

CRANFIELD UNIVERSITY
ROYAL MILITARY ACADEMY

Lt. Col. Francis D. Halleux, ir, MSc
BEL Bomb Disposal

Improvised Explosives, how to understand the Threat and assess
the Risks

Centre for Defence Chemistry
Department of Chemistry

PhD
Academic Year: 2019 - 2023

Supervisor: Dr Jean-François Pons
Associate Supervisors: Prof M.H. Lefebvre, Dr Ian Wilson
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the degree of Doctor of Philosophy

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ABSTRACT

The research undertaken for this thesis has contributed to address the risk posed by dual-use industrial chemicals as improvised explosives in Improvised Explosive Devices (IEDs). The novelty of this work was the investigation of the detonation properties of Urea - Hydrogen Peroxide (UHP), an oxidiser widely used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide, identified as a potential emerging threat, with very limited academic literature available on its explosive properties. This research project, which includes 150 instrumented firings, was also one of the first attempts to thoroughly characterise a tertiary explosive for risk assessment purposes. The detonability of UHP at small scale was first investigated, successfully validating an experimental setup and a charge geometry that closely approached large-scale behaviour and proved suitable to study other energetics. Consistent detonation performance parameters at large and small scale were determined from complementary experimental approaches, thermochemical calculations and numerical simulations. The collected academic data were further analysed in a Counter-IED (C-IED) perspective within the scope of a limited release technical-operational threat assessment (**not included in this manuscript**). This work has also provided valuable insights into the non-ideality of UHP, highlighting the limitations of the available characterisation methods and modelling tools. In terms of real-world impact, the results published in this body of work provide relevant knowledge to the scientific community, complementing the rather limited available academic literature with a comprehensive characterisation of UHP detonation performance. The outcome is also of great interest for the industrial risk management and process safety. This work was equally important to understand the threat and assess the risk posed by tertiary explosives in a C-IED context and address relevant recommendations to the worldwide intelligence services and the law-enforcement agencies.

Keywords:

Urea – Hydrogen Peroxide; Non-ideal Explosive; Detonation; Performance; Threat Assessment

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LIST OF ABBREVIATIONS AND SYMBOLS

AAP	Allied Administrative Publication
Al	Aluminium
AN	Ammonium Nitrate
ANFO	Ammonium Nitrate Fuel Oil
ASV	Attenuated Shock Velocity
AtN	Attack the Network
BA	Benzoic Acid
BKW	Becker-Kistiakowski-Wilson
Bstr	Booster
CI	Confidence Interval
C-IED	Counter-Improvised Explosive Device
CJ	Chapman-Jouguet
D	Diameter
d	Depth (Chapter 3)
DAX	Disc Acceleration eXperiment
D-BREIE	Data-Base of Range Evaluated Improvised Explosives
DG HOME	Directorate-General Migration and Home Affairs
DtD	Defeat the Device
$E_{b, equ}$	Equivalent bubble energy
EMRTC	Energetic Materials Research and Testing Center
ERDA	Explosives Research and Demonstration Area
EOD	Explosive Ordnance Disposal
EoS	Equation of State
$E_{s, equ}$	Equivalent shock energy
EU	European Union
EU-US	European Union-United States
FBI	Federal Bureau of Investigation
FINEX	Forensic International Network for EXplosives
FWDM	Fragment Weight Distribution Map
GOF	Glass Optical Fiber
HME	Homemade Explosive
HMTD	Hexamethylene Triperoxide Diamine
HP	Hydrogen Peroxide
HPOM	Hydrogen Peroxide Organic Material
ID	Inner Diameter
IE	Improvised Explosive
IED	Improvised Explosive Device

