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NUMERICAL SIMULATION OF EXPERIMENTS WITH COMMERCIAL EXPLOSIVES

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Introduction

The presentation discusses results obtained in the numerical simulation of experiments on the properties of the commercial explosive PZhV-20U.

A unique approach was used to describe experiments aimed to characterize

- **detonation velocity versus diameter of non-sheathed cylindrical charges**
- **the expansion of detonation-propelled copper sheathes**
- **explosive sensitivity to shock**

Calculated and experimental results agree well.

Calculations were done with MAH hydrocode which models sophisticated 2D flows with allowance for physical and chemical transformations.

COMPUTATIONAL SETUP

Equations of state for inert materials

Mie-Gruneisen equation

$$P = P_x + \gamma\rho\left(E - E_x\right) \ , \quad P_x = \frac{\rho_0 c_0^2}{n}\left(\delta^n - 1\right), \quad E_x = \frac{c_0^2}{n}\left(\frac{\delta^{n-1} - 1}{n-1} + \frac{1}{\delta} - 1\right)$$

P = pressure, E = specific internal energy, P_x and E_x are cold components, ρ_0 and c_0 are, respectively, density and sound speed for non-compressed material, $\delta = \rho/\rho_{0k}$, ρ_{0k} is crystalline density, γ and n are constants.

Used values of the parameters

Material	ρ_0, g/cm^3	ρ_{0k}, g/cm^3	c_0, km/s	γ	n
Fluoroplastic	**2.19**	**2.19**	**1.7**	1.883	**6.4**
Copper	**8.9**	**8.937**	**3.60**	2.67	**6.0**

Equations of sate for PZhV-20U

- **Non-reacting material:** Mie-Gruneisen equation with parameters ρ_{0k}=1.7975 g/cm^3, c_0=3 km/s, n=6.35, and γ=1.2366.

- **Explosion products:** an equation of state by V.F. Kuropatenko(*) with parameters D_{0k}=5.6 km/s and α=0.35. For the initial density ρ_0=1.2 g/cm^3, the calculated detonation velocity and Chapman-Jouguet pressure made, respectively, D_{CJ}=4.86 km/s and P_{CJ}=8.1 GPa.

- PZhV-20U decomposition was described with a **semiempirical two-stage detonation macrokinetics model** developed at RFNC-VNIITF. The model is based on the "hot spots" hypothesis proved in numerous experiments with heterogeneous explosives.

* An equation of state for dense explosive detonation products. J. Compbustion and Explosion Physics, 1989, V.25, #6, p. 112-117

Explosive decomposition model

Kinetic equation:

$$\frac{d\xi}{dt}=\begin{cases}-W\cdot\dfrac{\rho_{HE}}{\rho_{0k}^{1/3}\cdot\rho_{DP}^{2/3}}\cdot\left(\dfrac{1-\xi}{\theta}\right)^{2/3}\cdot\exp\left(-E_a/3E_t^*\right)\cdot U(\sigma), & \dfrac{\theta\cdot\xi}{\rho_{HE}}>\dfrac{1-\xi}{\rho_{DP}};\\ -W\cdot\left(\dfrac{\rho_{HE}}{\rho_{0k}}\right)^{1/3}\cdot\xi^{2/3}\cdot\exp\left(-E_a/3E_t^*\right)\cdot U(\sigma), & \dfrac{\theta\cdot\xi}{\rho_{HE}}\le\dfrac{1-\xi}{\rho_{DP}}.\end{cases}$$

$$W=W_0\left(\alpha+\frac{\beta}{1+\exp(\lambda(\mu-\xi))}\right),\qquad U(\sigma)=arctg\left(a\sigma+b\sigma^m\right).$$

$\sigma=P/P_{CJ}$; P_{CJ} is Chapman-Jouguet pressure.

E_a is effective activation energy.

