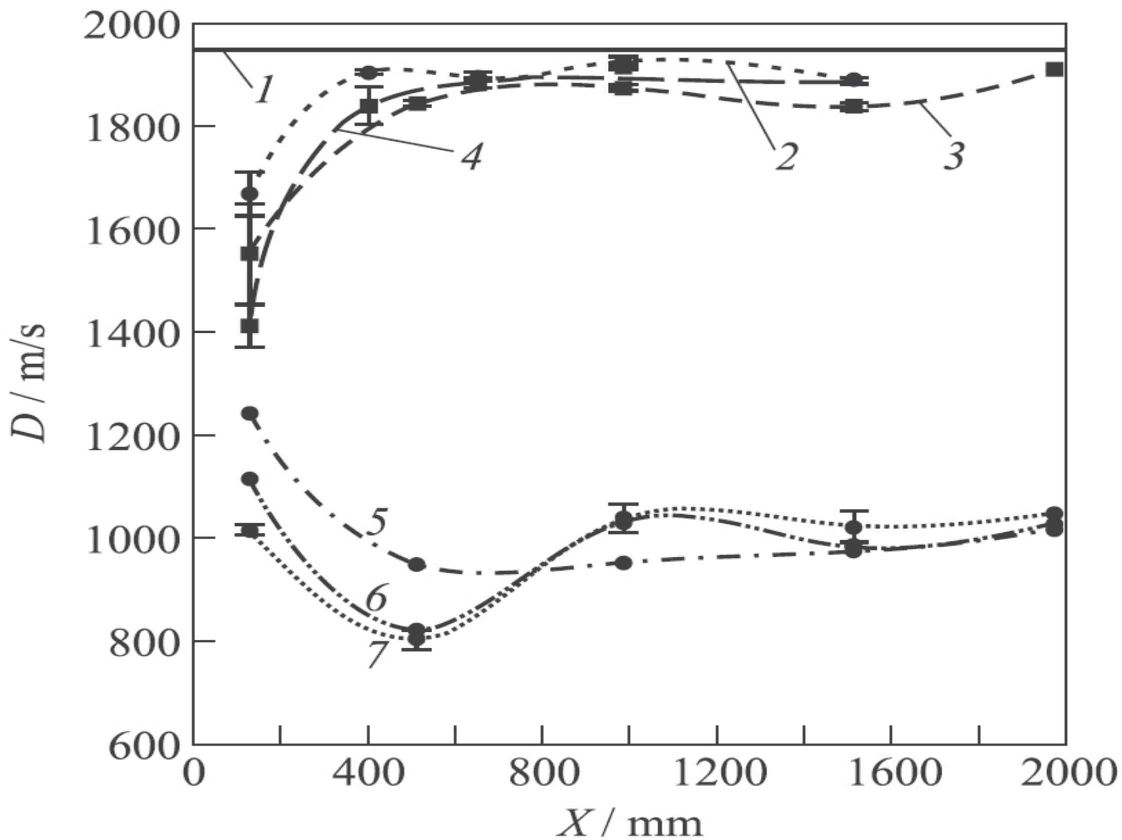


Critical energy of direct detonation initiation E_m as function of energy release time t. ν –energy release zone number of dimensions. Calculations for stoichiometric chlorine-hydrogen mixture. Energy release zone: 1 –cylinder of 2 mm in radius, 2 and 3 – spheres of 2.5 and 1 mm in radii. Experiment with cylindrical zone of energy release in stoichiometric mixtures of acetylene (4) and hydrogen (5) with oxygen



Schematic of the experimental set up

Influence of the initiation source energy on detonation initiation (two different scenarios of detonation formation)

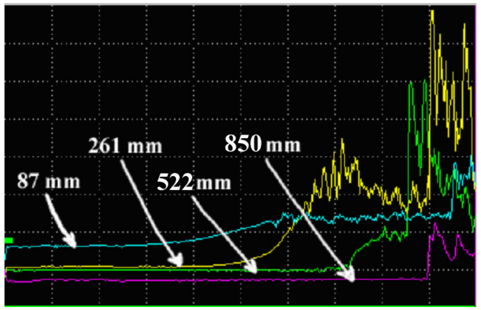


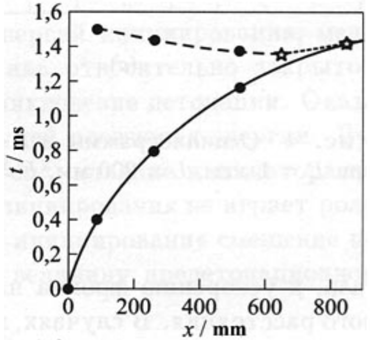
Measured shock and detonation wave velocity diagrams of detonation formation in quiescent H_2-air mixture: 1 – CJ velocity; 2 – E = 1440 J; 3 – 1250 J; 4 – 950 J; 5 – 900 J; 6 – 850 J; and 7 – E = 750 J

$$E_c = 0.91 \lambda \gamma P_0 M_{CJ}^2$$

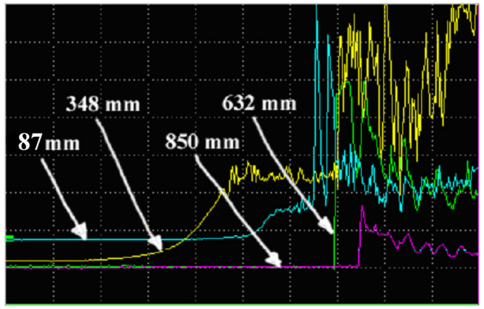
critical energy of direct planar detonation initiation, where λ is detonation cell size, and γ - detonable mixture specific heat ratio and pressure, M_{CJ}- CJ detonation Mach number

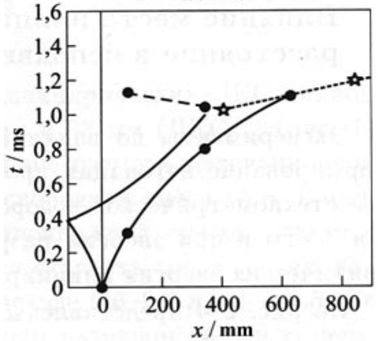
Dependence of detonation onset length on the ignition source location



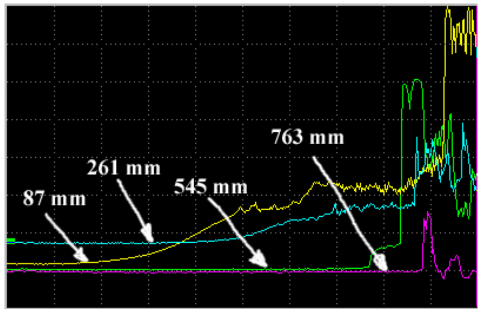


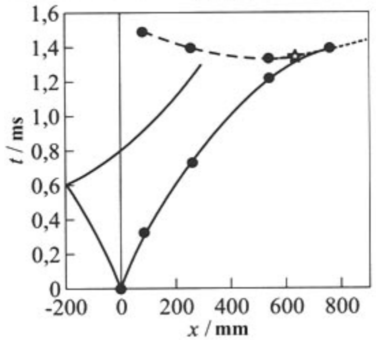
When L/d lower than 1.2 the shock wave have no time to form and reflect from the closed end of channel.





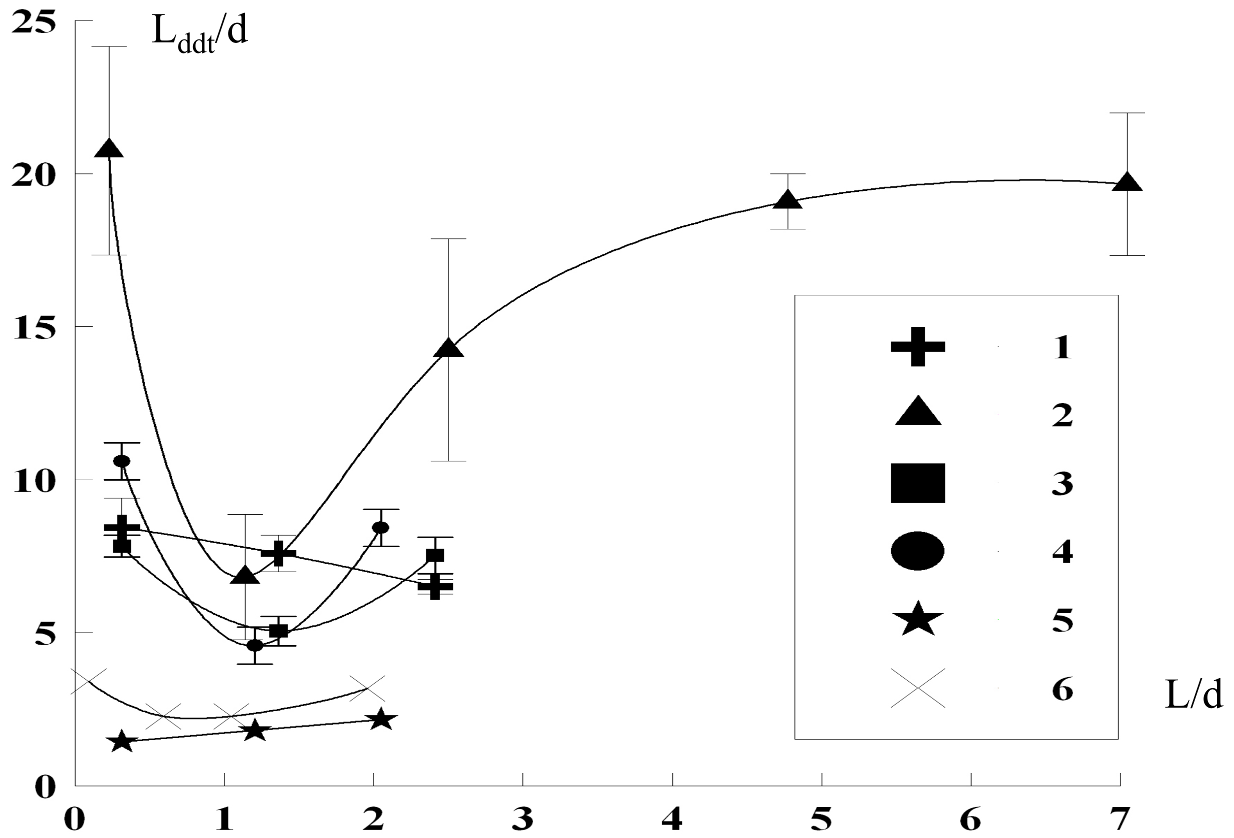
When L/d is equal to 1.2 the shock wave front catch up with the flame and the detonation arises. Predetonation length in this case is minimal.





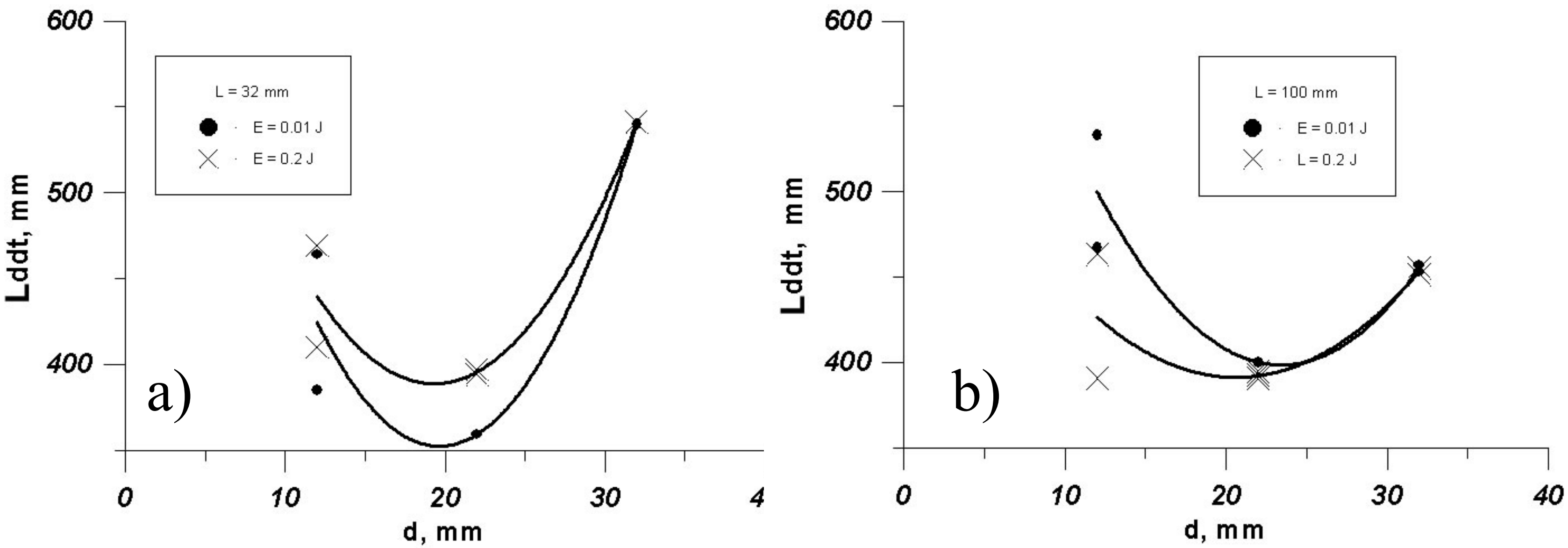
L/d higher than the 1.2 the shock wave front is not able to catch up with the flame before the detonation onset.