IW(M)	Impedance Window (Method)
JCAT	Joint Counterterrorism Assessment Team
JWL	Jones-Wilkins-Lee
L	Charge Length
LASL	Los Alamos Scientific Laboratory
LEMBE	Laboratory for Energetic Materials and Blast Engineering
M	Mass
M-BKW	Modified Becker-Kistiakowski-Wilson
Mg	Magnesium
NATO	North Atlantic Treaty Organization
NEQ	Net Explosive Quantity
OD	Outer Diameter
PCB	PicoCoulomb
P_{det}	Detonation pressure
PDV	Photonic Doppler Velocimetry
PE	Polyethylene
PI	Power Index
P_{max}	Side-on peak overpressure
PMMA	Polymethylmethacrylate
PtF	Prepare the Forces
PTFE	Polytetrafluoroethylene
PVC	Polyvinyl chloride
PVDF	Polyvinylidene fluoride
Q_{det}	Heat of Detonation
R	Range
RDX	Research Department Explosive, Cyclotrimethylene trinitramine
RMA	Royal Military Academy
ROC	Radius of Curvature
SEDEE	Service d'Enlèvement et de Destruction d'Engins Explosifs
TATP	Triacetone Triperoxide
t_b	First pulsation period
T_{det}	Detonation temperature
TMD	Theoretical Maximum Density
TNT	Trinitrotoluene
TPX	Polymethylpentene
UHP	Urea Hydrogen Peroxide
UN	United Nations
UNi	Urea Nitrate
V_{gas}	Volume of gas

VN	Von Neumann
VoD	Velocity of Detonation
W	Charge Weight
Z	Scaled distance
1DE (MM)	One-Dimensional Euler (Multi-Material)
2DE	Two-Dimensional Euler
Γ	Polytropic exponent
ρ	Loading density

1 Introduction

1.1 Background to the study - Improvised explosives

In today's military and civil conflicts, Improvised Explosive Devices (IEDs), considering their relative ease of use and mediatic impact, remain the weapon of choice of insurgents and, consequently, the most significant cause of casualties. A NATO approved definition for IED is "*a device placed or fabricated in an improvised manner incorporating destructive, lethal, noxious, pyrotechnic or incendiary chemicals and designed to destroy, incapacitate, harass or distract. It may incorporate military stores but is normally devised from non-military components*" (NATO AAP-06, [2021](#)). To address this enduring threat, NATO started in 2010 with a Counter-IED (C-IED) action plan based on three complementary pillars: *defeat the device* (DtD), *prepare the forces* (PtF) and *attack the network* (AtN).

The design of such an unconventional explosive weapon can range from 'simple' to 'sophisticated', depending on the imagination of the terrorist, the time and material available and potentially some form of knowledge or experience. The availability of raw materials is of utmost importance for the bomb maker and improvised explosives (Figure 1-1) will be considered when it is impossible or too risky to acquire, on the black market or through criminal networks, energetics from military stocks (military grade high explosive, mines, artillery shells, etc.) or rock blasting industry (dynamites, ammonium nitrate-based explosives, etc.). Improvised explosives (IEs) refer typically to homemade explosives (HMEs), not produced for commercial or military purposes and applications (Marshall and Oxley, [2009](#); Yeager, [2011](#); Doyle, [2013](#)). HMEs (Brady, [2011](#)) include conventional explosives manufactured illegally, such as Ammonium Nitrate Fuel Oil (ANFO), a typical commercial explosive mixture used in the mining industry but also misused by terrorists since the 70's, especially for large-scale bombings (Sterling Hall Bombing, Madison Campus, Wisconsin, 1970), and non-conventional explosives, such Triacetone Triperoxide (TATP), a sensitive primary explosive (Matyas and Pachman, [2013](#)) also referred to as the '*mother of Satan*' (Yeager, [2011](#)), already synthesised by Palestinian insurgents in the early 80's

and one of the most commonly encountered HMEs over the past 20 years (Paris 2015, Brussels 2016, Manchester 2017).