E_t^* is the thermal component of specific internal energy at the shock front

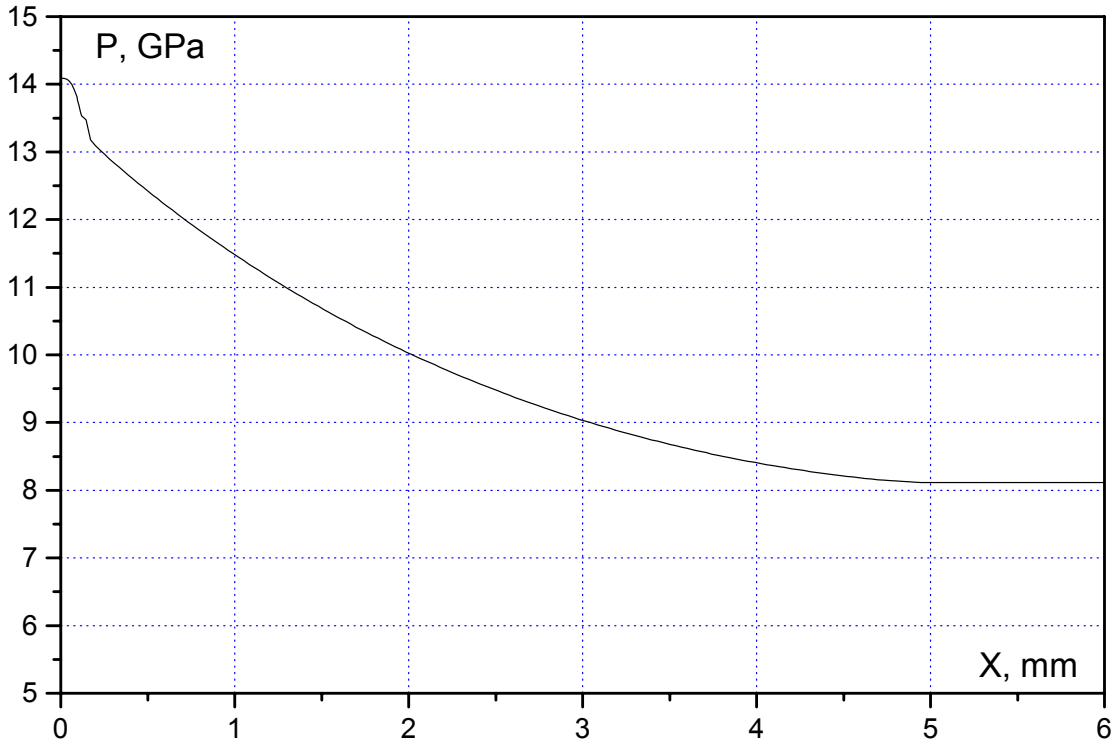
$U(\sigma)$ is a "dimensionless' velocity of the burning front

The factor $\exp(E_a/3E_t^*)$ defines the number of shock-activated hot spots.

The first stage of the model describes the combustion of hot spots and the second one treats surface combustion after the hot spots have merged.

Kinetic model parameters

W_0, μs^{-1}	E_a, kJ/g	a	b	m	θ	α	β	λ	μ
11.37	0.15	0.108	1.1	4.6	0.25	0.125	0.875	35	0.8



Calculated pressure profile for PZhV-20U stationary detonation

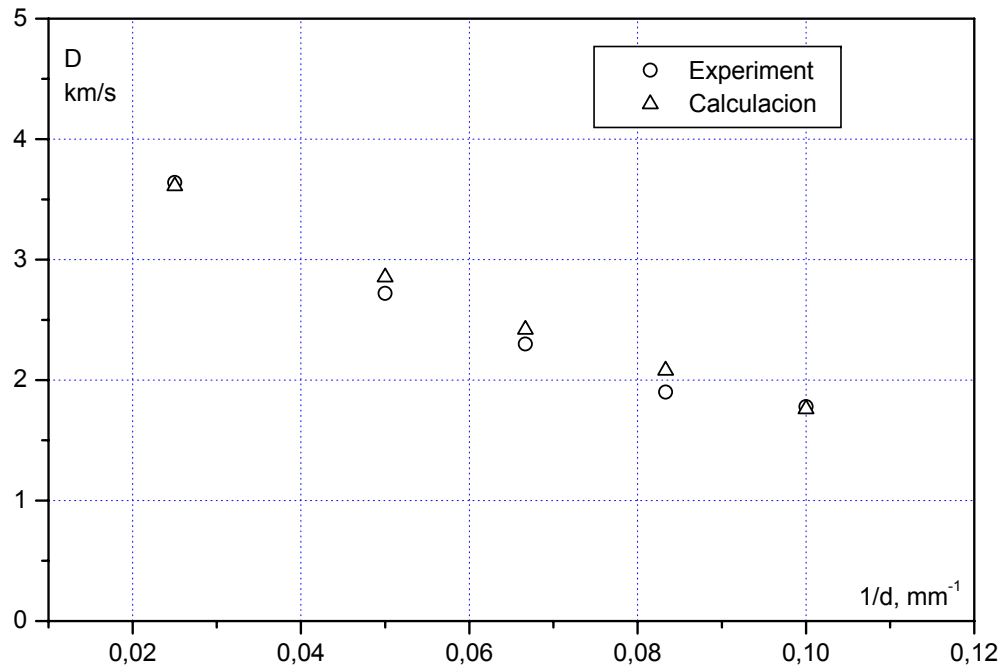
- **The calculated width of PZhV-20U reaction zone is ~5 mm.**