Dependence of predetonation distances Lddt on the distance L from spark plug to the detonation chamber closed end



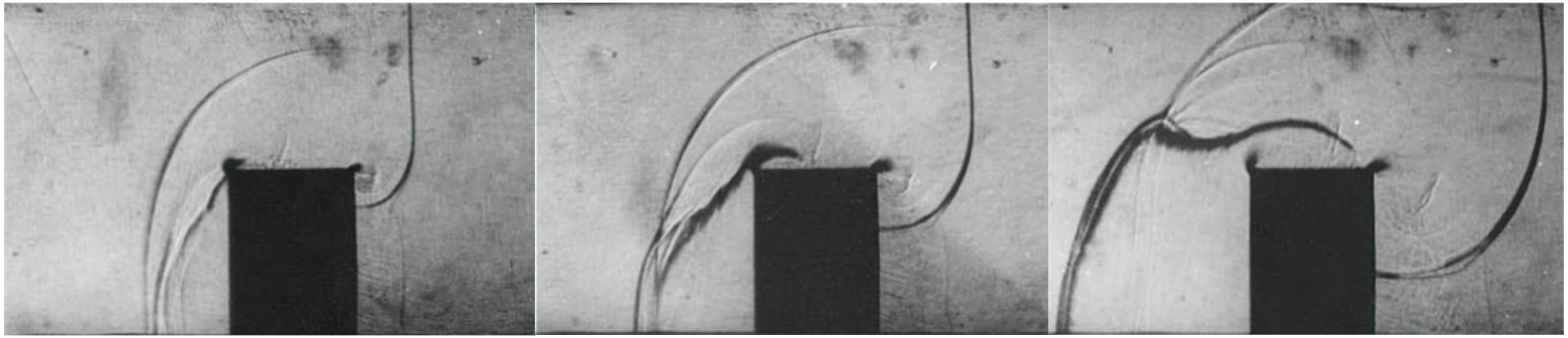
d - internal diameter detonation chamber. 1 - d = 83 mm, P = 1 atm., E = 0.2E_{cr}; 2 - d = 22 mm, P = 1 atm., E = 0.02E_{cr}; 3 - d = 83 mm, P = 1 atm., E = 0.1E_{cr}; 4 - d = 83 mm, P = 1 atm., E = 0.006E_{cr}; 5 - d = 83 mm, P = 3 atm., E = 0.009E_{cr}; 6 - d = 22 mm, P = 3 atm., E = 0.03E_{cr}

Influence of sidewall on DDT length in tube



Dependences of detonation onset length on the distance between the discharge gap and sidewall. a – L=32 mm, b – L=100 mm [43].

Detonation initiation by shock reflection from rectangular obstacles



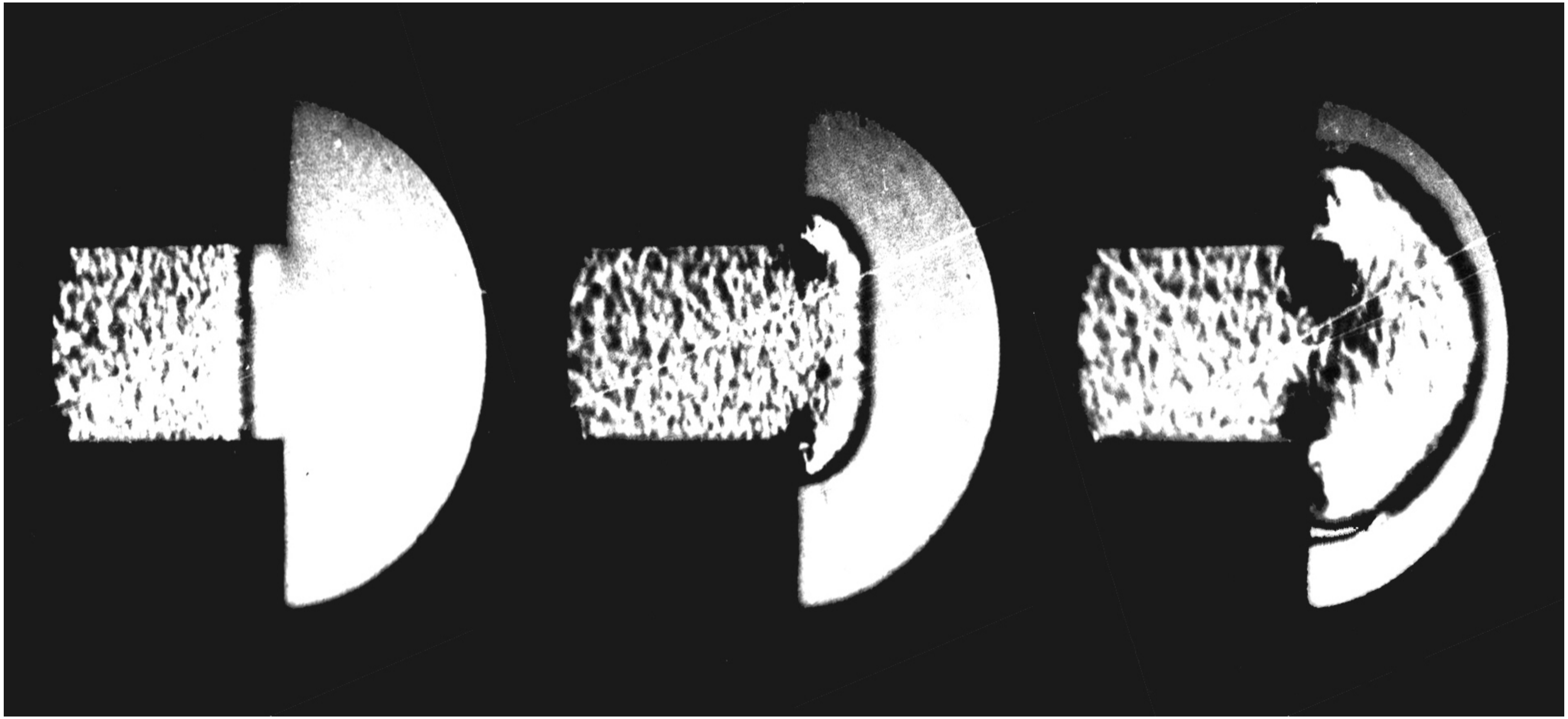
Sequence of schlieren images of shock wave reflection and detonation front growth with $2H_2 + O_2$ + 80%Ar.
$M_s = 2.48, P_0 = 5.26$ kPa, $\Delta t = 10$ μs

$$\eta = \frac{h}{a_r \tau_r}$$

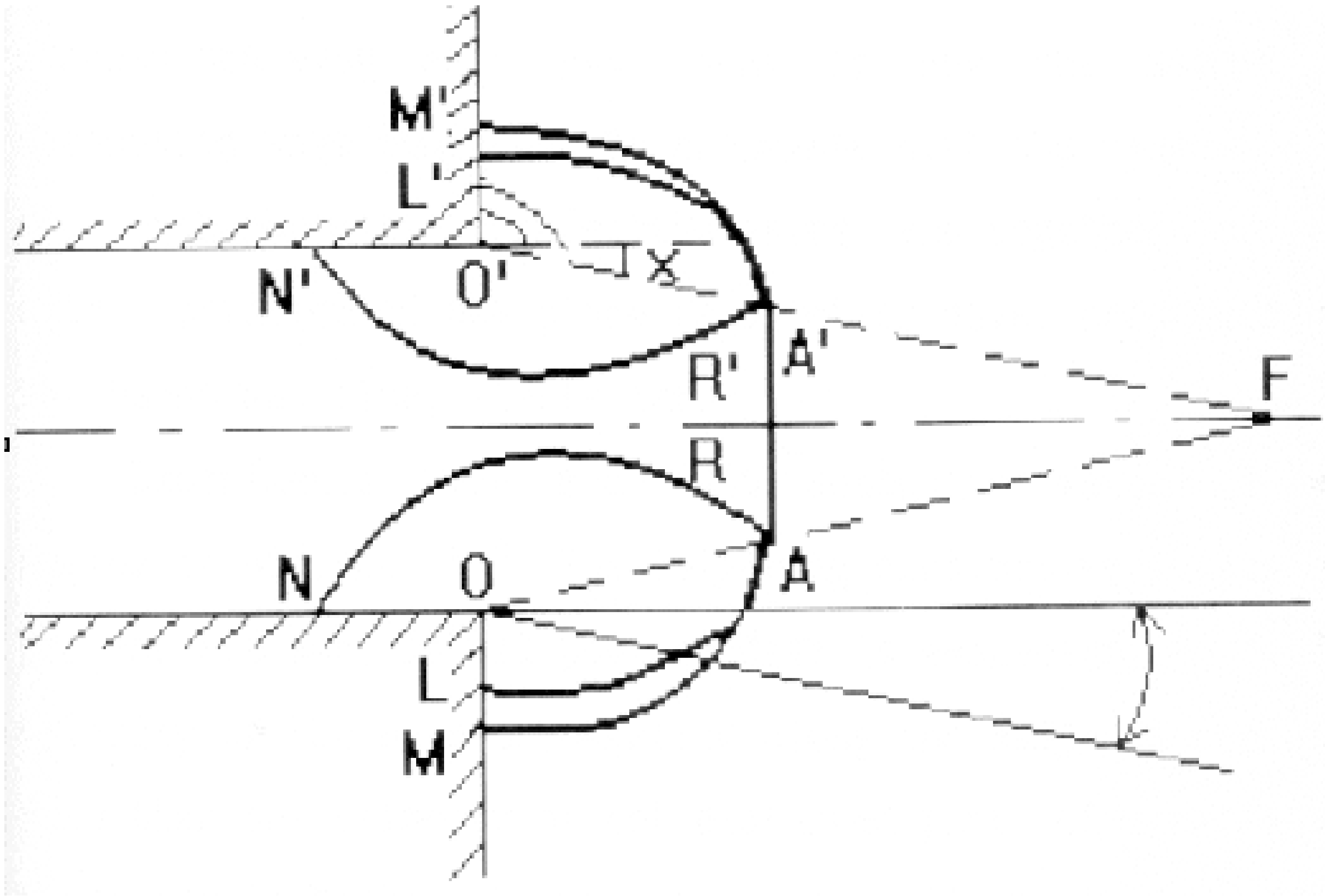
h - height of the obstacle, a_r and τ_r - the sound speed and ignition delay time in the undisturbed reflected shock region respectively

