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PRODUCTION OF NEW MATERIALS: SCIENCE,
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Explosive Production of New Materials

***SMALL EXPLOSION CHAMBER DESIGN AND
OPTIMIZED CONSTRUCTION BASED IN BLAST
PARAMETERS
for production of new metal-oxide materials***

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Summary

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- Underwater blast wave generators (WBWG)
- Vacuum explosion chambers

2. Design configurations and dimensions

- Past configurations
- Present vacuum chamber configuration and selected explosive

3. Applied models, design and results

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- Design assumptions, procedures and results

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- Emulsion explosive blasted in cubic meter containers
- PETN explosive blasted in 25 liter containers
- Emulsion explosive charge in 50 liter stainless steel barrel
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Design configuration and dimensions

Vacuum explosion chamber:

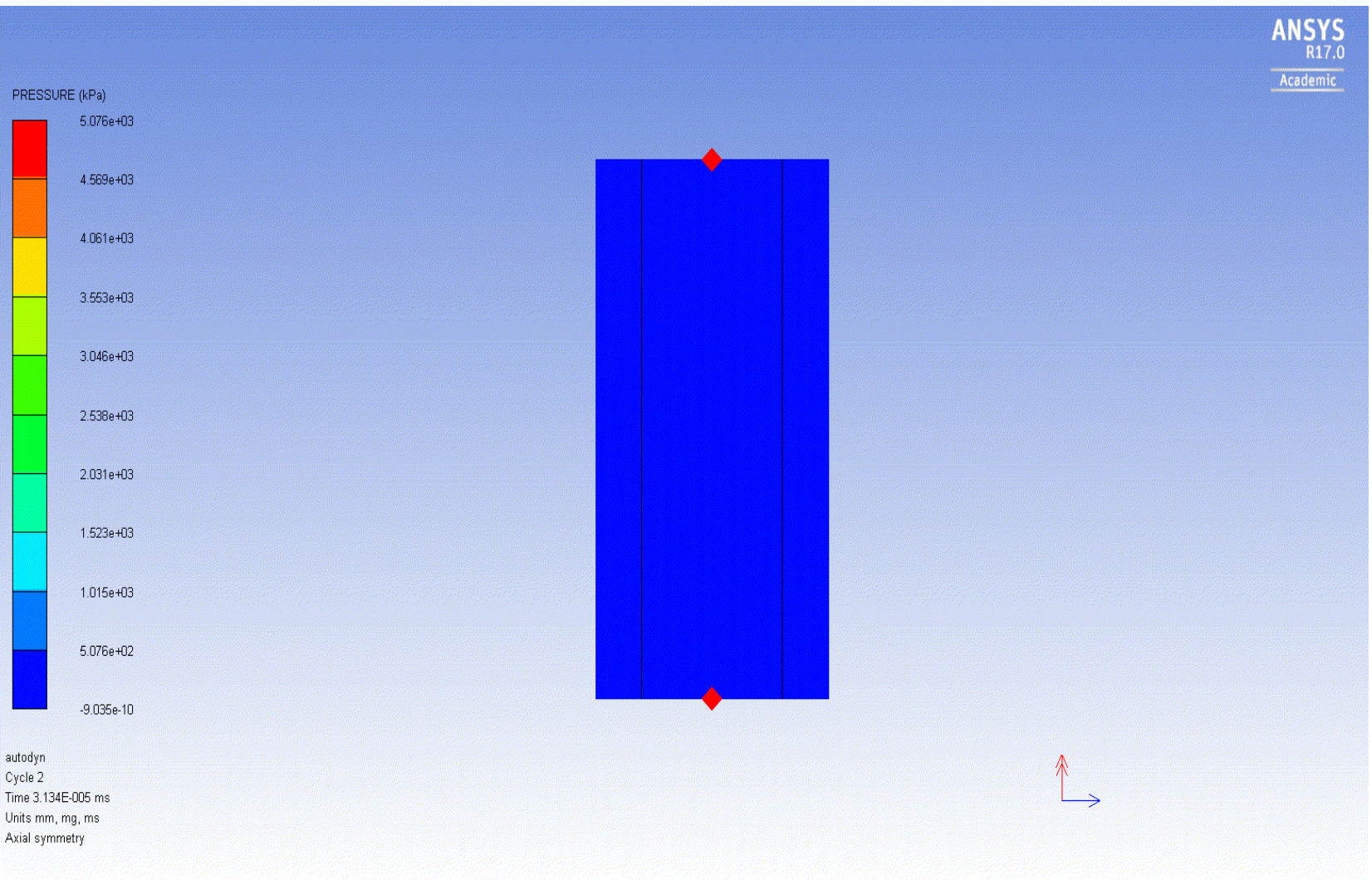
- Collecting detonation products
- No compression and shock by environmental atmosphere against wall of explosive chamber
- Increased mass explosive capabilities
- Strongly reduced contaminations

**Design parameters of explosion chamber
needs explosive environmental dense
material:**

water



Modelling opposite detonation example





Introduction

Main differences between confined underwater blast wave generators (WBWG) and the original blast wave generator (WBG):

- avoids the generation of high velocity fragments and reduces atmospheric sound wave;
- density of water 800 times greater than air, resulting in a much faster shock wave and sound velocity (4.5 times faster);
- pressure impulse in shock wave is 15-20 times higher
- produces a better blast impulse and surface area distribution;
- collect detonation products.