Non-sheathed cylindrical charges

- PZhV-20U, ρ_0=1.2 g/cm³
- *d* = diameter; length = 10*d*.
- Primer: a strong explosive of diameter *d* and 20 mm thick
- Initiation in a 6-mm-diam circle
- Outer surfaces are free boundaries.

d=10 mm	*L*, mm	17÷41	41÷66	66÷95
	$D_{эксп}$, km/s	2.09	1.76	1.78
	$D_{расч}$, km/s	2.08	1.85	1.76
d=12mm	*L*, mm	17÷48	48÷81	81÷113
	$D_{эксп}$, km/s	2.35	1.95	1.90
	$D_{расч}$,km/s	2.31	2.10	2.08
d=15 mm	*L*, mm	16÷56	56÷98	98÷145
	$D_{эксп}$, km/s	2.85	2.27	2.30
	$D_{расч}$, km/s	2.63	2.44	2.42
d=20 mm	*L*, mm	18÷73	73÷134	134÷194
	$D_{эксп}$, km/s	3.12	2.74	2.72
	$D_{расч}$, km/s	3.13	2.85	2.85
d=40 mm	*L*, mm	22÷145	145÷269	269÷390
	$D_{эксп}$, km/s	3.81	3.68	3.64
	$D_{расч}$, km/s	3.88	3.61	3.61