Detonation diffraction

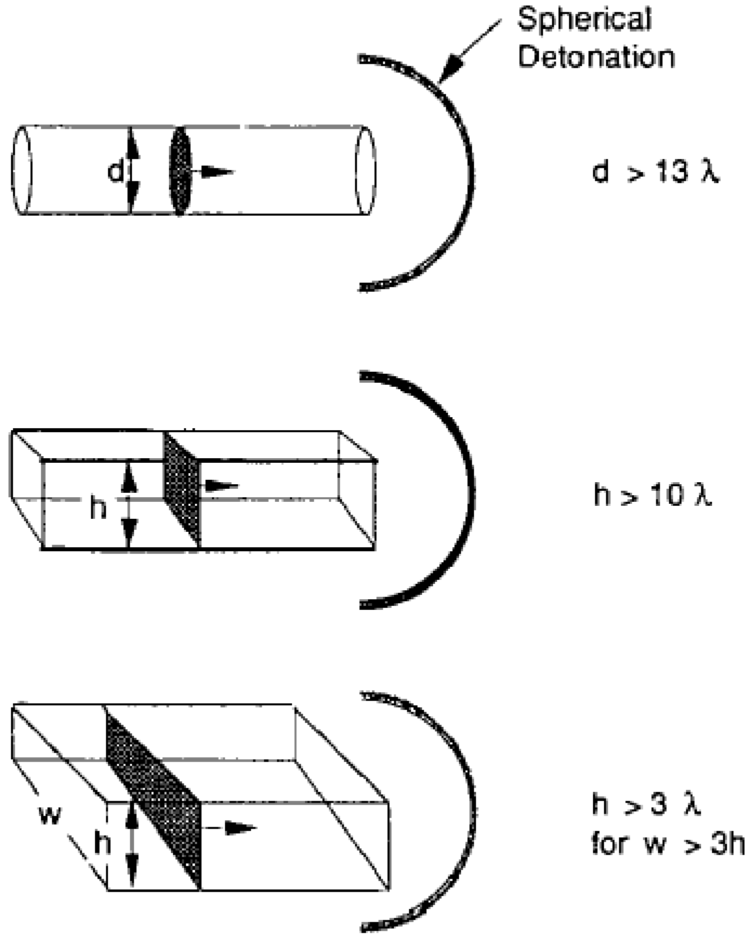
Detonation diffraction



Sequence of schlieren photographs showing detonation diffraction on the right angle in CH_4 + $2O_2$ mixture at initial pressure of 1 bar

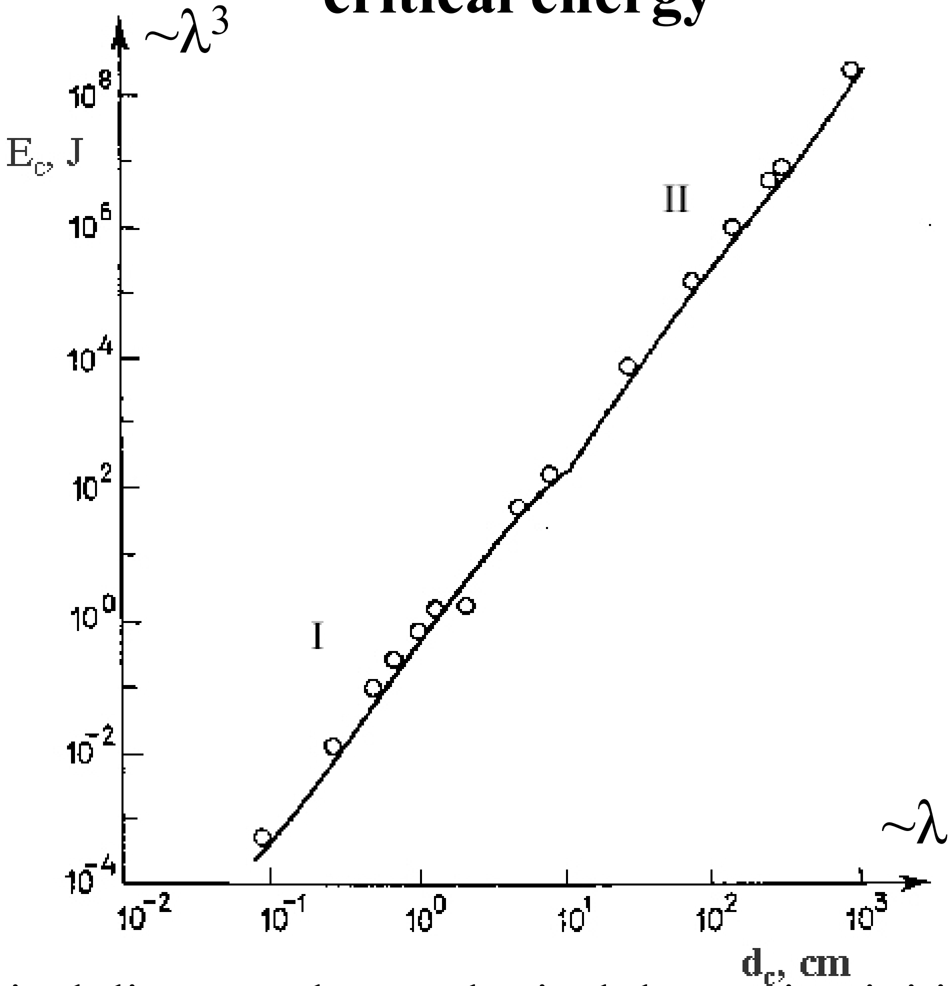


Schematic of detonation waves diffraction. M'A'AM – diffracted wave front, ARN and A'R'N' – fronts of reflected rarefaction waves, χ- angle of points A A' propagation



Requirements for successful transmission of a planar detonation into an unconfined three dimensional spherical detonation wave

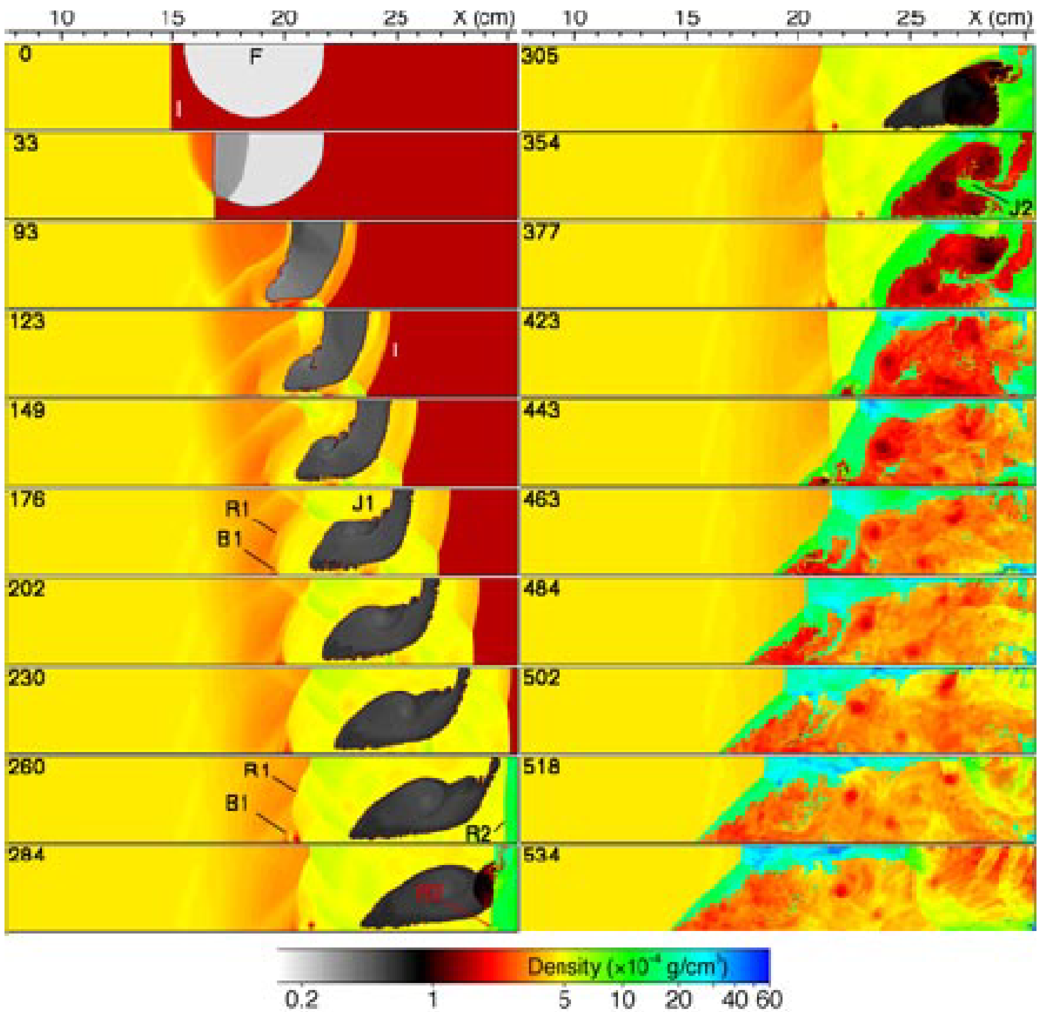
Correlation of diffraction critical diameter with detonation initiation critical energy



Dependence of critical diameter d_c on spherical detonation initiation critical energy E_c in mixtures of hydrocarbons with oxygen (I) and air (II)

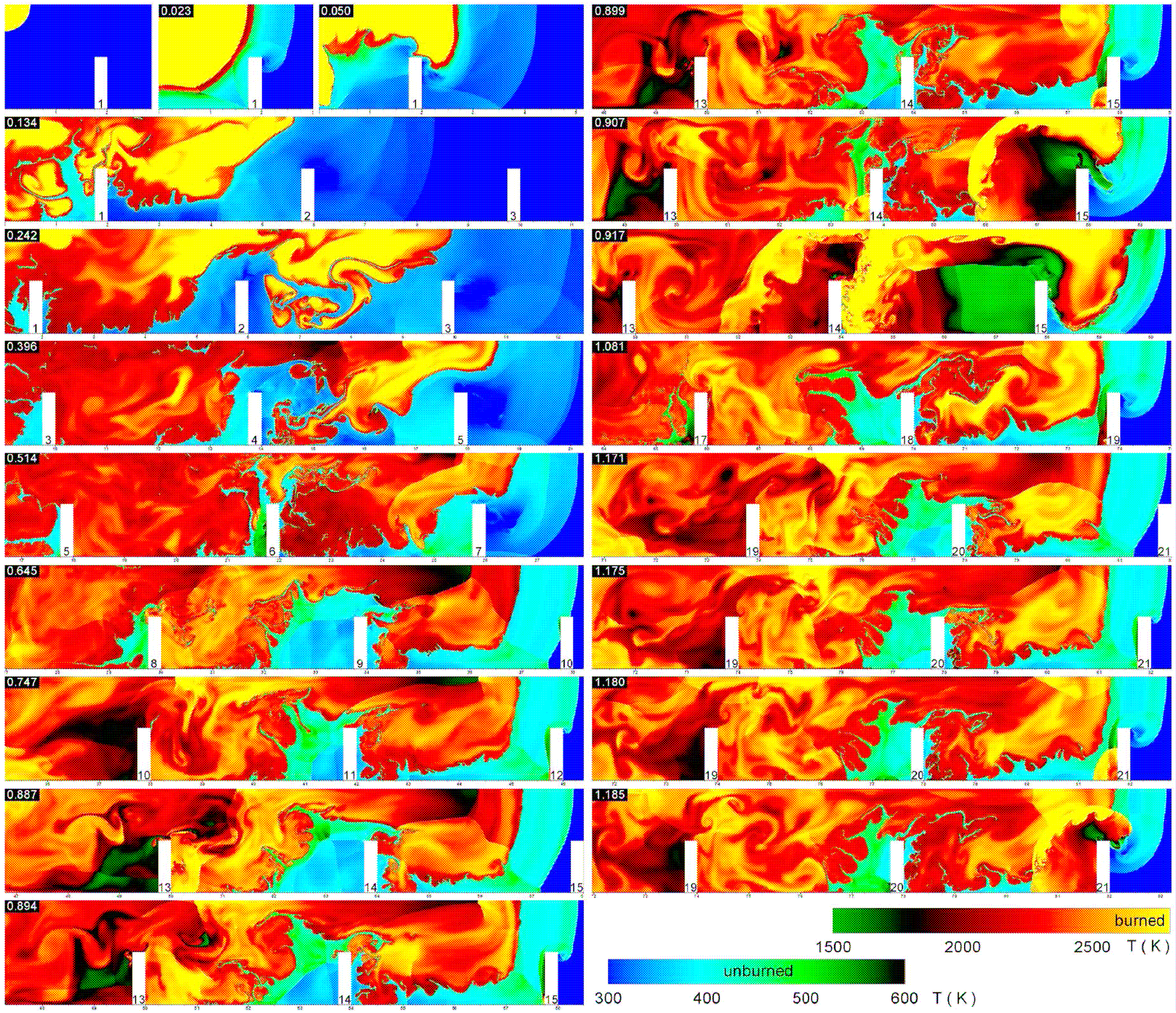
Numerical simulations of the detonation formation

Detonationless supersonic combustion formation at the interaction of shock wave with flame