Due to the interest of collecting detonation products, many developments were achieved for initial vacuum explosion chambers, having in the final detonation operation only the products of reactive media, without any contaminants from water or ambient air.

My gratitude of many fruitful discussions with INNOVNANO research group, in particular with Marisa Rodrigues here present. 5

Design configuration and dimensions

Selected explosives

Ammonium nitrate-fuel oil emulsion explosive composition:

NAME	COM. NAME	REF.	GLOBAL FORM.	DENS. [g/cm ³]		COLOR	PHYS. STATE
				Bulk	Effective		
Ammonium Nitrate	Porous Am. Nit.	AN	NH ₄ NO ₃	0.69-0.74	1.725	white	solid
Oil	Diesel Oil	Oil SAE 30	-	0.9		yellow	liquid
Microcrystal Wax	Galp P1	Galp P1	-	-	-	white	solid
Parafin Wax	Guerowax-70	Guerowax-70	-	-	-	yellow	solid
Sorbitan Monooleate	Span 80	Span 80	-	-		yellow	liquid
Sorbitan Sesquioleate	Arlacel 83	Arlacel 83	-	-		yellow	liquid
Hollow Glass Microballons	Q-CEL 400	Q-CEL 400	-	0.11	0.21	white	solid

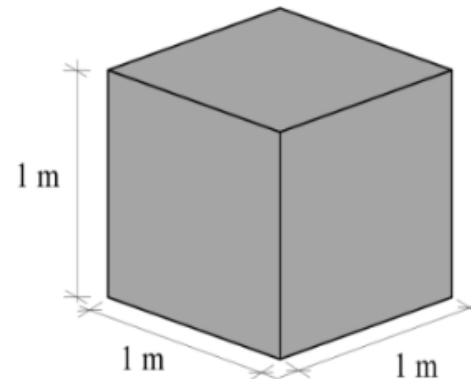
Global characteristics of PETN explosive:

NAME	COM. NAME	REF.	GLOBAL FORM.	DENS. [g/cm ³]		Melting point	Boiling point
				Bulk	Effective		
PentaErythritol TetraNitrate	Pentrite	PETN	C ₅ H ₈ N ₄ O ₁₂	0.69-0.74	1.77	142.9 C	180 C

Design configuration and dimensions

Past configuration

- plastic cubic meter container
- ammonium nitrate-fuel oil emulsion explosive placed in the center of an 20 mm aluminum tube
- pressure sensor was glued to the external wall





THOR predictions and JWL coefficients

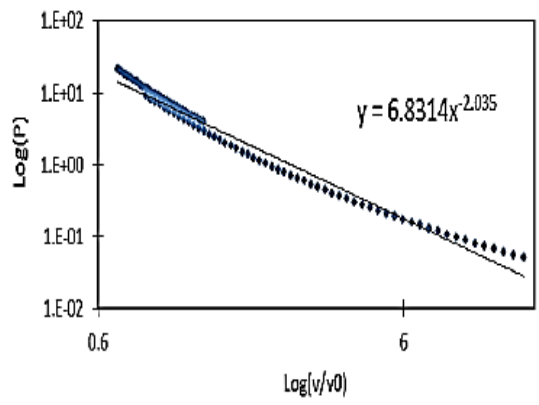
- Initial and final detonation products properties of PETN detonation using **THOR** code:

Initial conditions	CJ conditions	
Density $\rho = 1100 \text{ kg/m}^3$	$D_{CJ} = 5437 \text{ m/s}$	$T = 3847 \text{ K}$
$E_0 = -1682.85 \text{ kJ/kg}$	$P_{CJ} = 8.73 \text{ Gpa}$	$G = -2.59E+04 \text{ kJ/kg}$
$T = 298.15 \text{ K}$	$a_{CJ} = 4057 \text{ m/s}$	$\gamma = 1.1$
Pressure $= 10^5 \text{ Pa}$	$u_{CJ} = 1488 \text{ m/s}$	$\Gamma = 2.63$

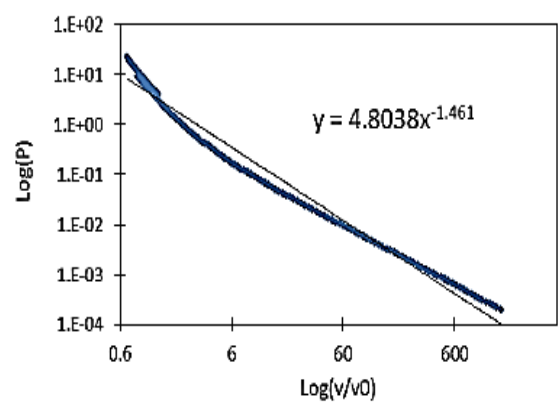
JWL equation of state for expanded detonation products:

$$P(v) = Ae^{-R_1 \frac{v}{v_0}} + Be^{-R_2 \frac{v}{v_0}} + C \left(\frac{v}{v_0} \right)^{-(w+1)}$$

Approach to Gruneisen coefficient, $\omega = \Gamma - 1$, where can be expressed $\Gamma = \Gamma_0 - \Gamma_1(v/v_0)$ (vd. Handley, 2011)



• Isen-adiab — Potencial (Isen-adiab)



• Isen-adiab total — Potencial (Isen-adiab total)

Adiabatic and isentropes curves, restricted and full, with P as function of adimensional volume (v/v_0) if a double logarithmic scale, where $v_0 = v_{CJ}$



Applied models, design and results

Calculation of JWL coefficients according to some restrictions:

- the Gruneisen coefficient from the exponential of the adiabatic curve;
- the Gruneisen coefficient from the exponential of the limit isentrope curve;
- the Gruneisen coefficient from the exponential of the total isentrope curve;
- the Gruneisen coefficient and the parameter C of JWL deduced by Caroline (Handley, 2011).