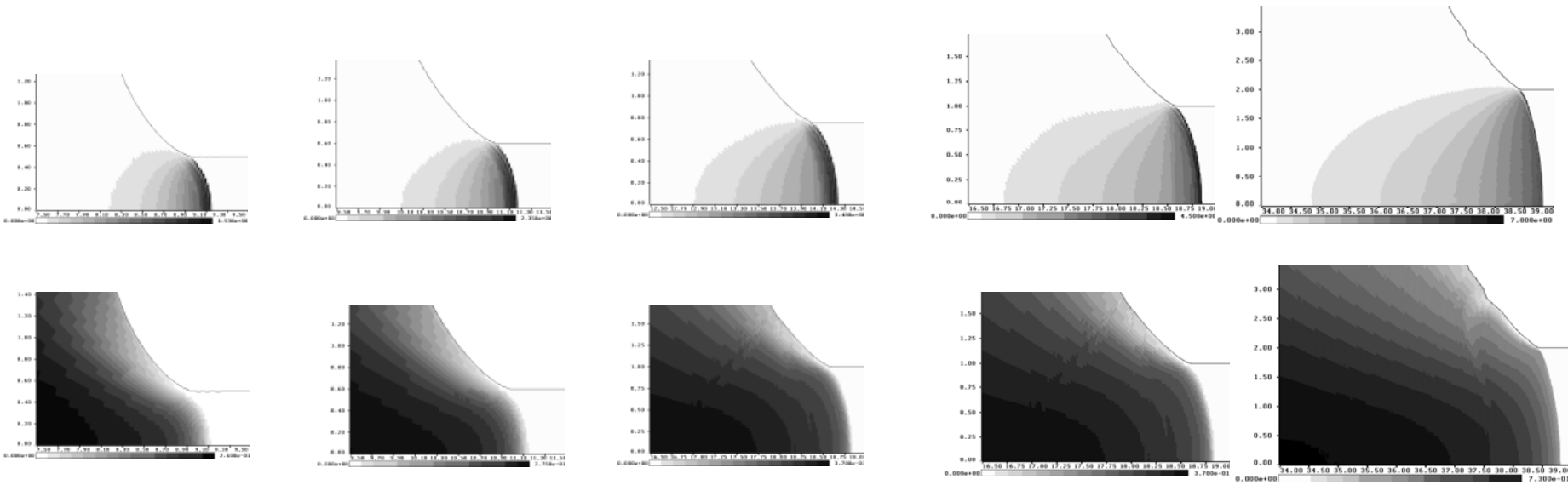
Detonation velocities



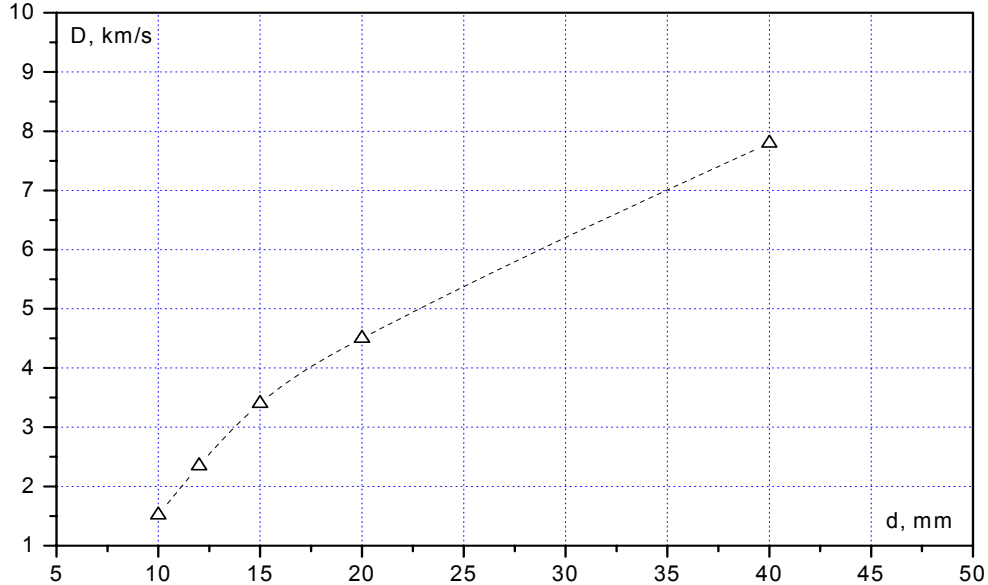
Detonation velocity versus charge diameter

- **The greatest difference between calculation and experiment makes 9.5%. It is seen for the 12-mm-diam charge.**
- **For both functions, extrapolation to $d = \infty$ gives D_{∞}=*(4.0-4.5) km/s.***

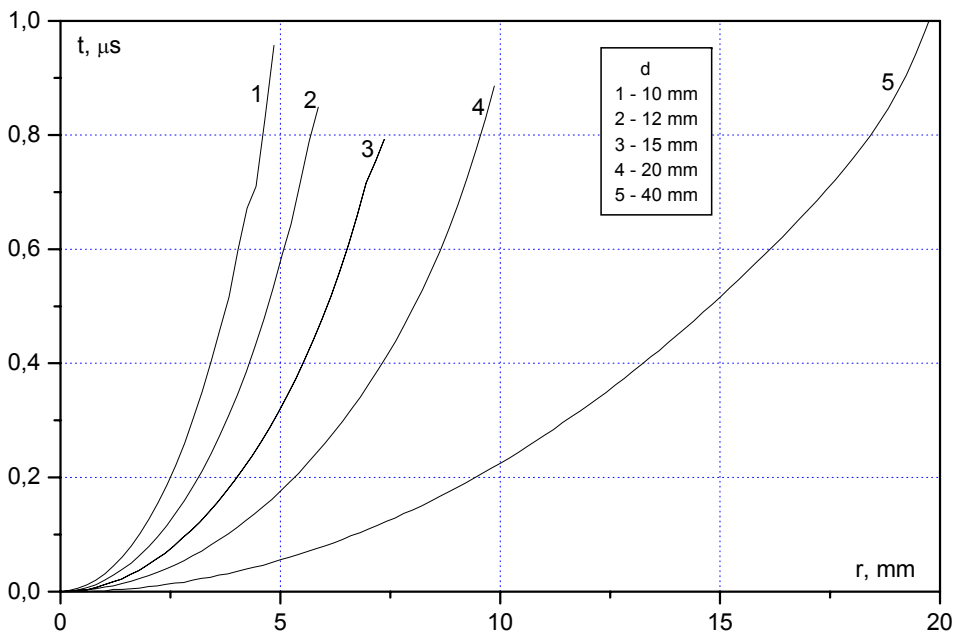
Steady-state pressures and concentrations for PZhV-20U charges



d=10 mm	*d*=12 mm	*d*=15 mm	*d*=20 mm	*d*=40 mm
t=46.0 µs	t=50.0 µs	t=56.0 µs	t=64.0 µs	t=106.0 µs