Calculated density fields showing the formation of supersonic combustion in ethylene/air mixture. Supersonic flame is forming after 450 μs. Intensity of incident shock wave Ms = 1.8. Time (μs) indicated in left top corner of each frame. Letters show incident shock wave (I), flame (F), reflected waves (R1, R2), fresh mixture pockets (J1, J2), and bifurcation structures (B1, B2), Oran E.S., 2003

Flame acceleration in the encumbered tube

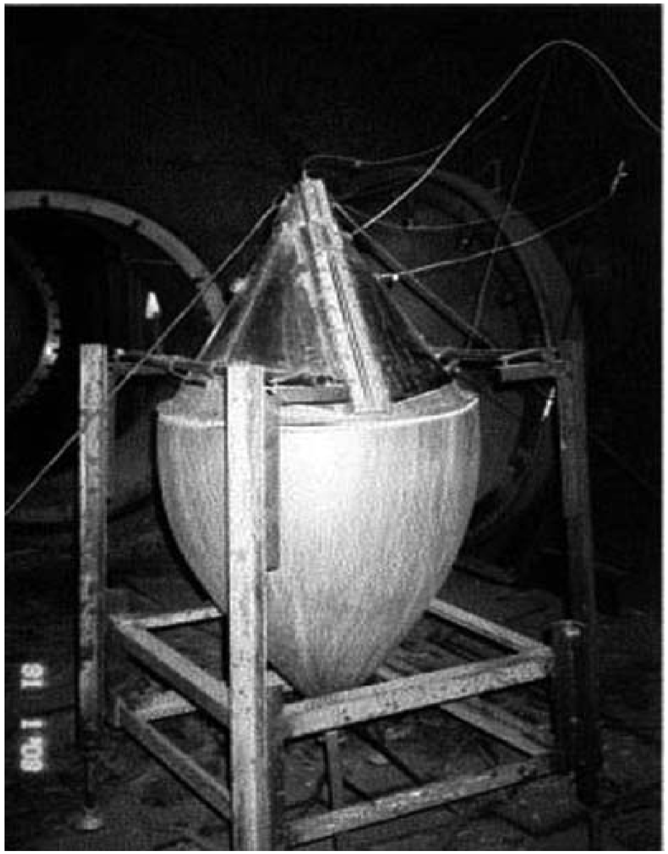


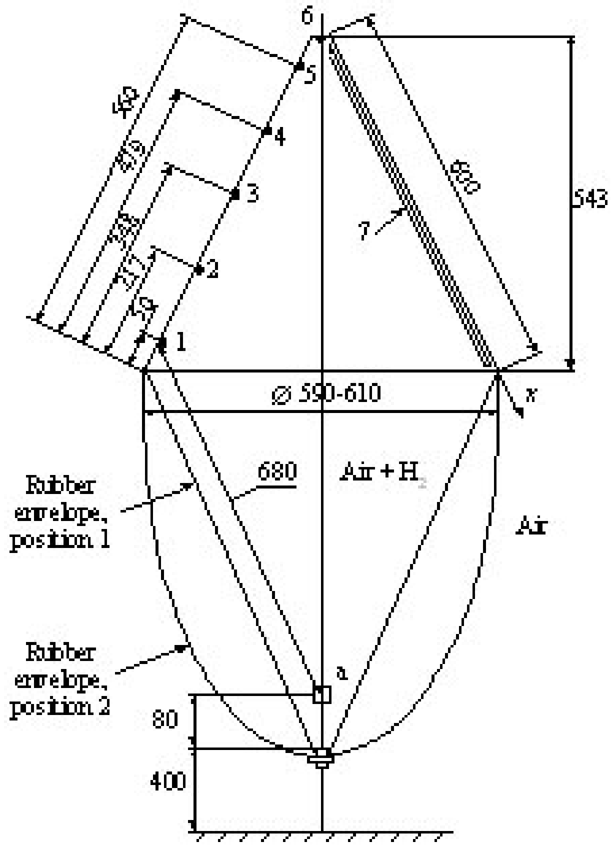
- Obstacles create velocity gradients and reflect shocks
- Velocity gradients and shock-flame interactions increase the flame surface area
- Burning rate increases, shocks become stronger

Calculated temperature fields showing flame acceleration in hydrogen/air mixture (Gamezo V.N. and Oran E.S., 2007)

Experimental and numerical research on large-scale combustion and detonation in confined volumes up to 900 m^3 for different conditions

Formation and development of combustion processes in conic cavity



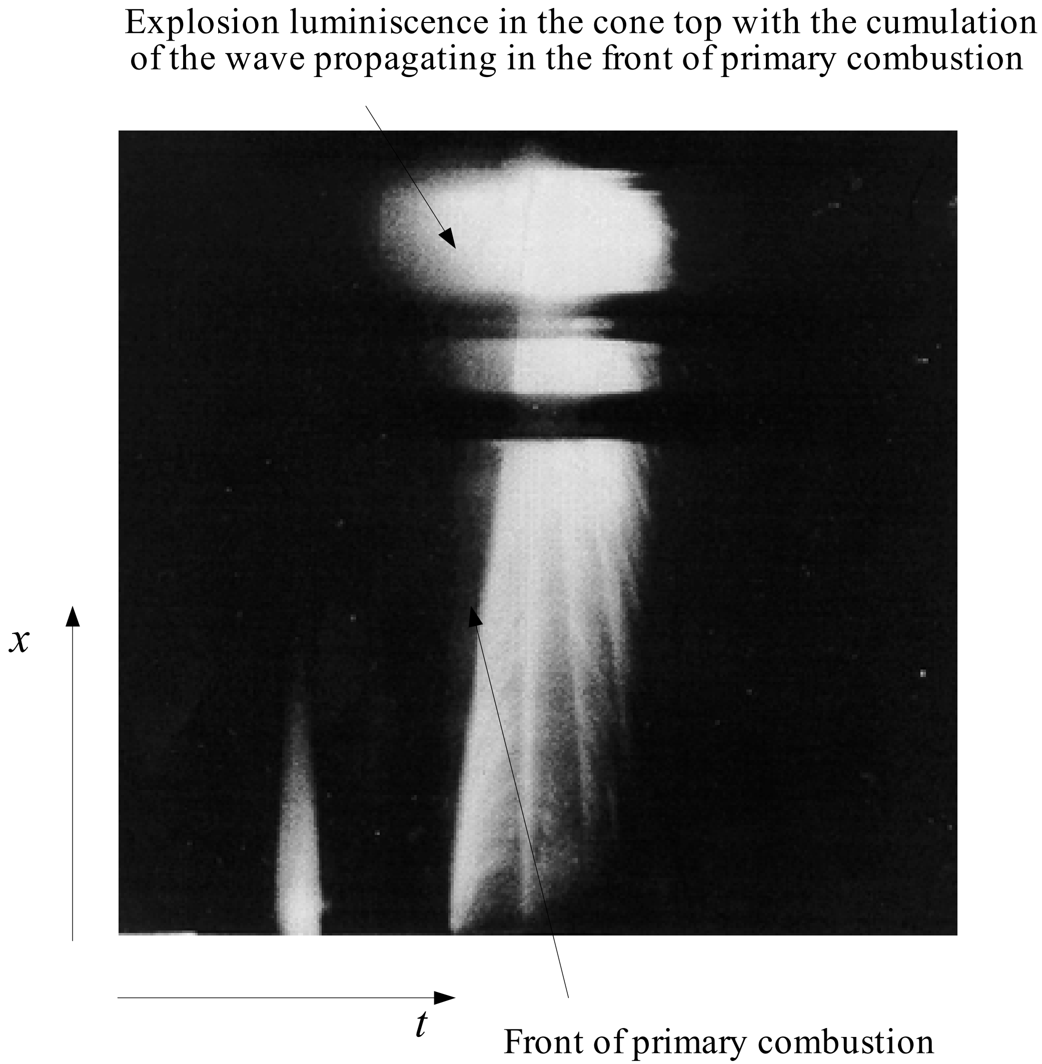


General view and scheme of experimental conic volume.
1-6 – pressure sensors, 7 – window-slot for high-speed photography (all dimensions are in mm)

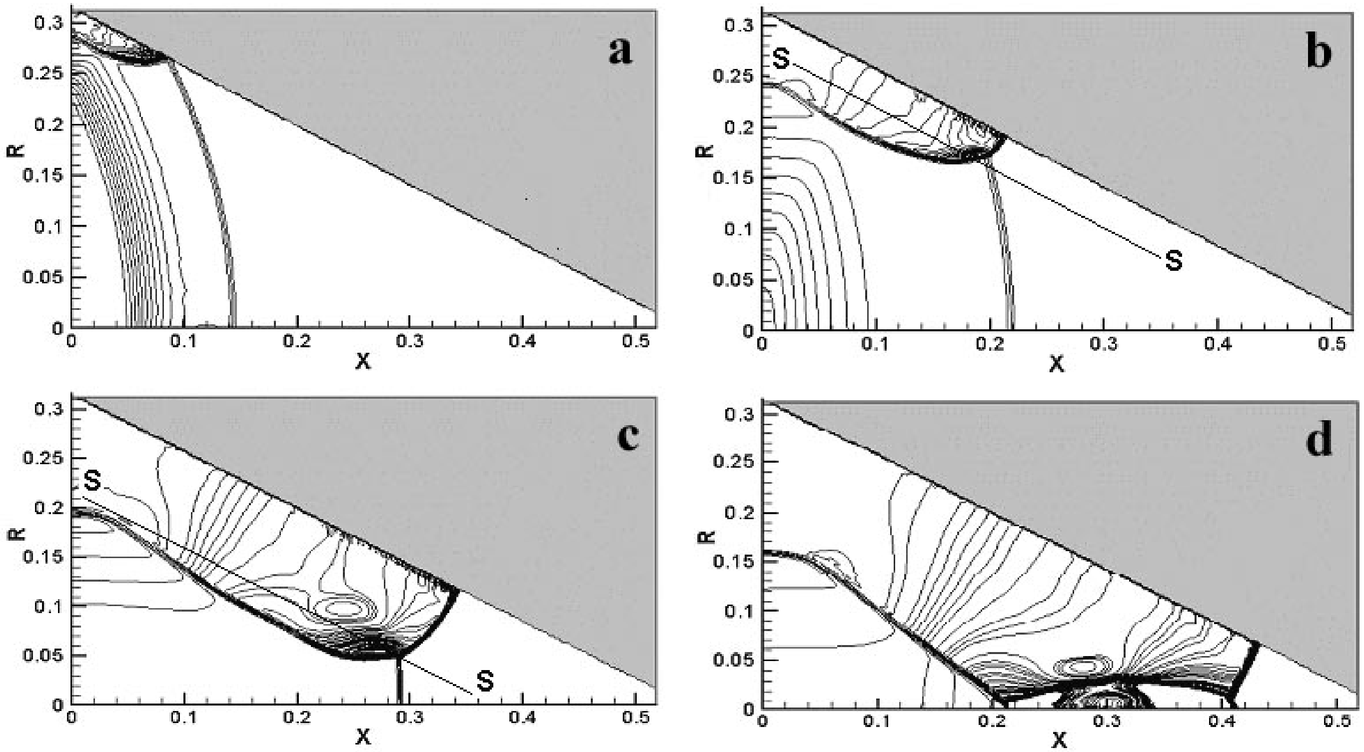
Formation and development of combustion processes in conic cavity

Parameter	Experiment #							
	1	2	3	4	5	6	7	8
Time t_1 of wave arrival to sensor *1*, µs	327	310	331	331.5	320	335	–	346
Pressure P_1, registered by sensor *1*, atm	56.7	42.2	56.7	40.0	47.8	51.2	–	41.4
Time t_6 of wave arrival to sensor *6*, µs	530	519	534	531	539	537	530	551
Pressure P_6, registered by sensor *6*, atm	625	515	1028	810	582	978	766	830

The pressure registered by sensors 1 and 6 for the stoichiometric hydrogen-air mixture and the realization time (process initiation by explosion of 3.5 g of RDX (hexogen)).