Test	ω	C	A	R1	B	R2	Deflection
		GPa	GPa		GPa		$\Sigma [P_{theor.} - P_{JWL}]^2$
1.0	1.602	6.81	800	8.29	50	5	26.93
1.1	1.602	6.81	1000	8.29	30	5	26.4
2.0	0.825	3.44	2486.75	8.2	41.54	2.59	25.5
2.1	0.825	3.44	2467.53	8.19	41.48	2.592	25.508
3.0	0.356	1.99	2354.65	7.93	47.78	2.385	25.421
3.1	0.356	1.99	2343.62	7.92	47.62	2.383	25.421
4.0	1.63	27.56	10	12	10	12	576

The presented results show the strong influence of exponent ω on the inclination deep of the curves. Best correlated results were achieved under conditions referred by res. 3.0 and 3.1, adopted for further calculations. Consequently these are the values taken in account for design pressure values of explosion chamber.

Applied models, design and results

In order to calculate the JWL coefficients to the used emulsion explosive, a complex method was established (Tavares et al., 2012).

Obtained results were calculated by successive steps:

- Correlating ANFO results with existing data in Autodyn® bibliography, in order to validate procedures
- Calculating JWL coefficients for emulsion explosive.

	Autodyn Bibliog.	ANFO	Emulsion explosive
ρ_0 (kg/m ³)	931	920	1187
A (GPa)	4.946 E 4	273.0	467.5
B (GPa)	1.891 E 4	77.33	97.57
C (GPa)	n. a.	851.9	909.4
R1	3.907	8.893	8.958
R2	1.118	1.733	1.348
ω	0.333	0.073	0.073
D_{CJ} (m/s)	4160	4812	5509
P_{CJ} (kPa)	5.15 E 6	5.45 E 6	7.85 E 6
E_{CJ} (kJ/m ³)	2.48 E 6	5.25 E 6	3.75 E 6

Applied models, design and results

Pressure of shock wave dependence of distance, from centre of detonation:

$$\Delta p = A \left(\frac{r_0}{r} \right)^\alpha \quad \text{for TNT, } \rho = 1.6 \text{ g/cm}^3: \\ A = 37 \text{ GPa}, \alpha = 1.5$$

P-t profile of shock wave:

$$p(t) = \Delta p e^{-t/\theta} \quad \text{for } t < \theta$$

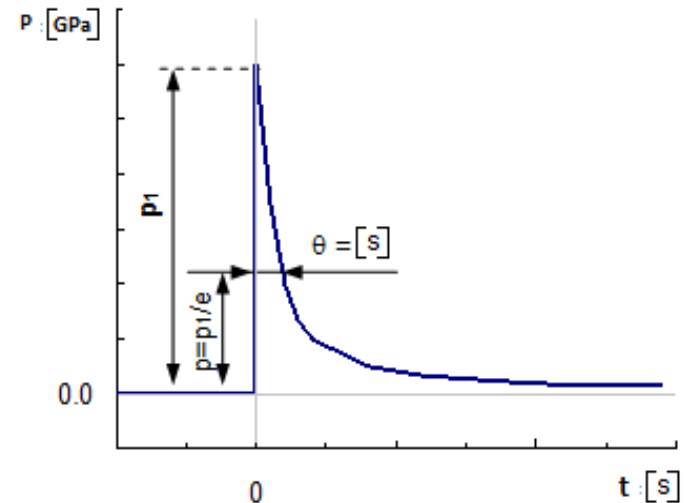
$$p(t) = \Delta p 0,368 \frac{\theta}{t} \quad \text{for } \theta < t < 5 \times \theta \text{ to } 10 \times \theta$$

$$\theta = B_1 \left(\frac{r}{r_0} \right)^\beta \frac{r_0}{c_0} \quad \text{TNT, } \rho = 1.6 \text{ g/cm}^3: \\ B_1 = 1.4, \beta = 0.24$$

Pressure impulse:

$$I = \int_0^t p dt = 1 \cdot 10^5 \left[\Delta p \theta (1 - e^{-t/\theta}) \right]$$

$$I = \int_0^t p dt = 1 \cdot 10^5 \left[\Delta p \theta \left(0,632 + 0,368 \ln \frac{t}{\theta} \right) \right]$$



θ is so-called time constant or characteristic width of peak (it describes exponential pressure drop with time, and it is $p(t)$ width at which maximum pressure decreases to value p_{\max}/e).

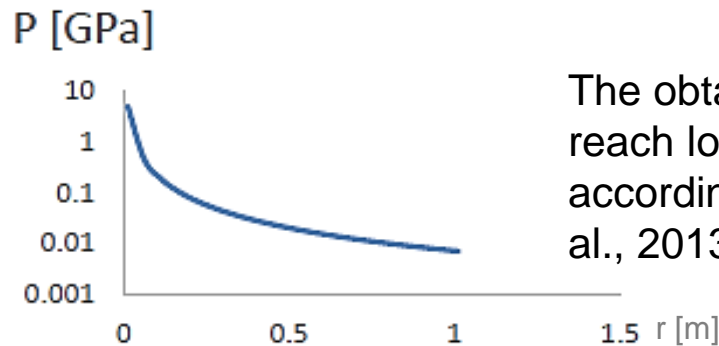
(vd. M. Sucaska, 2007)



Dynamic simulations – general equations

With these expressions, it is possible to define limit dimensions for our designed WBWG. Detonation products properties of PETN explosive, calculated as a function of initial density, allow the determination of its detonation products shock polar.