Pressure at the shock front

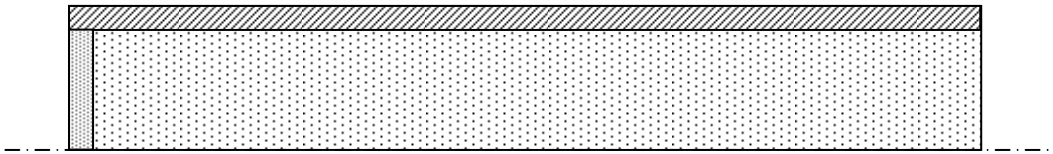


Wave travel time through PZhV-20U

d, mm	P_f, GPa	$1-\xi$, %
10	1.52	26.0
12	2.35	27.5
15	3.40	30.0
20	4.50	37.0
40	7.80	73.0

Pressure at the shock front and burning

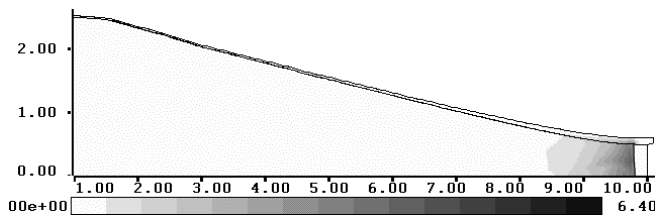
Sheathed charges



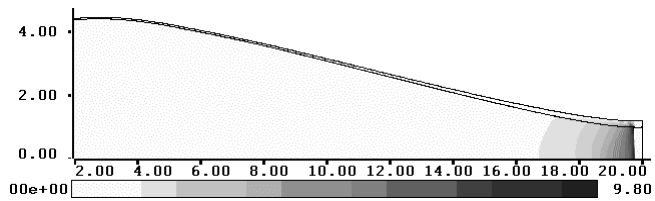
Computational configuration

- d=10, 20 and 40 mm; ρ_0=1.2 g/cm^3.
- The sheath is 0.1d thick.
- Initiation in a 3-mm-diam circle

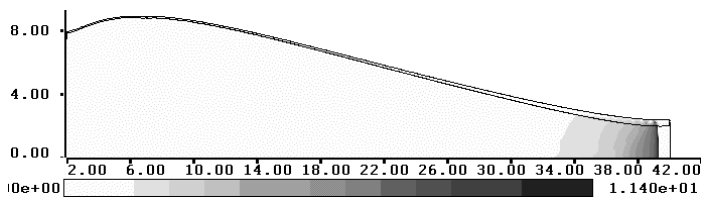
d=10 mm
t=30 μs



d=20 mm
t=50 μs



d=40 mm
t=92 μs



Calculated pressures

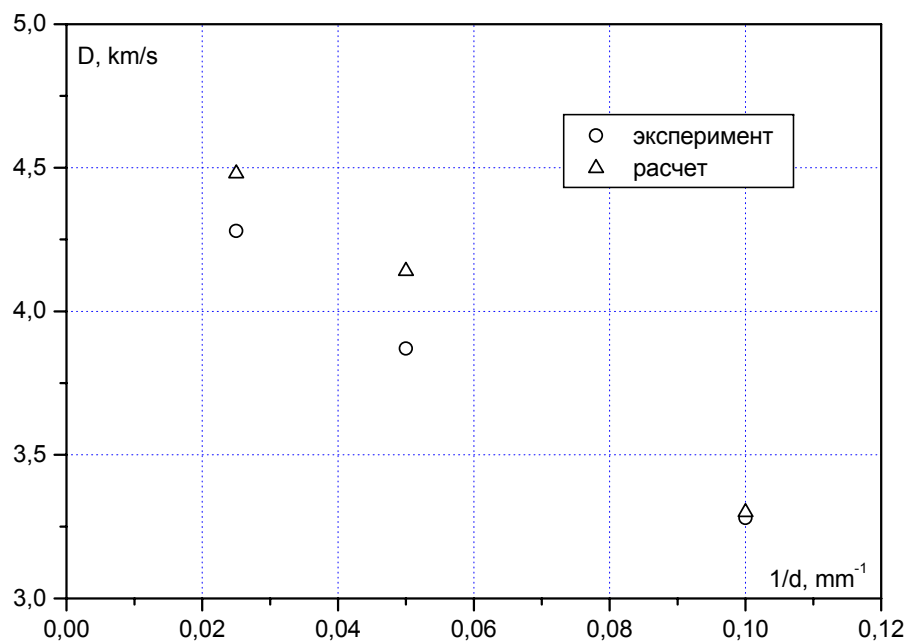
- Отставание фронта на боковой границе относительно центральной точки составляет ~0.015d.
- PZhV-20U burning makes 50%, 68% and 84% for d=10, 20 and 40 mm, respectively.