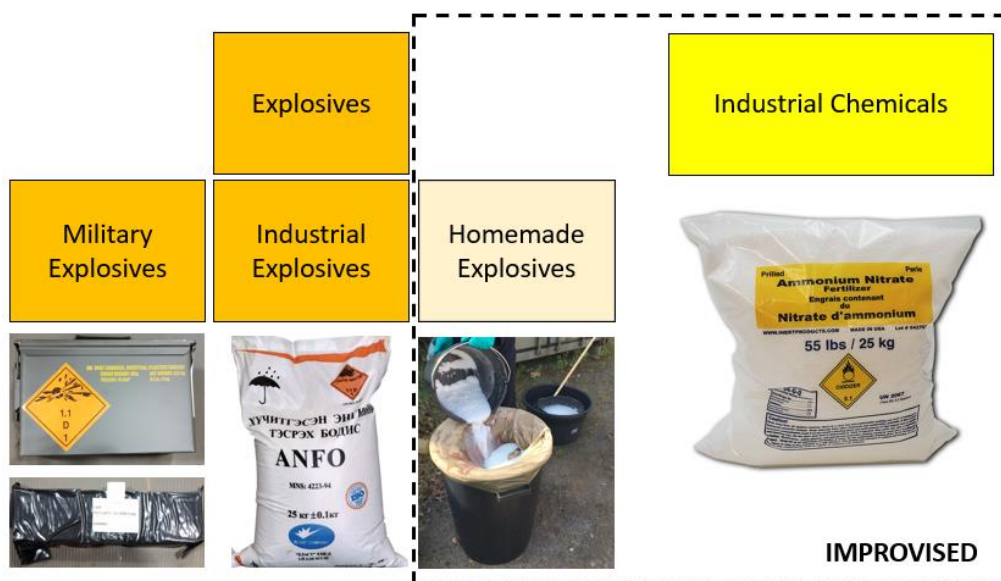


Figure 1-1: Potential explosive charge in IEDs.

Additionally, some industrial chemicals with explosive properties (Merrifield and Roberts, [1991](#); Lewis, [2004](#)), not intended to be used as explosives, could also be considered as improvised explosive charges in a terrorist context. These dual-use energetics are typically low-performance explosives with large critical diameters and do not exhibit any ability to detonate below a certain critical mass which can be as considerable as 10 to 100 kg. Considering their very low level of sensitivity to external stimuli, such as shock sensitivity, they belong to the tertiary explosives group as they need a booster charge to detonate (Meyer et al., [2007](#); Yeager, [2011](#); Doyle, [2013](#)). For those reasons, they are most of the time not considered explosives and not addressed in a generic way by international regulations, potentially making them or their precursors directly commercially available without quantity limitations.

In the fight against terrorism, the importance of addressing tertiary explosives is clear. Even if an industrial chemical is not classified as an explosive because it is not likely to detonate accidentally, it can be used purposely as a tertiary explosive detonated with a bespoke booster in an explosive device, posing a threat to human life and to the environment. This threat should hence be precisely

assessed to evaluate the need for enforcing control on its accessibility on the market. Among dual-use chemicals, fertiliser grade ammonium nitrate (AN), whose detonation properties have been extensively studied for risk assessment purposes (Bauer et al., [1982](#); Hubbard and Marshall, [1996](#)), is nowadays regulated (EU [2019/1009](#)), as a consequence of previous industrial disasters (Prugh, [2020](#)) and its use in terrorist context (Marshall and Oxley, [2009](#); Yeager, [2011](#); Doyle, [2013](#)), as an explosive or an explosive precursor. When this research project started in 2019, Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide (UHP) widely used in the dental, cosmetic and pharmaceutical industry as a solid source of Hydrogen Peroxide, had been identified as an emerging threat (EU-US, [2019](#); JCAT, [2020](#)), with very limited academic literature available on its explosive behaviour (Matyas et al., [2017](#)), encouraging further research to provide relevant knowledge for the scientific community, the industry, the law-enforcement agencies and the intelligence services.