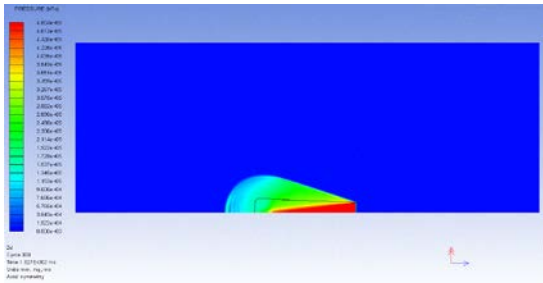
- Detonation velocities were calculated using $D=1.608 + 3.933\rho_0$ (D given in km/s and ρ_0 in kg/dm^3) given by LASL, 1980.
- Acoustical approach from detonation products of PETN to the shock polar pressure of water allow the calculation of $A=5.12$ GPa for the initial density of PETN of $1170 \text{ kg}/\text{m}^3$.
- Assuming preceding A value and the $\alpha=1.5$ value it was possible to determine transmitted shock pressure inside water container, as a function of radius distance from central charge.



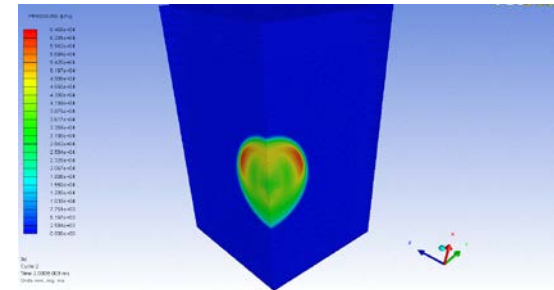
The obtained results seems to show the possibility to reach low final pressure values ($P < 0.6$ MPa) according to the previous experiments (Ambrósio et al., 2013).

Autodyn® 2D and 3D simulations

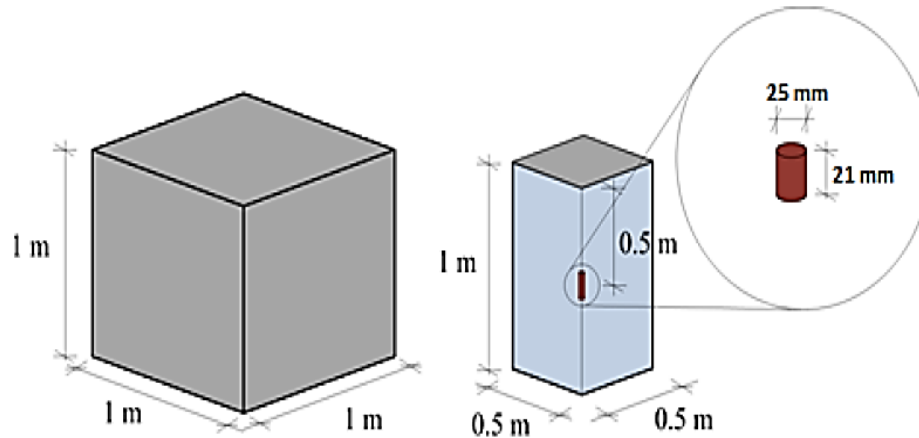
Autodyn simulations are performed in two configurations:



- detonation progression inside cylindrical charge of 2.5 cm diameter and 2.1 cm long, in 2D simulation.



- expansion of detonation products at the end of detonation, inside a cubic meter water tank, in 3D simulation.

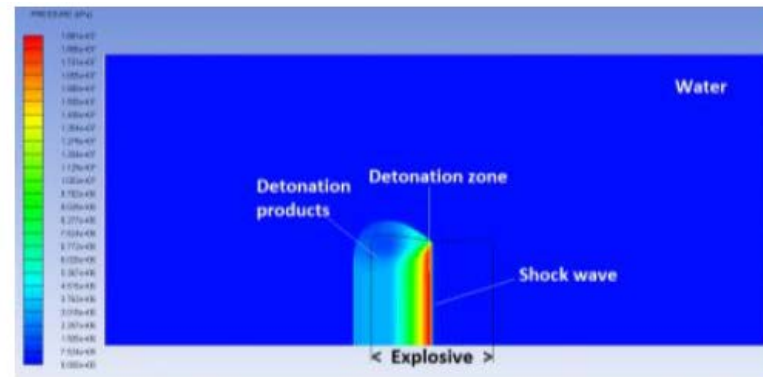
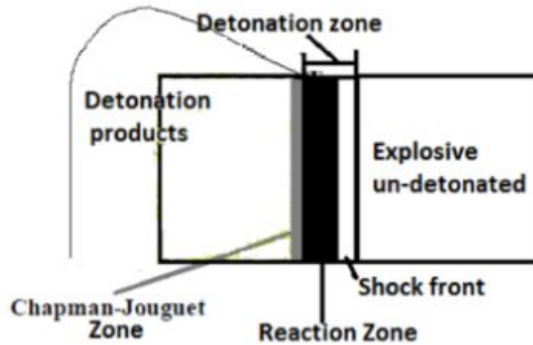


Assuming a 15.5g PETN (with a density of 1.5g/cm³), and for Autodyn® data:

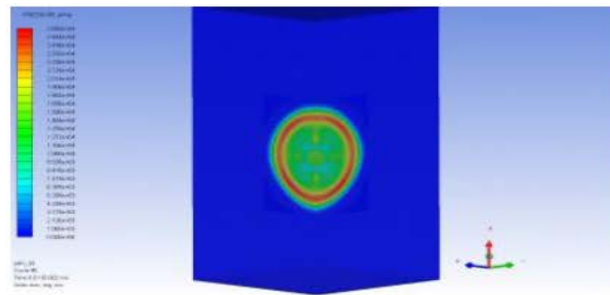
- $A = 625.3 \text{ GPa}$,
- $B = 23.29 \text{ GPa}$,
- $R_1 = 5.25$,
- $R_2 = 1.6$,
- $\omega = 0.28$.