d mm	*D*, km/s		R_f, mm		P_f, GPa	
	Calculation	Experiment	Calculation	Experiment	Calculation	Experiment
10	3.30	3.28	49	36	6.4	–
20	4.14	3.87	167	122	9.8	6.7*
40	4.48	4.28	357	250	11.4	7.5*

Detonation parameters for sheathed PZhV-20U charges

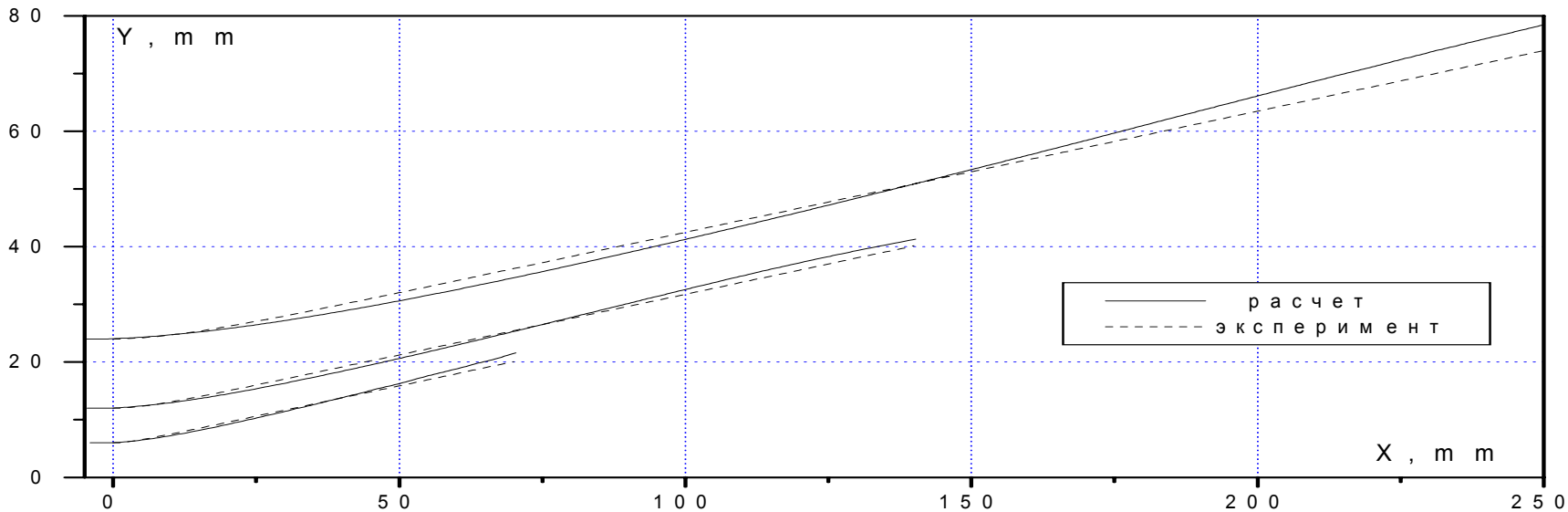
R_f, and P_f are, respectively, the radius of curvature and pressure at the shock front.

*** effective Chapman-Jouguet pressure**



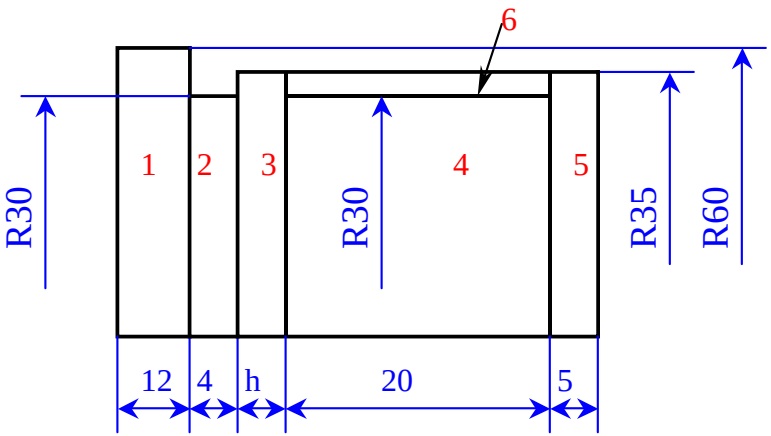
Detonation velocity

- **extrapolation to $d = \infty$ gives D_∞ = (4.7-5.0) km/s**



The outer surface of the copper sheath for PZhV-20U charges of diameters *d*=10, 20 and 40 mm