Luminescence propagation of a in the focusing zone of the cone

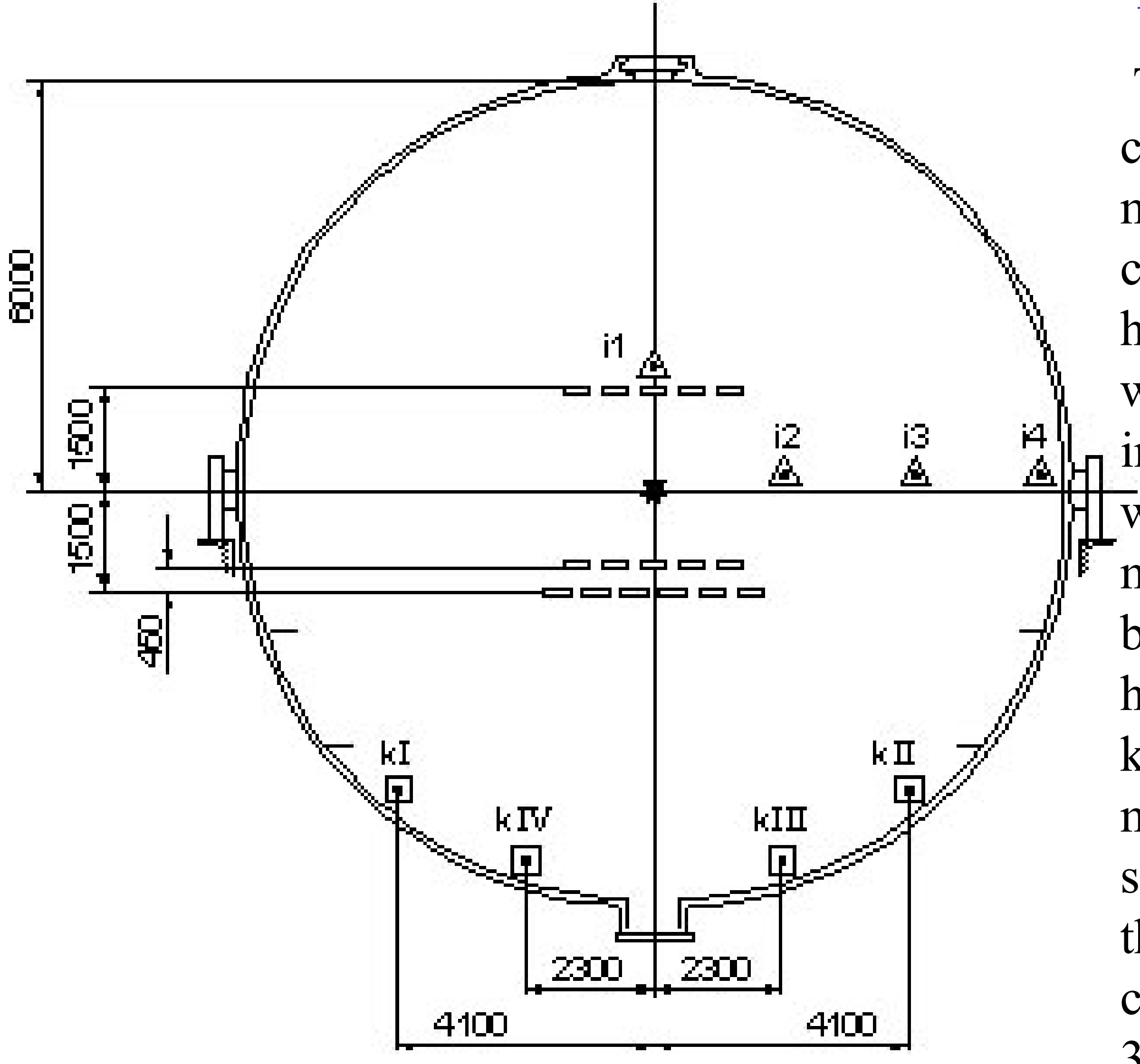


Pressure isolines in the cone cross section at different time moments (a – t = 0.05 ms; b – t = 0.125 ms; c – t = 0.2 ms; d – t = 0.25 ms).

The maximum pressure, obtained in this configuration, reached 1900 atm.

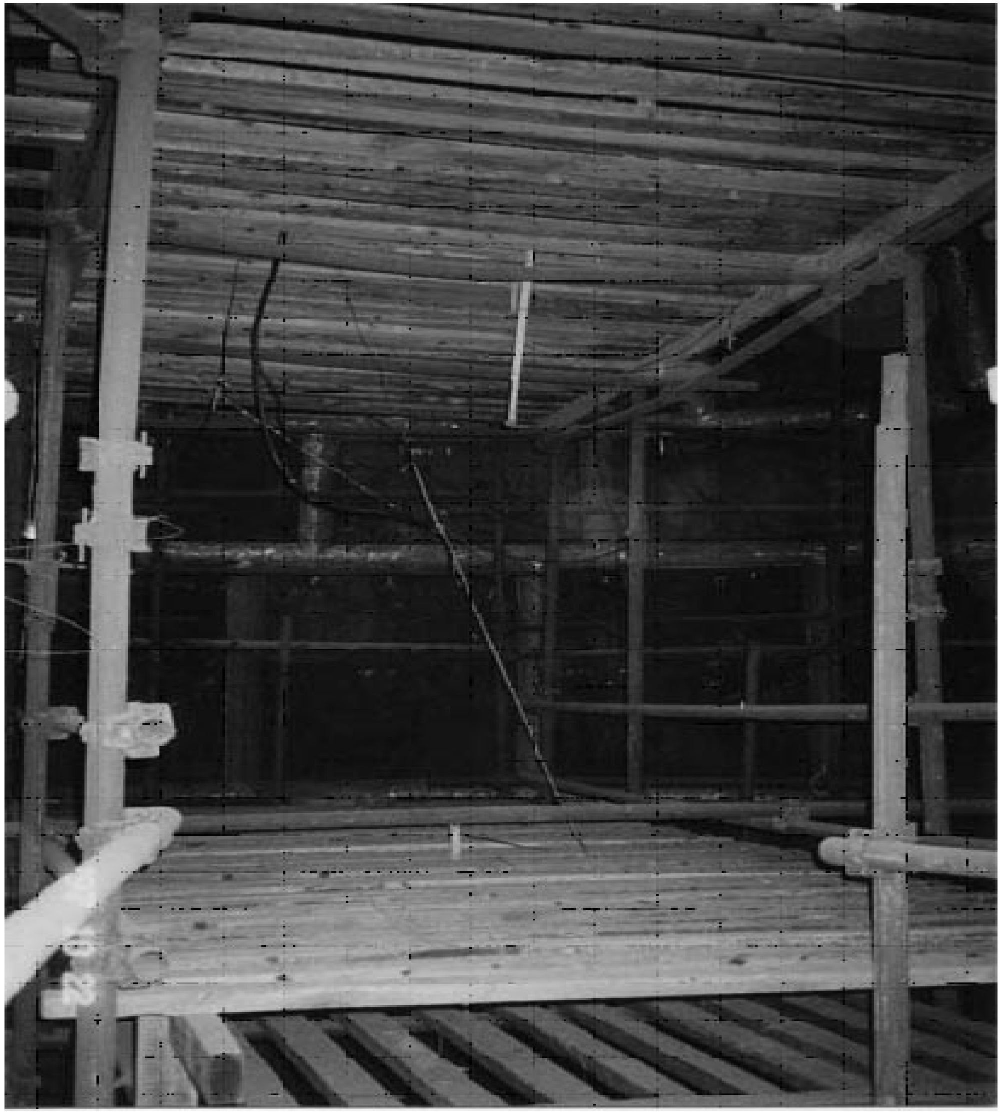
(Ivanov M.F., 2007)

Experiment in a spherical chamber of large volume

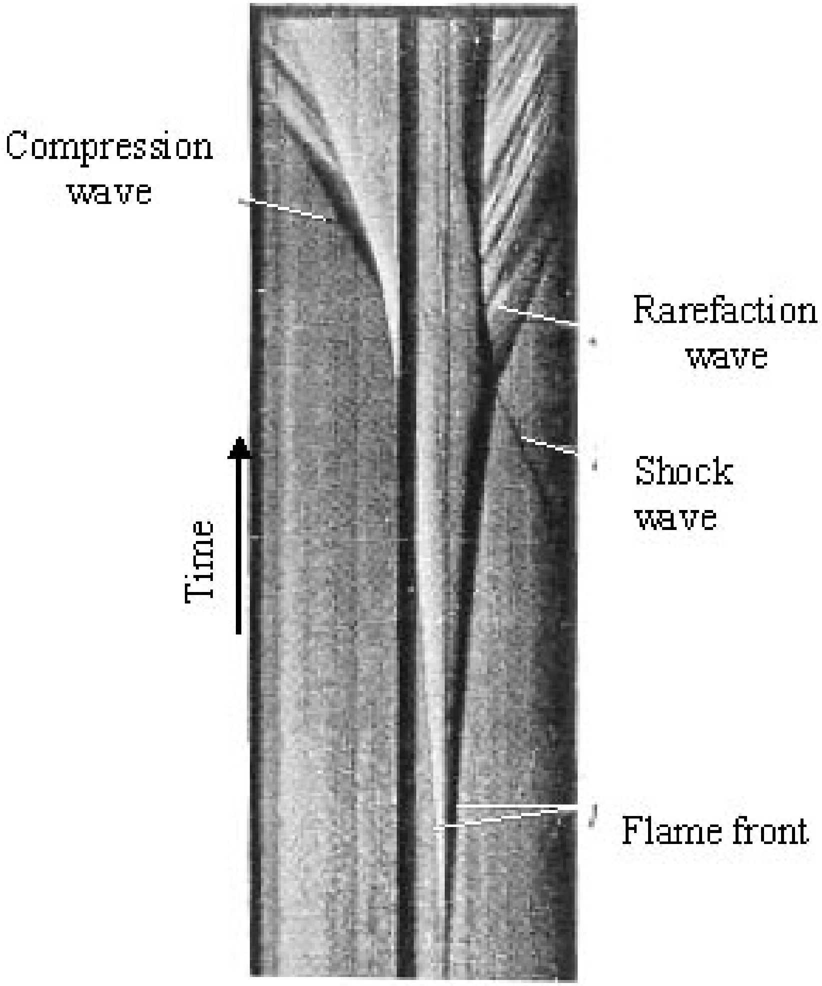


Scheme of sensor arrangement in the explosive chamber (all dimensions are in mm)

The mixture pressure in the chamber was 1.4 atm, and the mixture had stoichiometric composition. Measuring hydrogen contents in the mixture, which was carried out repeatedly in the course of 100 hours during which the mixture was maintained, showed that in the bottom part of the chamber, the hydrogen concentration steadily kept the value of 25.4%. The mixture must have been stratified, and in the top part of the chamber the hydrogen concentration could have reached 32.6%.



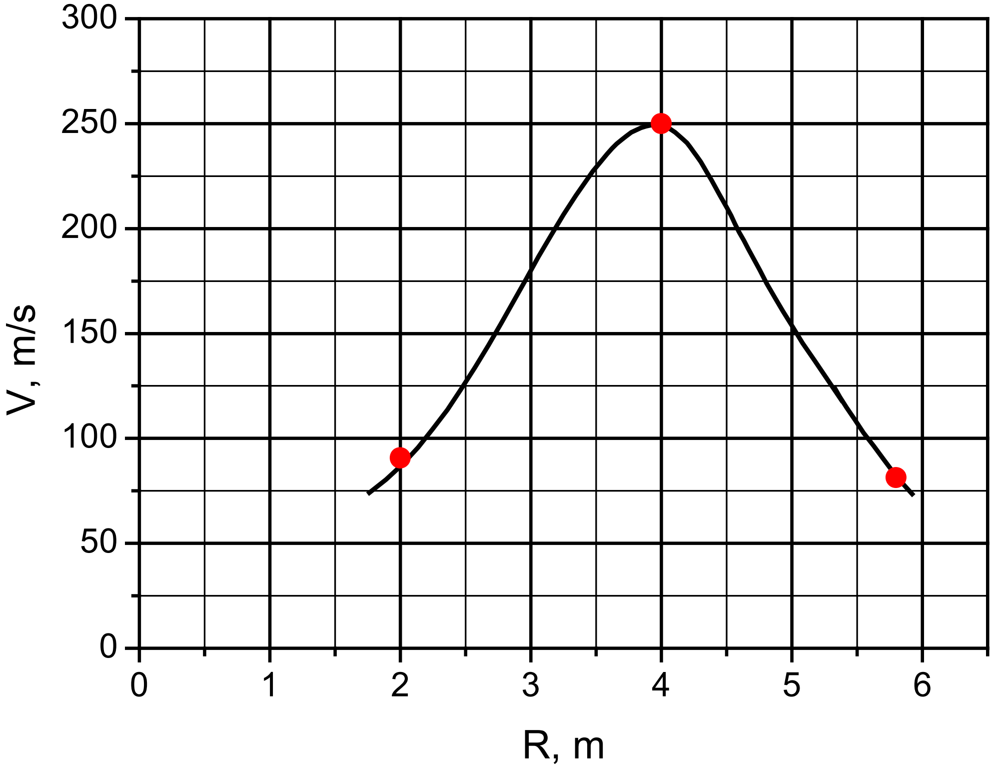
Chamber interior before the experiment



At the ignition of a mixture in the center of the chamber, there are weak shock waves formed which, being reflected from the wall, three times interact with the flame front and amplify due to reaction intensification. The amplified wave is reflected from the wall before a wave of primary combustion reaches the wall; secondary combustion is initiated, turning into an explosion similar to that observed in the shock tube.