To tackle the threat of improvised explosives, national and international research programs have been launched over the past 20 years, such as the Data-Base of Range Evaluated Improvised Explosives (D-BREIE) project at New Mexico Tech's Energetic Materials Research and Testing Center (EMRTC) (Yeager, [2011](#)) or the Forensic International Network for EXplosives (FINEX). The collected information is no more limited to official restricted bulletins and scientific data are progressively available in peer-reviewed publications dedicated to the study of improvised explosives. Of course, as highlighted in this thesis, a clear distinction must be kept between scientific knowledge available in the open literature and restricted information which should not fall into the wrong hands. This field of investigation remains however particularly challenging (Maienschein, [2012](#)), providing a range of opportunities to address existing research gaps. More research is needed to characterise the threat of IEs by extending the understanding of these compositions, as such formulations do not follow conventional explosive performance and safety standards, or to assess the risk by predicting the effects of IEs, knowing that they generally do not follow standard detonation theory.

1.2 Aim and Objectives

The overall aim of the work presented in this thesis was to address the risk posed by dual-use industrial chemicals (Merrifield and Roberts, [1991](#)) as improvised explosives in IEDs, by characterising, as a relevant case study, the detonation properties of Urea - Hydrogen Peroxide (UHP), an oxidiser produced at large scale in the chemical industry, identified as a potential emerging threat (EU-US, [2019](#); JCAT, [2020](#)), with very limited academic literature available on its explosive properties (Matyas et al., [2017](#)).

This was achieved by focusing on the following individual objectives:

1. Demonstrate detonability at small scale and optimise experimental setup to closely approach large-scale behaviour (**Chapter 2**)
2. Determine detonation performance parameters at large and small scale (**Chapter 3**)
3. Compare detonation performance parameters from advanced characterisation methods (**Chapter 4**)
4. Assess the risk, from previous academic characterisation and complementary operational testing (**Chapter 5 – not included in the manuscript**).

Improvised explosives, how to understand the threat and assess the risks? This research question was hence answered in two steps. The academic characterisation of UHP (**Chapters 2-3-4**), which followed a coherent sequence from initial detonability assessment to detonation performance and advanced characterisation, each chapter including a bespoke literature review, was complemented by a comprehensive technical-operational study (**Chapter 5 – not included in the manuscript**), using the previously collected academic data to feed the C-IED threat assessment. The thesis structure aligned to chapter titles is depicted in Figure 1-2.