Gap-test systems



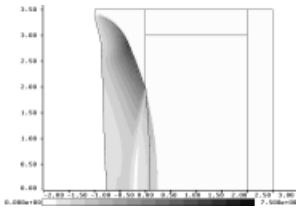
1 – cap
2 – primer
3 – fluoroplastic
4 – PZhV-20U
5 – fluoroplastic
6 – foam plastic

Computational configuration

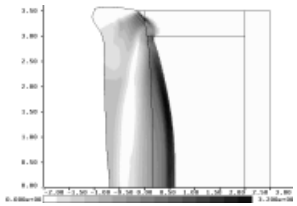
- **Initiation in a 3-mm-diam circle**
- **PZhV-20U, ρ_0=1.2 g/cm^3**
- **A gap of thickness *h* between the primer and PZhV-20U is filled with inert material; *h*=10, 15 and 20 mm.**

Pressure profiles at different times

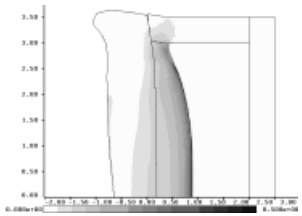
t=5 μs



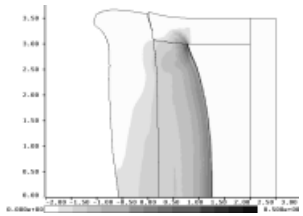
t=7 μs



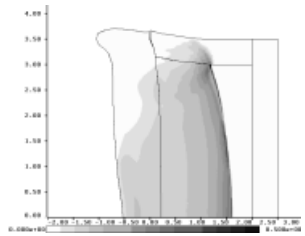
t=8 μs



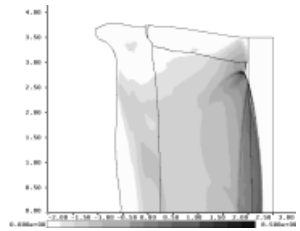
t=9 μs



t=10 μs

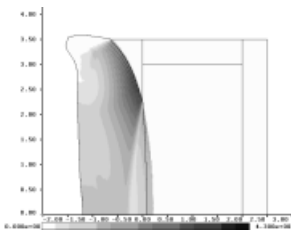


t=12 μs

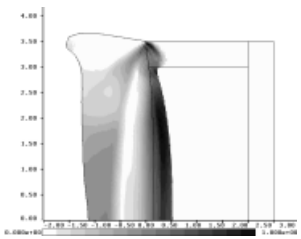


h=10 mm

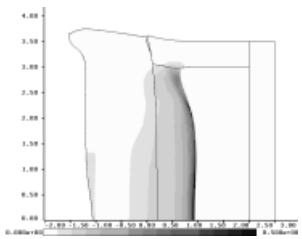
t=7 μs



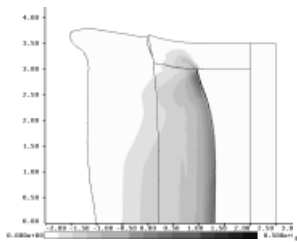
t=9 μs



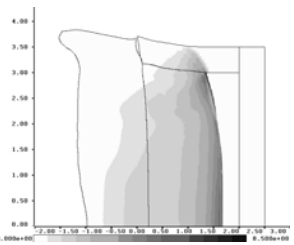
t=11 μs



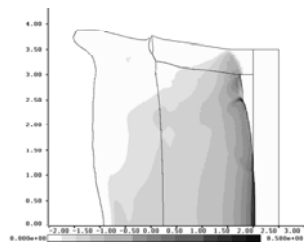
t=12μs



t=13 μs

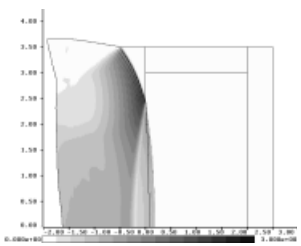


t=14 μs

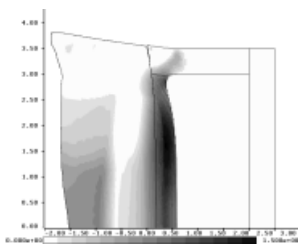


h=15 mm

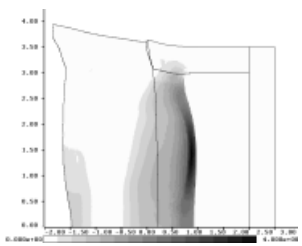