- At CJ point:
- $D_{CJ} = 7450 \text{ m/s}$,
 - $P_{CJ} = 22 \text{ GPa}$,
 - $E_{CJ} = 8.56E+6 \text{ KJ/m}^3$

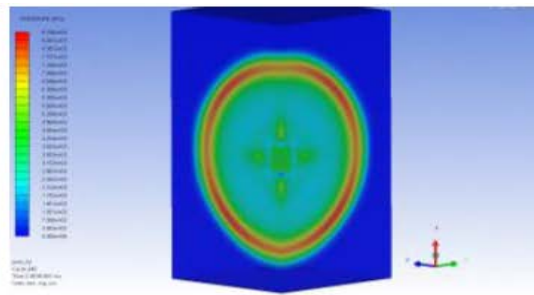
Autodyn® 2D and 3D simulations



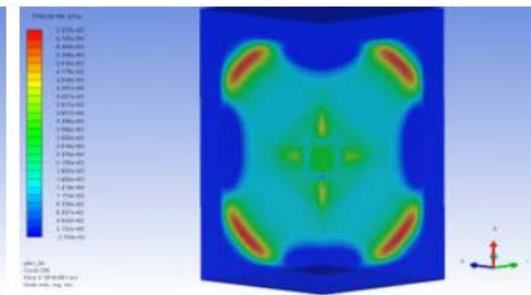
In a 2D configuration, it can be assumed that detonation wave travels through the explosive material from left to right. The shock front is followed by the chemical reaction zone. Behind it are located the dense and hot gases from the detonation products. The increase volume of the gases of the products generates higher pressure values, generating a shock wave inside surrounding material (water).



i) non-dimensional volume reaches the value of $165 v/v_0$



ii) Expansion products touch the wall of the water tank



iii) Expansion products reaches the corners of the water tank

Design procedures, results and assumptions

Using preceding presented values of JWL expansion model, the explosion can be designed according these values with AD-Merkblätter Standards procedures. According to AD-Merkblätter Standards Series B1, considering a cylindrical shape, the final design pressure parameter can be obtained through the chamber wall thickness equation:

$$s = \frac{D_0 \cdot p}{20 \frac{K}{S} \cdot v + p} + c_1 + c_2 \quad \longrightarrow \quad p = \frac{20K \cdot v \cdot s}{S(D_0 - s)} - c_1 - c_2$$

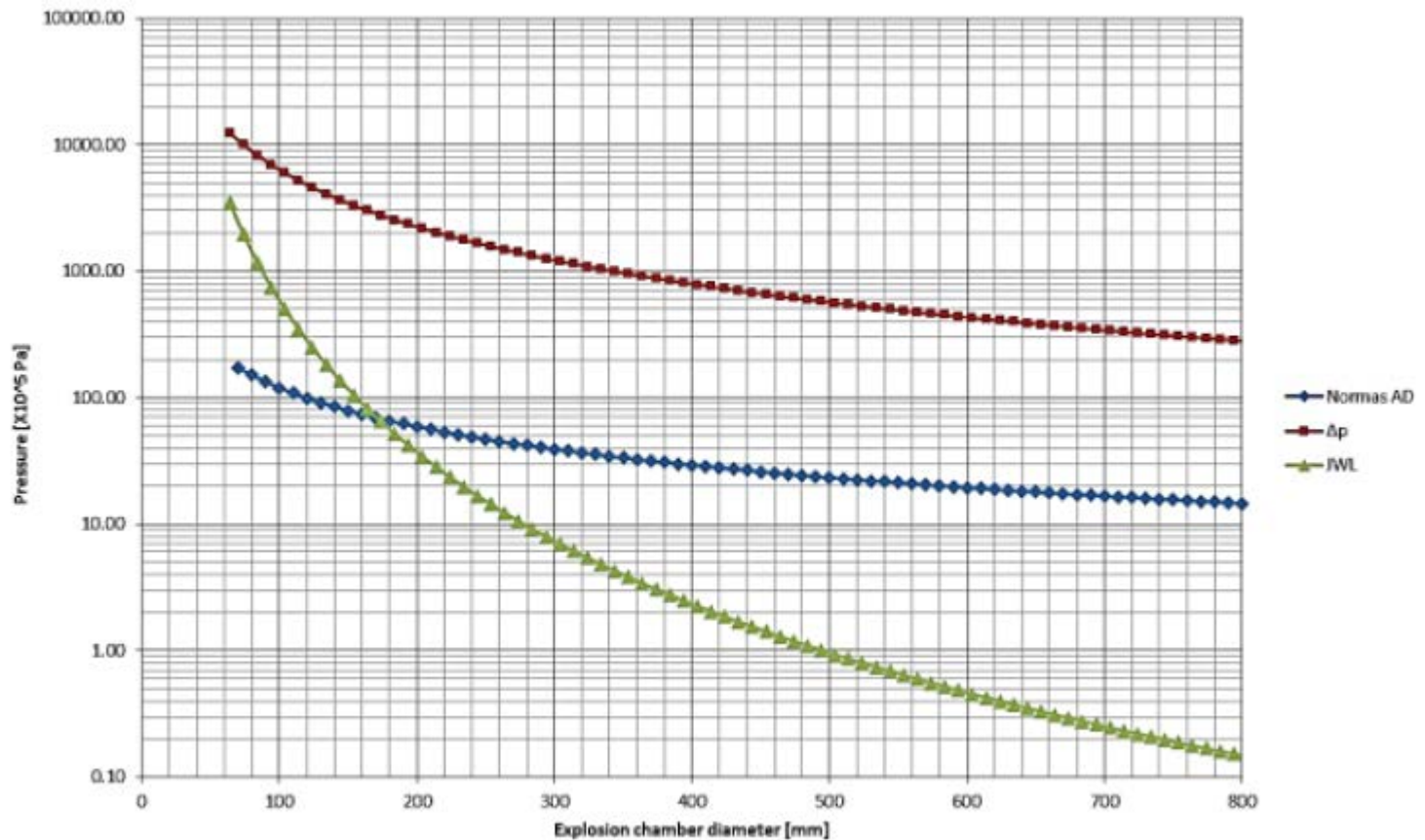
The pressure evolution can be plotted by:

- Simplified expression, referred as ΔP ,
- Applying JWL model, referred as JWL,
- AD-Merkblätter Standards, referred as AD, as a function of diameter of explosion chamber for a given mass of explosive charge.

Applied JWL EoS coefficient values:

w	C	A	R_1	B	R_2
	GPa	GPa		GPa	
0,328	3,6	90	5	90	2,879

Design procedures, results and assumptions

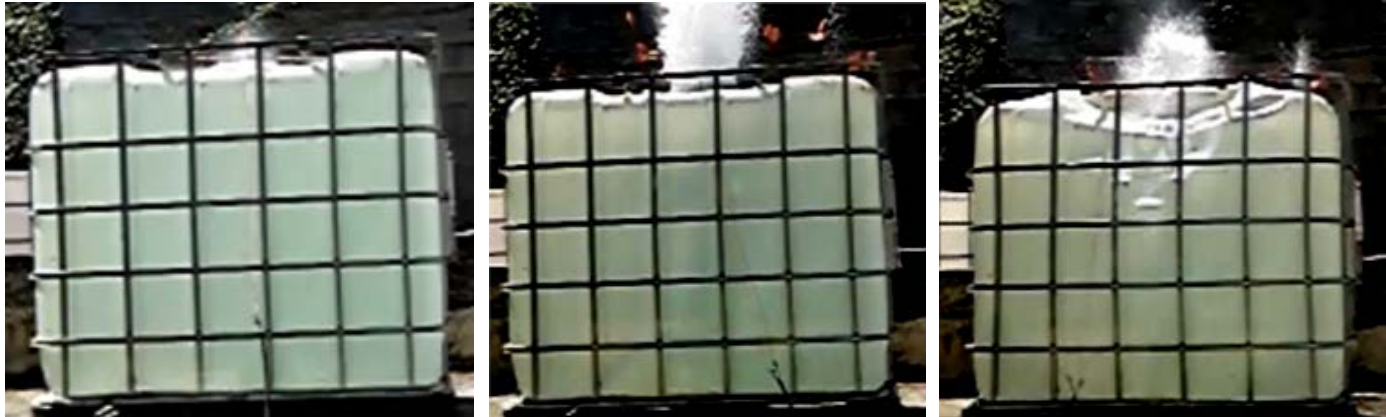


The evolution of pressure, as function of charge diameter, for a mass charge of 60 g of emulsion explosive. The explosive chamber can be designed for this explosive charge, as long as the diameter is larger than 180 mm (assuming JWL model, where pressure evolution values for JWL cross AD results).

Previous results – Emulsion explosive in cubic meter container



External deformation of plastic container and observed reflections for the 3 tested charges (5g left, 10g centre and 15g right).



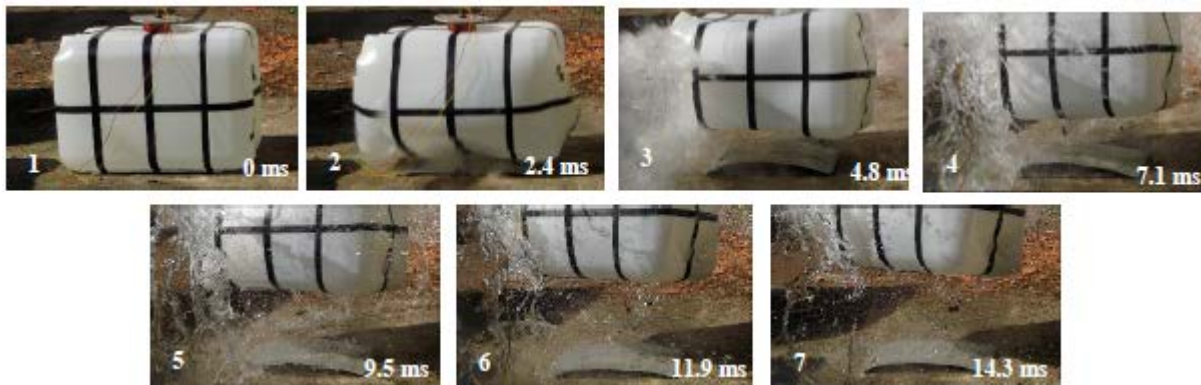
From these results it can be observed:

- detonation of small charges generate elastic deformation of plastic wall, without any permanent deformation;
- four reflection shock movements of plastic container are clearly observed with 10 g charge;
- 15 g charge generates permanent deformation – all the other charges generate elastic deformation;
- keeping inlet open allows a dissipative pressure decreasing process, observed clearly under 15 g charge; it allows the non-destruction of 17 container

Previous results – PETN explosive

Experimental study shows the deformation and blasting of 25 litter container for 2 classes of different explosive charges:

- using only the standard detonator (0.6g PETN charge + primary explosive \Leftrightarrow 0.8 g of PETN) without any supplementary charge,
- using the same conditions of the previous test, but now adding 3g PETN (from a detonating cord) to the standard detonator.



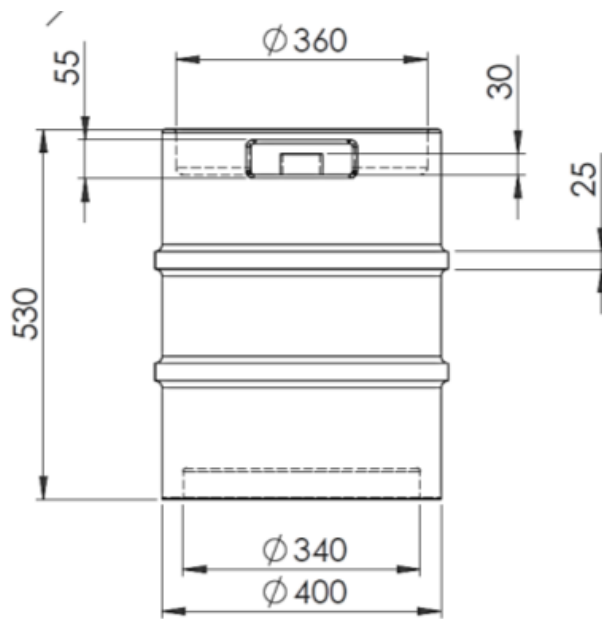
Obtained results prove the validity of simulations, confirming central blasting phenomena process for the generation of an exterior blast generator. Main blast wave expands initially according an “equatorial” disc. The blast process, latter on, is expanding for all directions. Sinusoidal shapes of lateral walls were observed. Measured pressure levels are lower than theoretical expected values. Plastic 25 litter containers are ruptured at final, but not destroyed, confirming predicted values. 18



Design configuration and dimensions

Present vacuum chamber configuration for collecting detonation products

- stainless steel closed explosion chamber (50 liter beer barrel with a 3 mm wall thickness)
- Possibility to collect detonation products without any contamination and avoiding drying operations



Emulsion explosive in a 50lt steel barrel

The barrel was charged successively with increasing charges, starting from a commercial nº 8 detonator and adding emulsion explosive charges of 5g, 10g, 15g, 30g and 60 g.



The initial vacuum condition and electric detonator connection was achieved with the assembled piping system.

Explosive mass	Barrel initial volume [litter]	Barrel final volume [litter]
Detonator nº 8	50	50
Detonator + 5 g	50	50
Detonator + 10 g	50	50
Detonator + 15 g	50	50,10
Detonator + 30 g	50,10	50,20
Detonator + 60 g	50,20	50,50

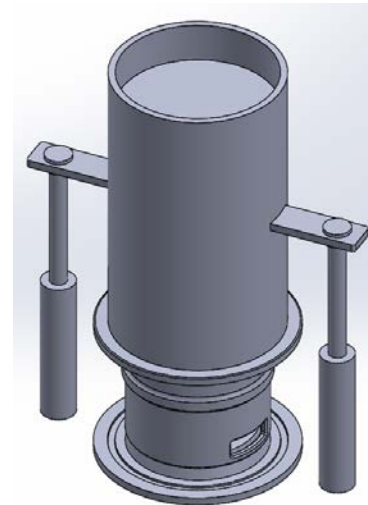
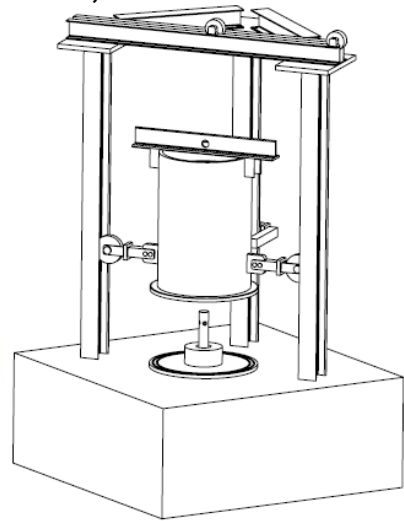
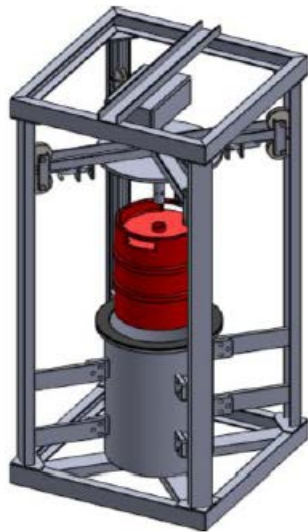


The final barrel condition, after explosive detonation of 60 g charge, where it can be seen the existing fractures in plastic coating surface. Only with this charge level was verified surface modifications, but any structural damage or modification.