Interaction of shock wave with the flame front
(Salamandra and Sevastyanova, 1963)

Flame acceleration in a large volume

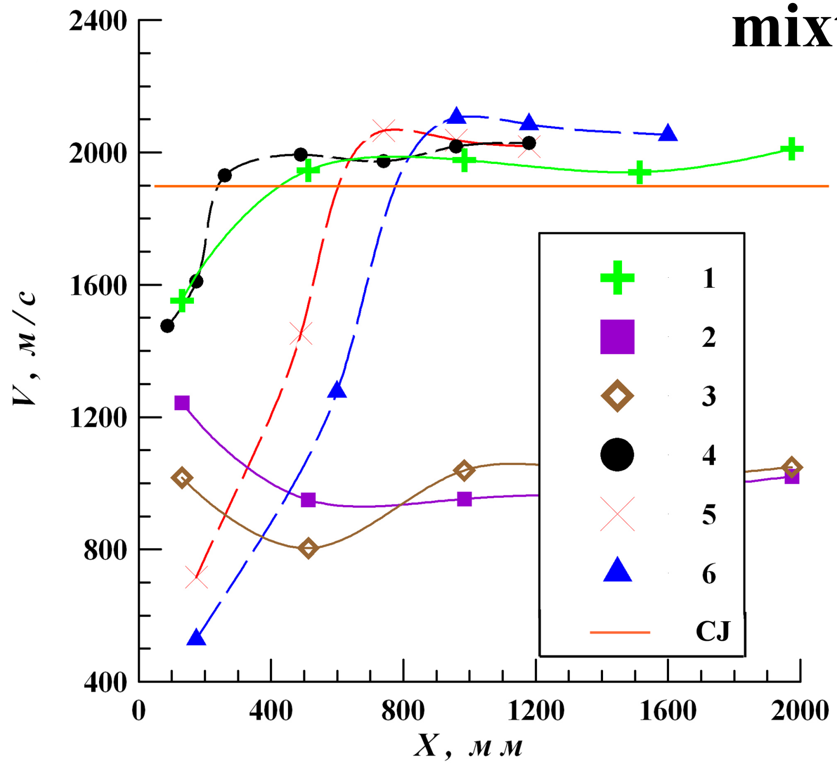


Velocity of flame front propagation inside the chamber

A considerable acceleration of flame accompanied by its turbulization and formation of shock (instead of transonic) waves, which noticeably change the parameters of the environment ahead the flame. Due to a higher velocity, these waves repeatedly interact with the wall. Disturbances in the medium and its heating not only cause the change of flame propagation regime, but also create conditions for initiation of ignition centers and explosion before primary flame front, which is similar to what was observed in top area of the conic cavity.

Detonation initiation in flow

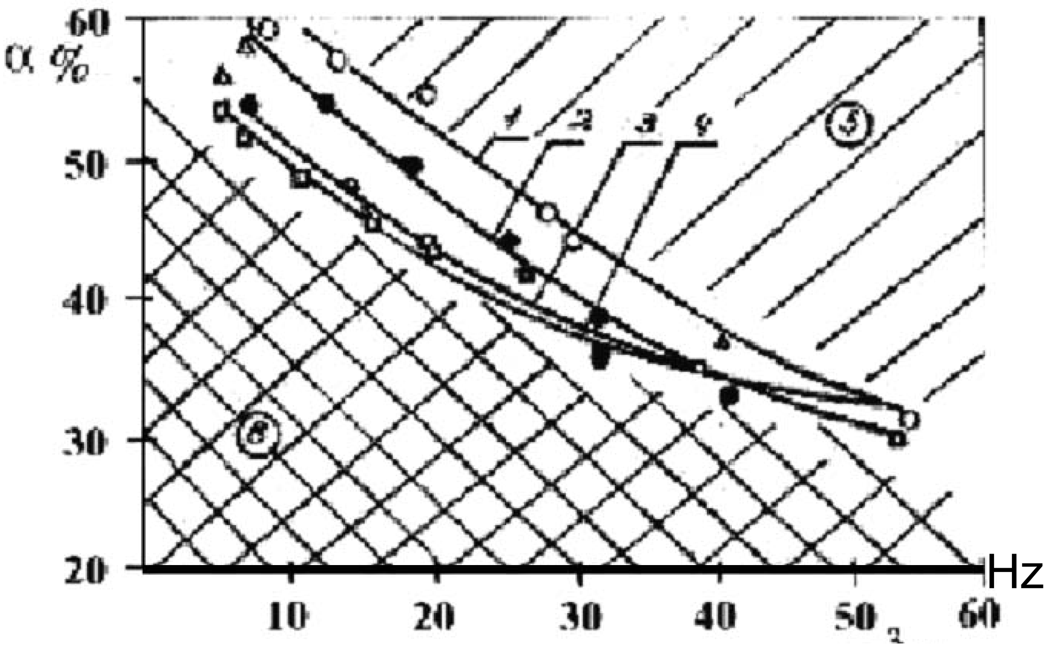
Dependence of detonation onset length on the initiation source energy in quiescent and moving mixtures



Velocities of shock and detonation waves in quiescent (1,2,3) and moving (4,5,6) mixture. 1 – E=1.35 E_{cr}, 2 – 0.97 E_{cr}, 3 – 0.65 E_{cr}, 4 – 0.95 E_{cr}, 5 – 0.5 E_{cr}, 6 – 0.25 E_{cr}

In “moving mixture” (50 m/s) 25% of E_{cr} is enough for direct detonation initiation.

Dependence of detonation onset length on the flow velocity



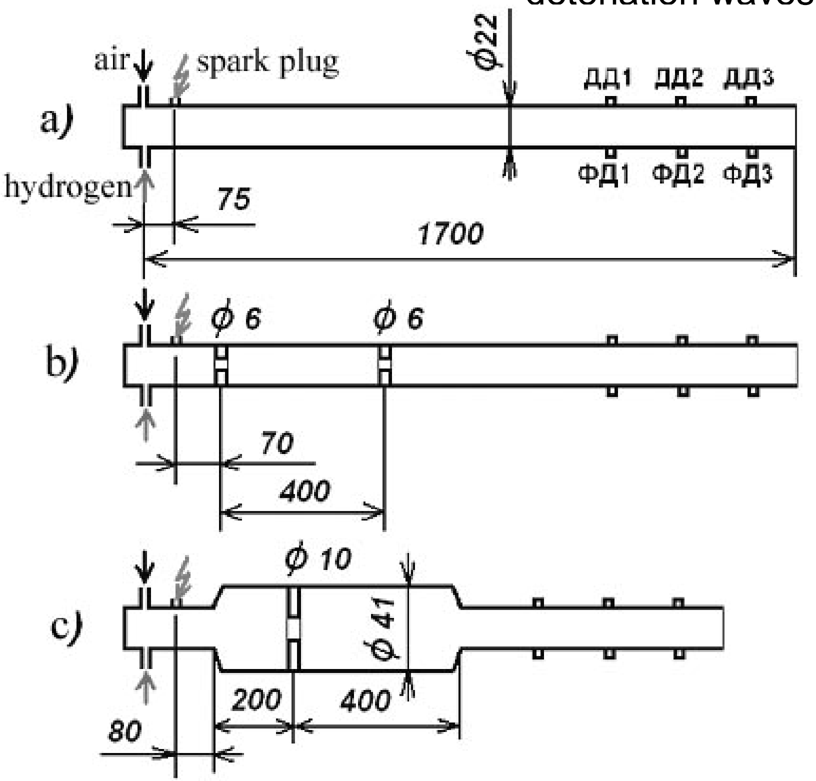
Limit values α as function of Re: 1 – ER = 0.625, 2 – ER = 0.71, 3 – ER = 1, 4 – ER = 1.2. Region 5 – detonation, 6 – no detonation

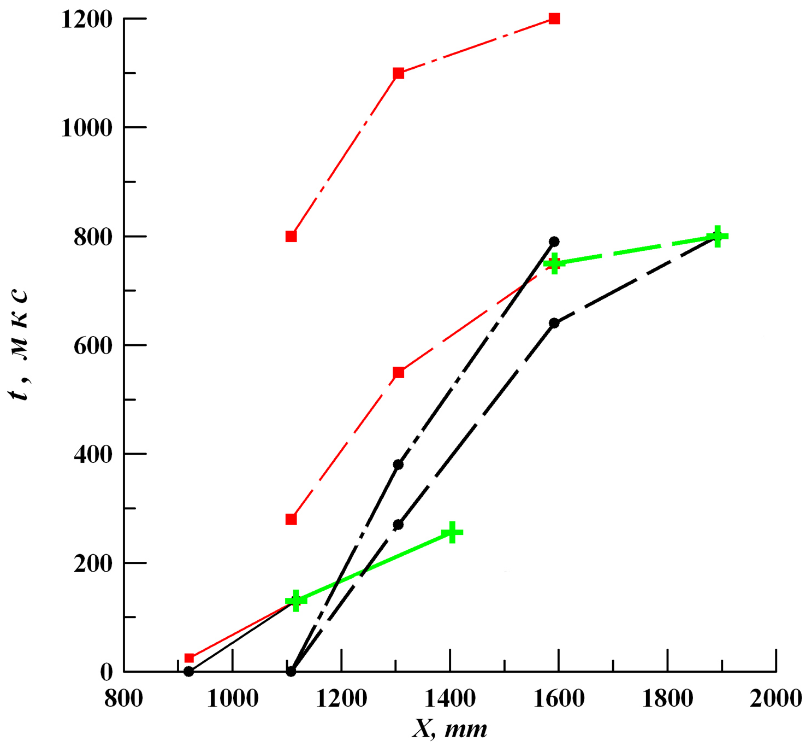
At the detonation formation in the flow of combustible mixture, flow characteristics may affect the detonation onset length and parameters. The influence of flow turbulence on deflagration-to-detonation transition was investigated experimentally in moving $CH_4+O_2+N_2$ mixtures in detonation chamber of 7 m in length and 36 mm in diameter. Methane/air mixtures of various ratio α enrichment with oxygen,

$$\alpha = Q_{O_2} / (Q_{O_2} + Q_{N_2}) \cdot 100\,\%$$

Influence of ring obstacles and expansion chambers on detonation formation

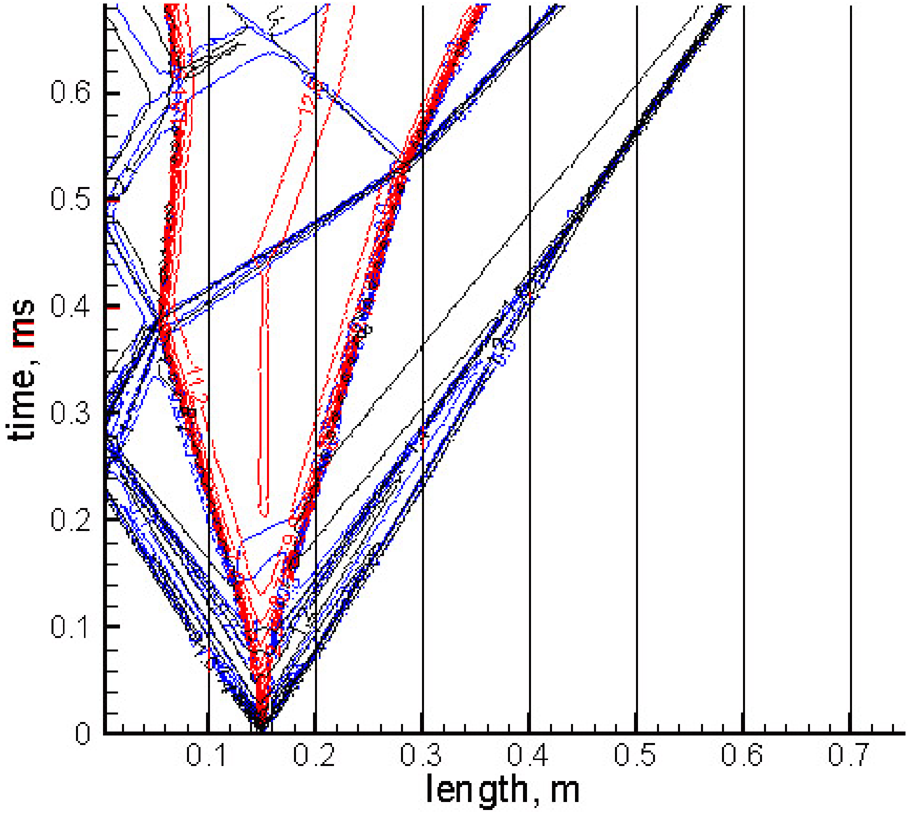
Detonation chamber schemes (left) and x-t-diagrams of flame fronts (red lines), shock waves (black lines) and detonation waves (green lines) (right)





Arrangement in the channel with the stoichiometric hydrogen-air mixture of annular obstacles with blockage ratio of 0.92 and extension chambers with extension ratio of 2.56 can cause the decrease of predetonation distance more than 2 times.