t=9 μs



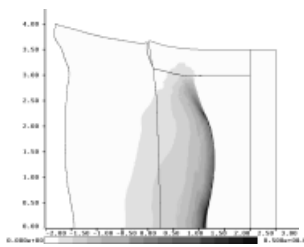
t=12 μs



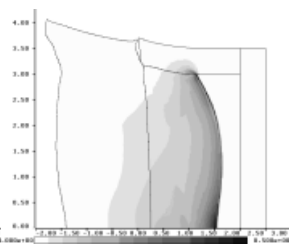
t=14 μs



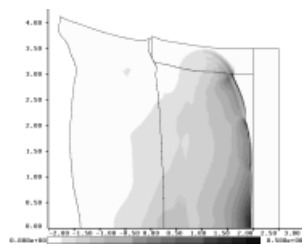
t=15 μs



t=16 μs

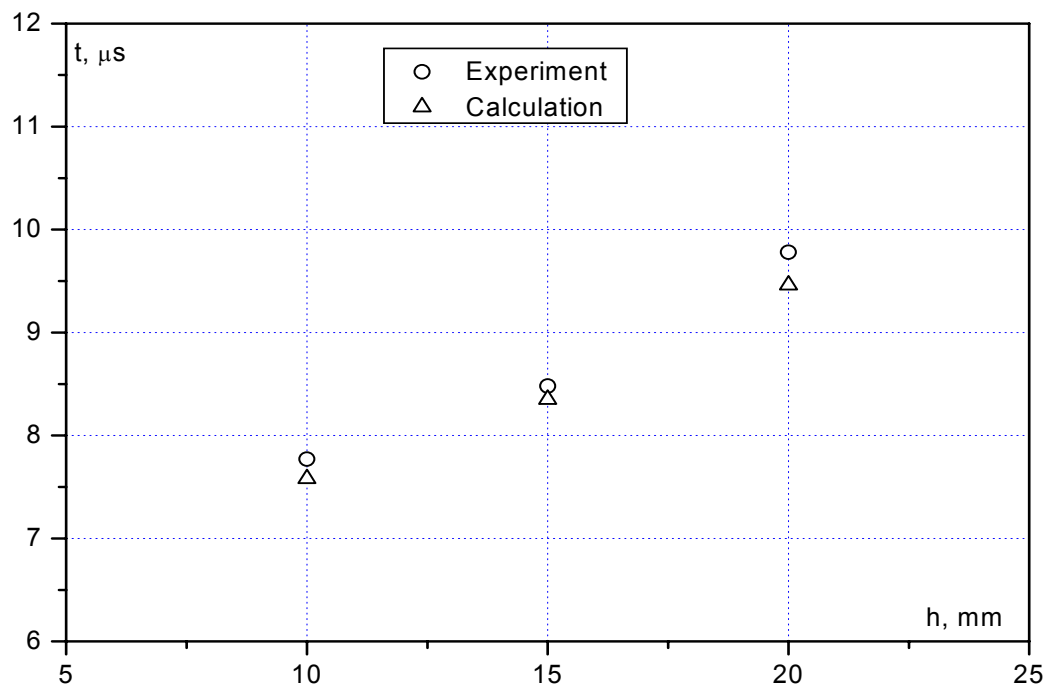


t=17 μs



h=20mm

h, mm	*τ, μs*	
	Calculation	Experiment
10	7.58	7.77
15	8.35	8.48
20	9.46	9.78



Calculated and experimental wave travel time through PZhV-20U

CONCLUSION

- **Our calculations on detonation velocities in PZhV-20U charges and their initiation by divergent shock waves of different intensities agree well with experiment.**
- **The outer surface of sheathes at the final stage of detonation is reproduced quite accurately, proving validity of the equation of state for detonation products.**
- **Our calculations helped obtain the shape of the shock front and detonation parameters for PZhV-20U charges used in different experiments. Calculated and experimental pressure profiles for PZhV-20U stationary detonation agree well.**
- **With appropriate normalization against experimental data, our explosive decomposition model can be used for other explosives.**