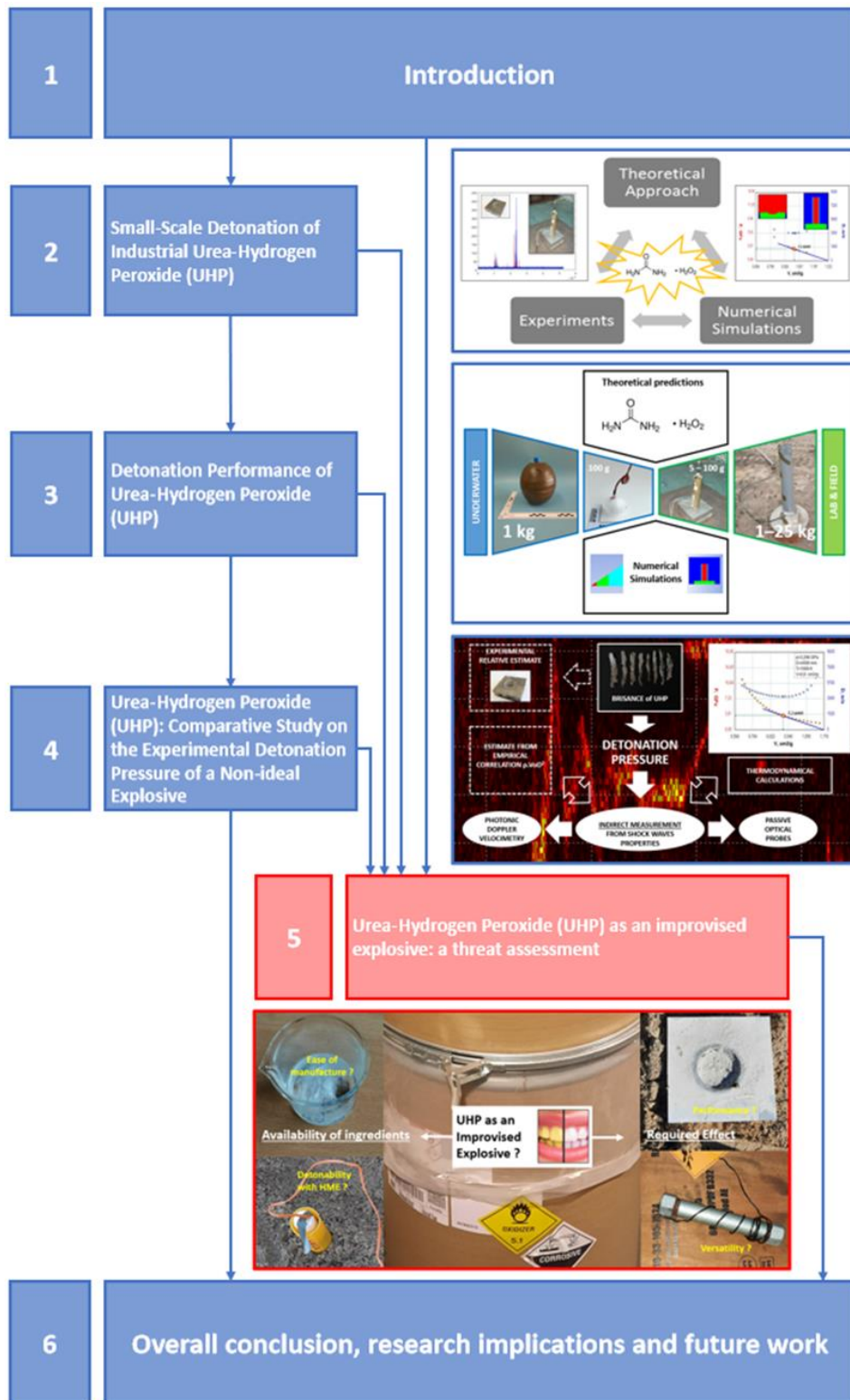


Figure 1-2: Thesis structure aligned to chapter titles, highlighting the coherence of the work and the distinction between academic (blue) and restricted (red) information. Due to its sensitive nature, Chapter 5 is not included in the manuscript.

1.3 Dissemination of the results

The research project (**Chapter 1**) and the proposed methodology were presented (poster), together with some preliminary results (**Chapter 2**) at the *6th Defence & Security Doctoral Symposium* (2020), receiving a 1st prize award (Appendix A). A first research article (Appendix B), addressing the lab-scale campaign (**Chapter 2**), was published in *Propellants, Explosives and Pyrotechnics* (Halleux et al., 2022a).

Preliminary results from the detailed performance characterisation (**Chapter 3**) were presented in 2022 at the *24th New Trends in Research of Energetic Materials Conference* (poster and published proceedings, Appendices C and D, Halleux et al., 2022b) and the *8th Defence & Security Doctoral Symposium* (poster, Appendix E). A second research article (Appendix F) was published in *Propellants, Explosives and Pyrotechnics* (Halleux et al., 2023a).

Initial investigations to determine the detonation pressure using indirect methods (**Chapter 4**) were presented (poster and published proceedings, Appendices G and H) at the *1st International Explosive Conference* (2022), *Future Developments in Explosives and Energetics* (Halleux et al., 2023b). A third research paper (Appendix I), presenting a comparative study on the experimental detonation pressure, was published in *Propellants, Explosives and Pyrotechnics* (Halleux et al., 2023c).

All the academic data feed a threat assessment related to the use of UHP as an improvised explosive, prepared in the format of a **separate** limited release document (**Chapter 5**). Preliminary results were presented at the *10th EU-US Explosives' Experts Seminar* (2022), a restricted security forum, and synthesised in an internal report for DG Home.

Finally, the general approach of the project and some of the key findings (**Chapter 6**) were presented in 2023 at the *Terrorism Risk Assessment, Modelling and Mitigation Seminar Series* (TRAMMSS), organised by Cranfield University.