Numerical simulations of detonation formation in quiescent and moving mixture

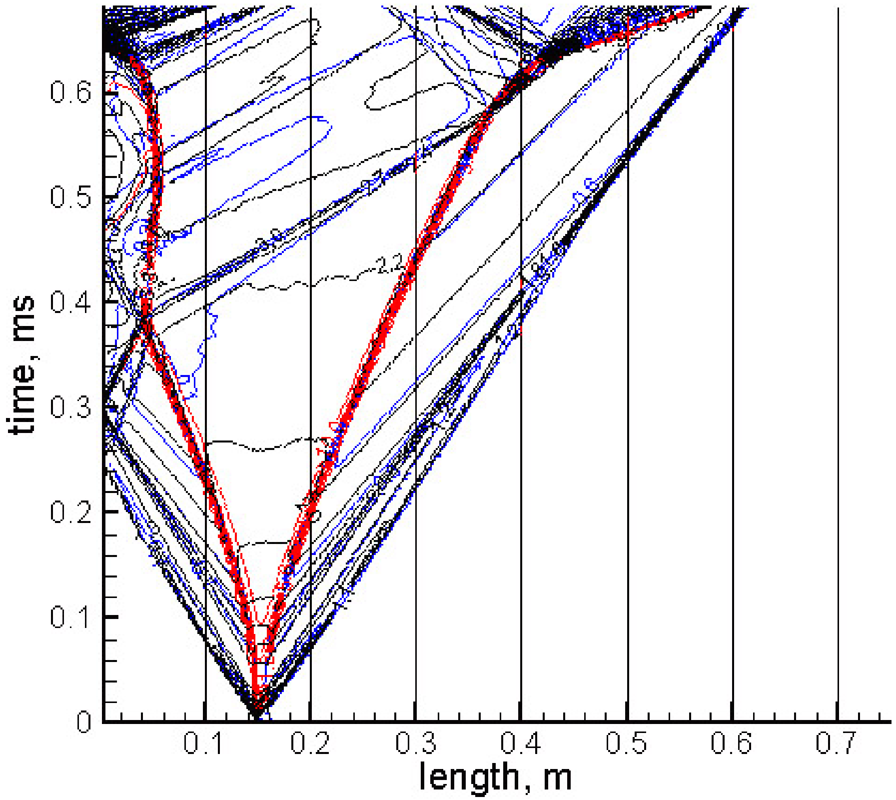


X-t diagram of combustion development in quiescent mixture. Black – pressure isolines, red – temperature isolines, blue – Mach number isolines

V=0 m/s

Shock wave reflected from the detonation tube closed end interacts with flame front but detonation doesn't form.

Detonation onset at the interaction of reflected shock wave with flame front

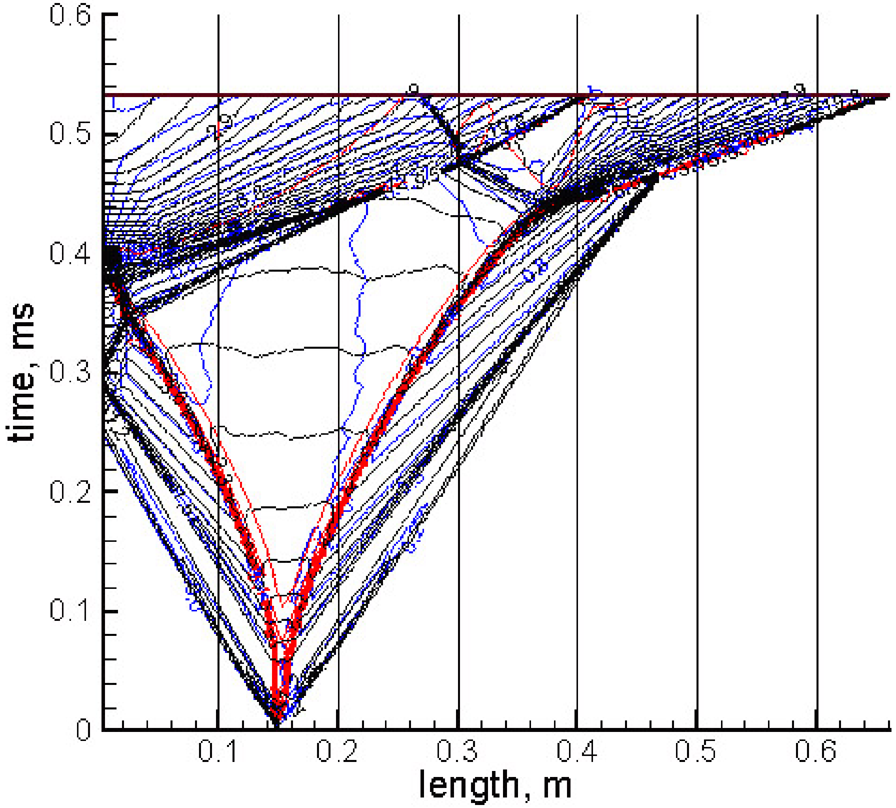


X-t diagram of detonation formation in combustible mixture flow of 35 m/s. Black – pressure isolines, red – temperature isolines, blue – Mach number isolines

V=35 m/s

Shock wave reflected from the tube closed end interacts with flame front. Detonation arises as result of this interaction. In the time moment of 640 μs one can see classical detonation onset. Detonation propagates downstream, retonation propagates upstream.

Detonation onset as a result of flame front acceleration

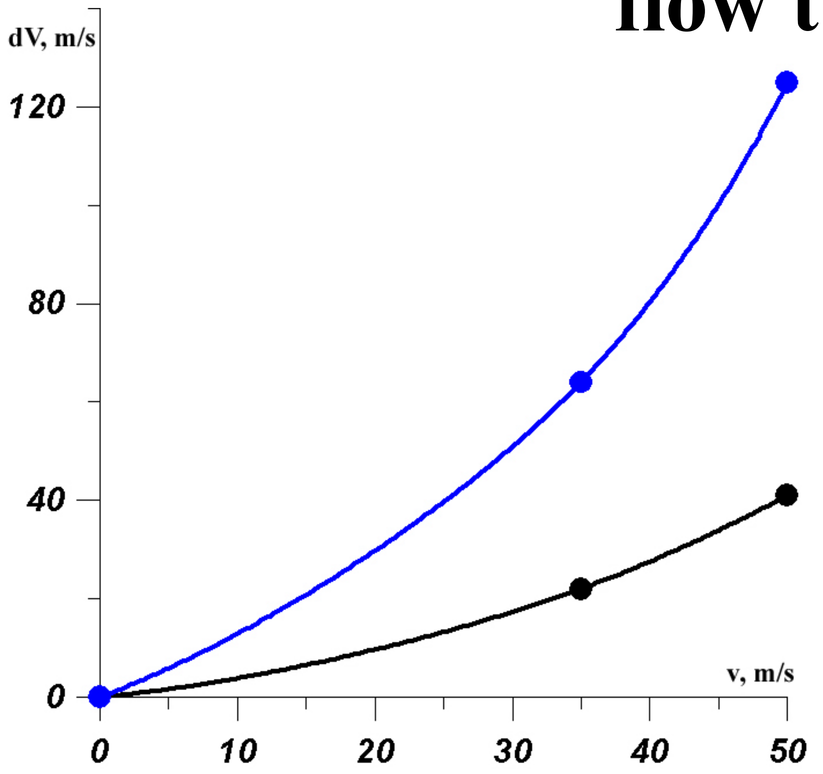


X-t diagram of detonation formation in combustible mixture flow of 50 m/s. Black – pressure isolines, red – temperature isolines, blue – Mach number isolines

V=50 m/s

In the time moment 440 μs detonation wave arises before interaction of reflected shock wave with flame front. One can see classical detonation onset. Detonation propagates downstream, retonation propagates upstream.

Shock and detonation velocity proficit caused by flow turbulence

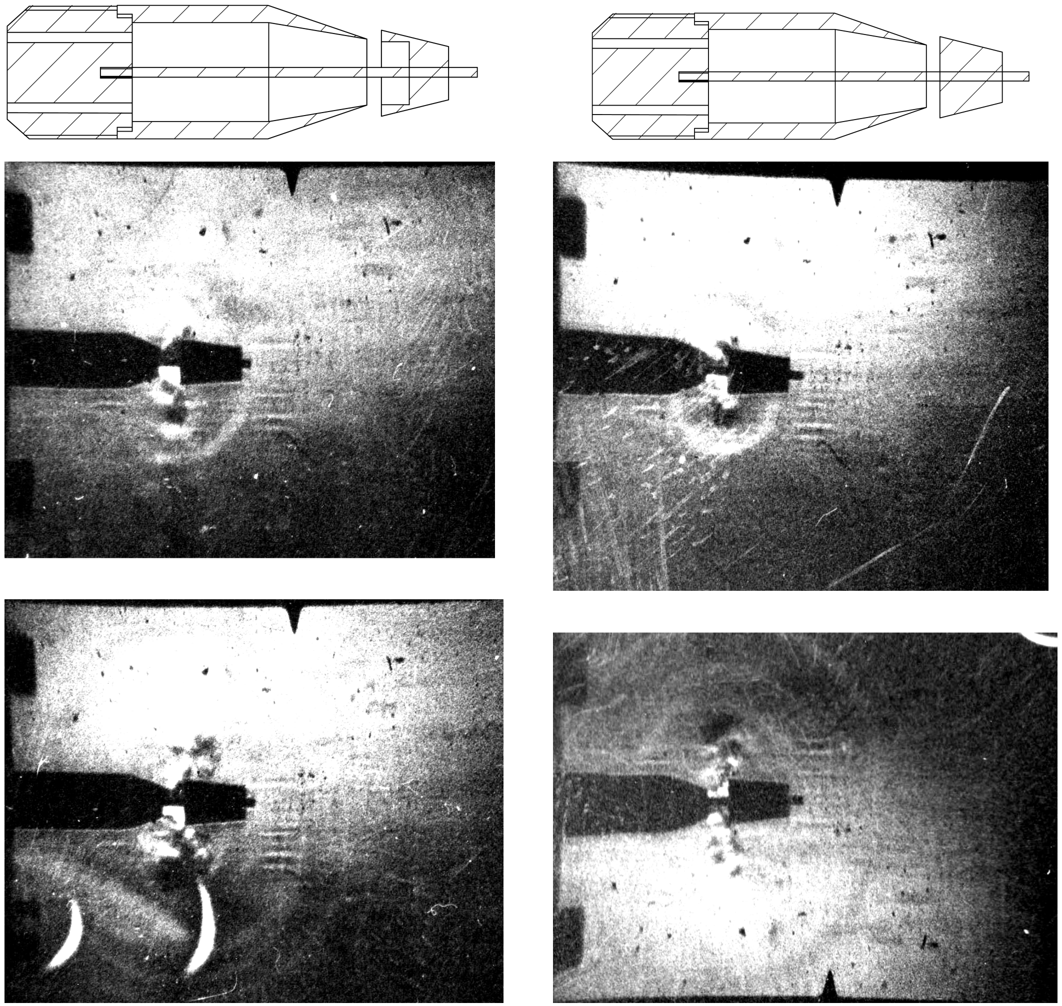


Dependences of shock wave (black) and detonation wave (blue) velocities proficit on the flow velocity

Flow turbulence provides proficit in velocities of shock and detonation waves. The possible reason is higher heat release due to increased combustion rate.