Assembled final construction

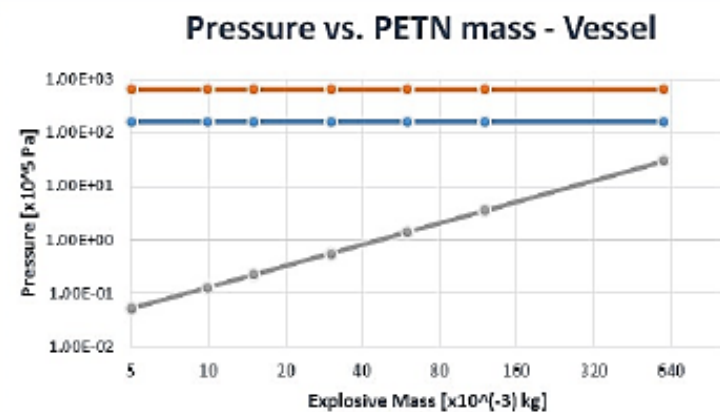
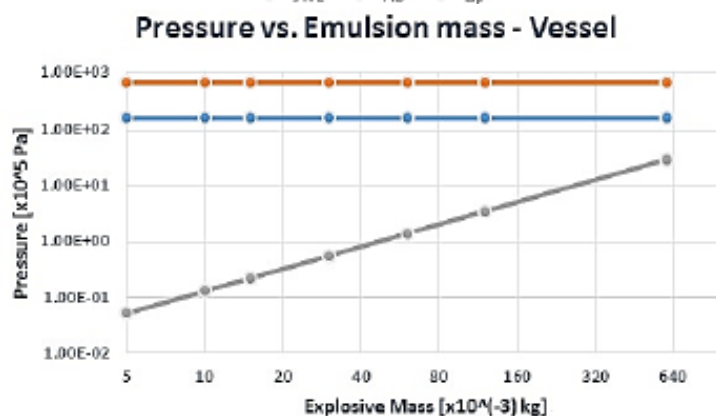
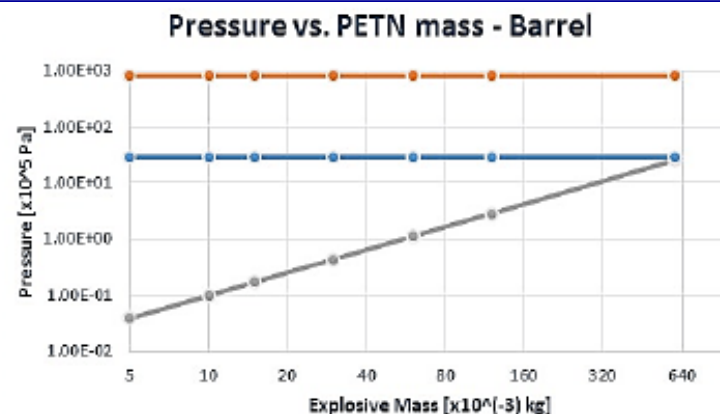
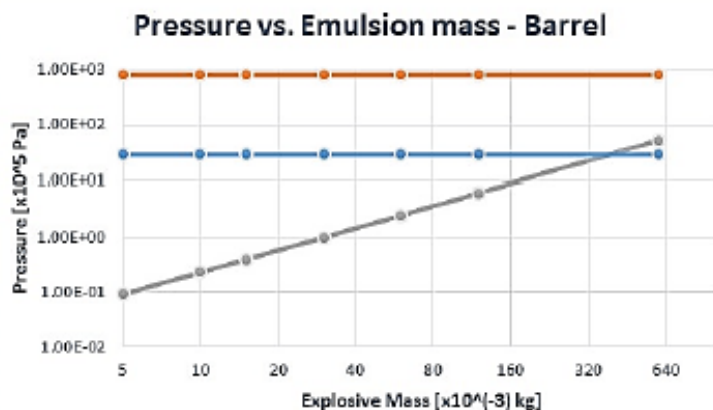
Some considerations taken designing the explosive chamber:

- vertical or horizontal chamber,
- how to perform the opening and closing,
- ensuring vacuum conditions,
- materials to use,
- connections,
- stability,
- safety,
- costs.





Pressure vs. Explosive charge



- The calculations led us to a 20 mm thickness steel cylindrical wall.
- Chamber with a 0,5m diameter and an equivalent length of 1,5 diameter



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Modelling heterogeneous explosive propagation



Conclusions

The present study shows the design and behaviour of plastic and a steel close chamber, after detonation of cylindrical explosive charge.

Predictions were defined from THOR results, performed using JWL parameters, and used in Autodyn® 2D and 3D simulations. For the design limits of the chamber AD-Merkblätter Standards was used.

The used explosive were ammonium nitrate-fuel oil emulsion explosive and PETN.

Wall thickness was discussed and final dimensions were optimized to 3 mm, from a commercial beer barrel of 50 liter volume. The barrel can be enclosed inside a cover explosion chamber of 20mm of wall thickness.

The results obtained prove the validity of assumed simplifications and design procedures of pressure evaluation of small explosive chambers.

Explosive mass were tested up to 60g inside the barrel, allowing to easily collect the detonation products, and 300g using only the vessel, always under vacuum conditions.



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**Thank you
for your attention**