2 Small-scale detonation of industrial urea-hydrogen peroxide

2.1 Abstract

The adduct of Urea and Hydrogen Peroxide (UHP), also called Carbamide Peroxide, is industrially produced as a solid source of hydrogen peroxide for bleaching, disinfection, and oxidation reactions. As a chemical combination of fuel and oxidiser, UHP has explosive potential but it is unclear whether it could sustain a detonation at small scale. In the configuration we tested, we succeeded in recording self-sustained detonation at relatively small scale under heavy confinement, measuring a maximum experimental velocity of detonation of 3860 m/s at an optimum 1.1 g/cm³ loading density. UHP can sustain a detonation, even at the 100 g scale, but this is strongly dependant on booster size, confinement material, loading density, charge length and diameter. According to our performance assessment, pure UHP exhibits the behaviour of a non-ideal tertiary explosive. Maximum calculated detonation pressures are below 10 GPa, the order of magnitude for commercial blasting explosives. Small-scale results are consistent with literature values from large-scale experiments, although literature on the matter is quite limited. The proposed experimental method can be used to quantify the detonability and performance of other industrial materials that may have energetic properties, or small samples of homemade explosive compositions, avoiding time-consuming, expensive and potentially hazardous large-scale experiments.

2.2 Introduction

The 2020 Beirut explosion of an estimated 2750 tons of Ammonium Nitrate was one more tragic illustration of the explosive potential of industrial oxidising chemicals (Van de Velde et al., [2008](#); Stennett et al., [2020](#)), which are strictly regulated against illicit use and require specific industrial risk control processes. Hydrogen Peroxide (HP) is another typical example of an oxidiser, widely misused by terrorists over the last 20 years for the synthesis of TATP and HMTD (Lefebvre et al., [2004](#); Matyas and Pachman, [2010](#); Contini et al., [2012](#); Matyas

and Chylkova, [2020](#)) or in mixture with organic material (HPOM) (Rarata et al., [2019](#)). HP can also be explosive on its own at high concentrations (Lewis, [2004](#)), which also stimulates current research on novel, green, nitrogen-free, peroxide-based explosives for the mining industry (Rarata and Smetek, [2016](#); Onederra and Araos, [2017](#)). Urea can be directly added to hydrogen peroxide to form an adduct (UHP), which is industrially produced as a solid and stable source of hydrogen peroxide for bleaching, disinfection, and oxidation reactions. As a chemical combination of fuel and oxidiser (Akhavan, [2011](#)), UHP has explosive potential but the available academic literature about its explosive properties is surprisingly limited. To the best of our knowledge, the explosive potential of UHP was first reported by Hussein (Hussein et al, [2016](#)) and Matyas (Matyas et al, [2017](#)). Hussein studied the relative explosive strength of mixtures containing urea and/or peroxide, using ballistic mortar techniques and thermochemical calculations. Matyas characterised comprehensively the explosive and thermal properties of UHP. He demonstrated its detonability, recording an experimental velocity of detonation (VoD) of 3778 m/s for a 30 kg charge. However it is unclear whether UHP could sustain a detonation at the 100 g scale. In this paper, we investigated the detonability of commercial lab grade UHP (97%) at small scale. We studied the effect of parameters such as charge diameter, charge length, loading density and confinement material, together with initiation and boosting material in order to confirm the possibility of detonation at common commercial scales and below, extending previous large-scale publications. Further UHP performance assessment includes witness plate indentation (Smith, [1963](#); Mader, [2008](#)) and VoD measurements using Optimex 64 (Pachman et al., [2017](#)).

2.3 Experimental Section

Our methodology (Figure 2-1) combined theoretical calculation, numerical simulation and a comprehensive experimental campaign, consisting of 40 firings. Theoretical predictions and numerical simulation results were compared with experimental data, obtained at small scale.