Mitigation of hydrogen explosions

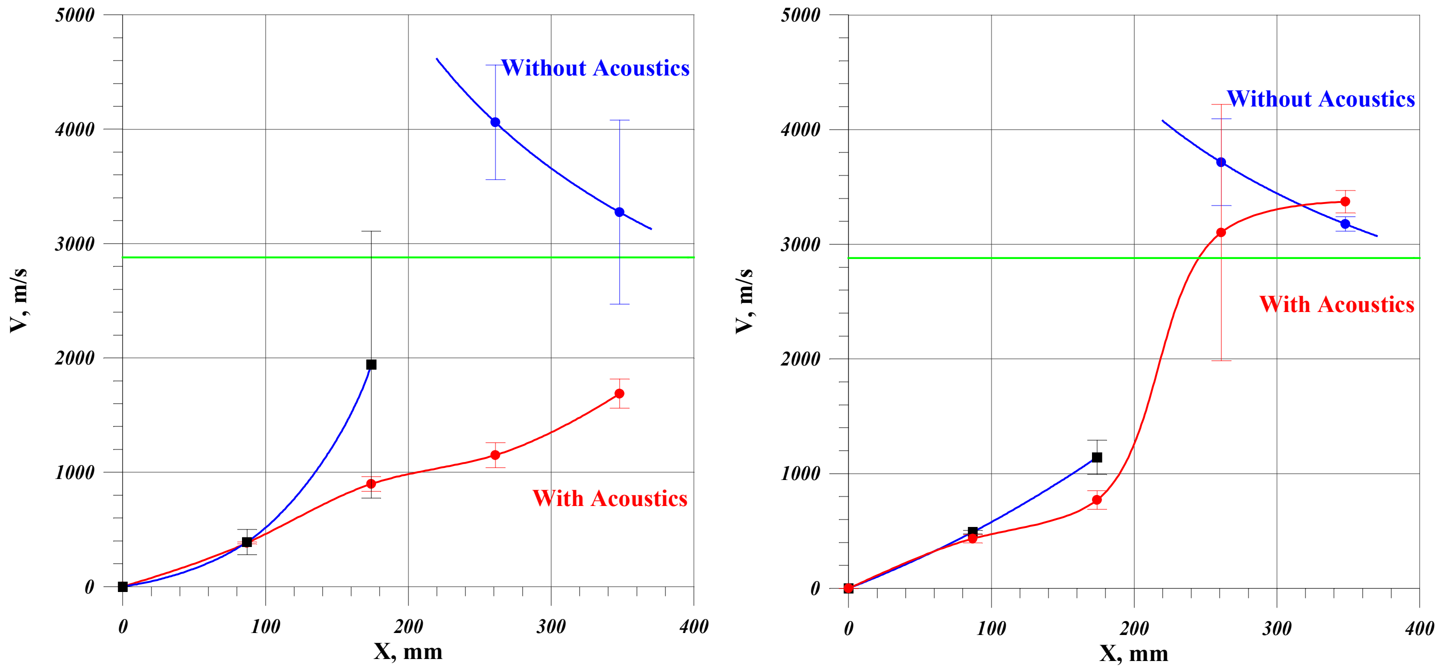
Acoustic action on deflagration-to-detonation transition



The results of visualization show that the only difference in the flows from the injectors consists in the presence of strong acoustic field with a frequency of about 17 kHz with the outflow of gas from the Hartman generator.

Shadow photographs of flows from the Hartman generator (left) and the radial injector (right)

Detonation development prevention with the acoustic

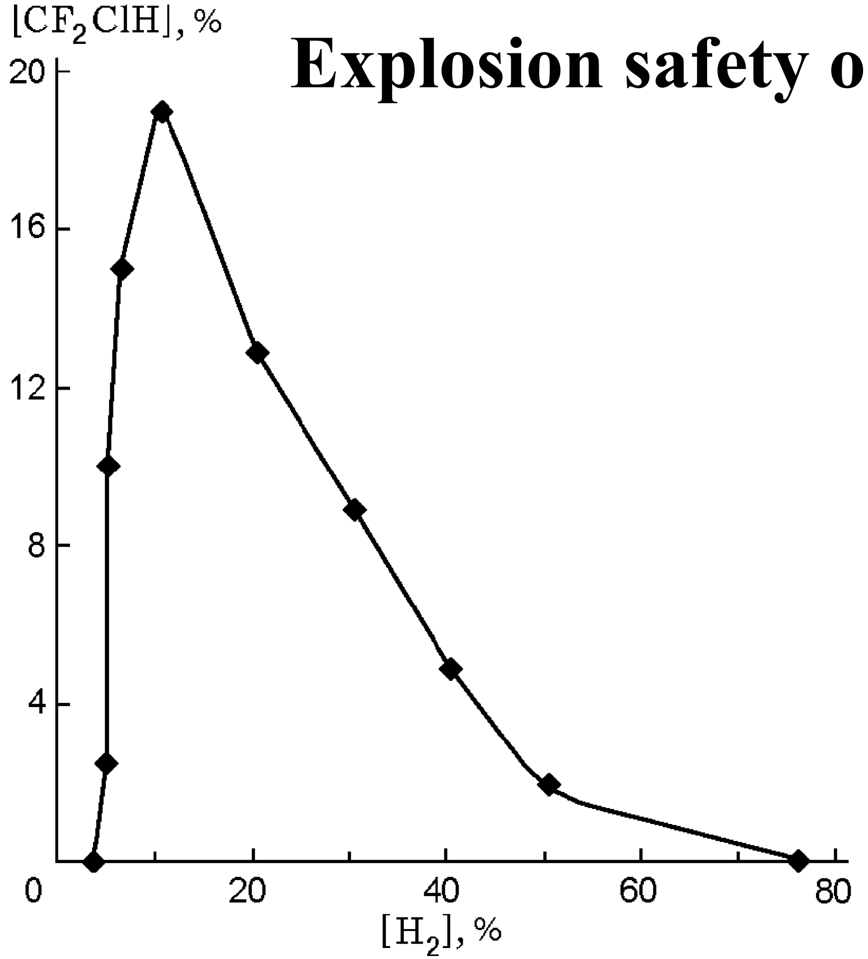


Distributions of the velocities of shock and detonation waves in the presence of acoustic field (red line) and without it (blue line) at pressures P_{DCC} = 1.4 atm and P_{DCC} = 1.9 atm (left and right) ER = 1.1. Green line - speed of detonation wave, calculated according to the theory of Chapman - Jouguet

Acoustic action on the transient turbulent flow contributes to the relaxation of large-scale vortex structures and to the transition of flow to the stationary turbulent. Also, acoustic field intensifies the gas diffusive transfer, which leads to the relaxation of pressure gradients, temperature and concentrations of active radicals.

Chain-branching reactions inhibition

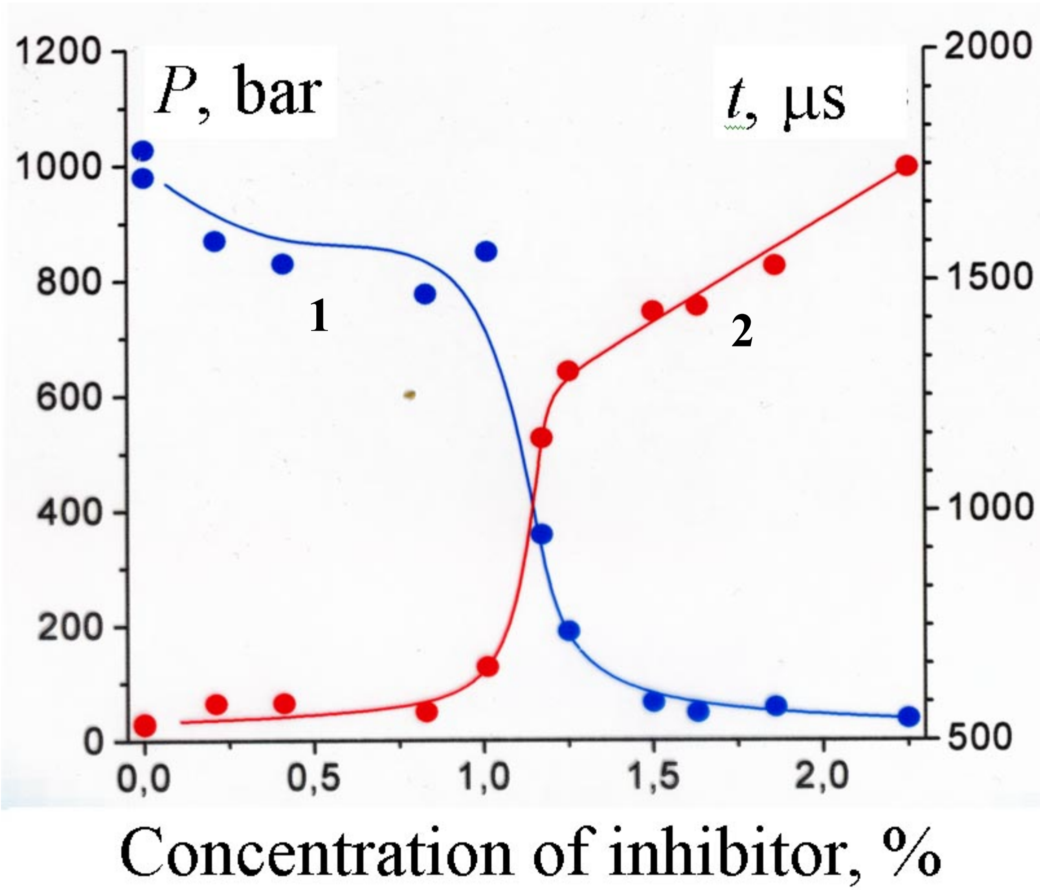
Explosion safety of hydrogen-air mixtures



Critical concentration of difluorochloromethane, which eliminate the explosion, versus the H_2 content in the hydrogen-air mixture

The determining factors are the branching-chain mechanism and the competition between multiplication and loss of active intermediate species. This show that inappreciable additives (tenth of percent) of inhibitor reduce the intensity of explosion considerably and even completely eliminate it.

Experiments in conic cavity



Pressure (1) and the arrival time of the pressure wave (2) in the top of the wedge depending the concentration of inhibitor (Azatyan V.V., 2004).

P_{max} drop is particularly strong in the range of 0.95 - 1.25% additive, which reduced the maximum pressure from 800 atm to less than 100 atm. In the interval of additives value the most dramatic change in the shock-wave velocity at the cone top occurs. This result may be explained only with chain-branching flame propagation mechanism.

Conclusions 1

•It is shown that flow velocity and initiation energy value are effect on detonation formation in the combustible mixture flow. Detonation onset in the flow to be considered taking into account flow characteristics that may affect it noticeable.

•Numerical simulation had shown essential influence of turbulent transfer of hot gas and active radicals on detonation onset distance. The main result is that the initial turbulence of flow essentially affects the deflagration to detonation transition. Predetonation distance decreases with increase of initial flow velocity. It is concerned with the influence of turbulence on the flame acceleration.

•The effects of detonation reflection, cumulating and initiation at the shock wave reflection from the rigid surface can cause the detonation with the parameters of pressure and velocity exceeding the CJ ones in the order of value or more.

Conclusions 2

•It was shown that non-stationary combustion regimes were most dangerous and significant in terms of their power effect on construction elements. Instability of non-stationary combustion front results in forming disturbances, waves and streams before the front. In closed and cumulating volumes wave intensification creates secondary combustion centers – explosions whose parameters exceed the values predicted by the Chapman-Jouguet conditions for stationary detonation (with normal initial conditions approximately fivefold).

•Strong acoustic field with a frequency of 17 kHz does not influence the initial stage of development of combustion, but at the final stage it prevents the formation of detonation.

•The determining factors of hydrogen-air flames propagation are the branching-chain mechanism and the competition between multiplication and loss of active intermediate species. Inappreciable additives (tenth of percent) of inhibitor reduce the intensity of explosion considerably and even completely eliminate it.

Thank you for your attention!