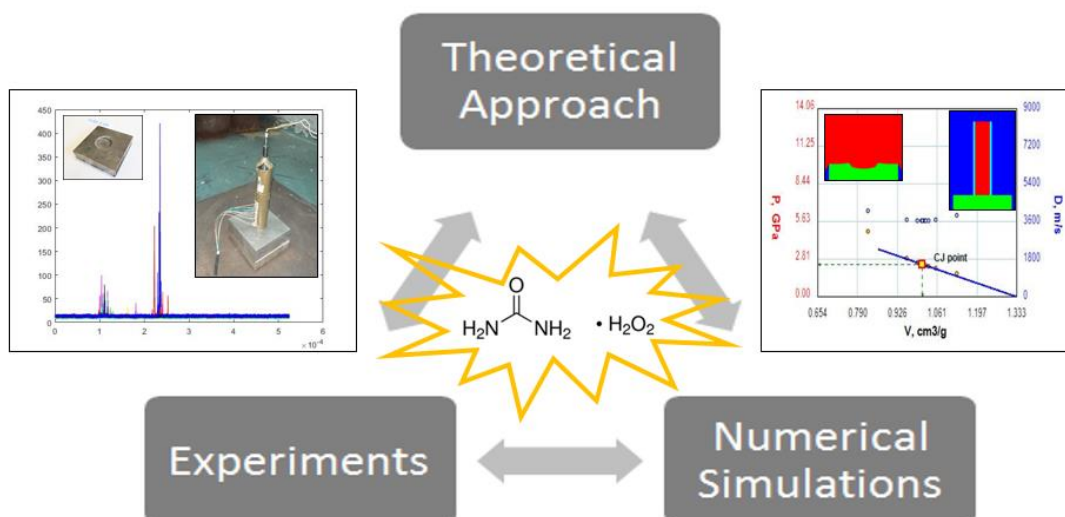


Figure 2-1: Research methodology.

The experimental approach preceded the numerical approach in order to experimentally validate a setup that enabled self-sustained detonations to be recorded. This geometry was then numerically simulated in Ansys Autodyn.

We used commercial lab grade UHP (97%) from a single lot purchased from ALFA AESAR – L13940.36. The particle size distribution was determined by dry sieving (Table 2-1).

Table 2-1: Particle size distribution.

Particle size (µm)	Sample retained (%)
>1000	15.5
1000-800	41.4
800-600	28.1
600-400	14.5
400-200	0.5

In accordance with Matyas' recommendations regarding thermal stability (Matyas et al., [2017](#)), UHP was stored at 5 °C when not in use and left in ambient conditions for one hour prior to the preparation of each charge.

2.3.1 Theoretical Approach

We used thermodynamic code Explo5 (V6.05) calculations (Suceska, [2018](#)) in order to determine the ideal detonation parameters, based on the chemical equilibrium steady state detonation model, and compare them with the values obtained experimentally. The standard enthalpy of formation of UHP was calculated from calorimetry measurements. A Parr 6200 isoperibol calorimeter (operated under 3 MPa O₂) was calibrated with Benzoic Acid (BA) reference and 10 single measurements were carried out on 1.75 g pellet samples (80% UHP - 20% BA as combustion aid), with no combustion residues observed. The standard enthalpy of formation at 298.15 K was calculated by applying the manufacturer standard methods for thermodynamic calculations. The theoretically based equation of state (EoS) molecular fluid EXP-6 (Fried et al., [2002](#)) was selected instead of Becker – Kistiakowski – Wilson (BKW) EoS to give better predictions of detonation velocity and pressure at densities below 1.2 g/cm³. We also used the Explo5 built-in algorithm (Peter et al., [2016](#); Vasilescu et al., [2020](#); Sucéska et al., [2021](#)) with 2250 K freezing temperature to estimate the Jones-Wilkins-Lee (JWL) coefficients and feed our hydrocode simulation (Section 2.3.3).

2.3.2 Experiments

2.3.2.1 Preliminary Testing

The objective of the preliminary testing was to define and validate a setup that enabled self-sustained detonation to be achieved. We used charge masses ranging from 2 g up to 100 g UHP, under light or heavy confinement material, initiated by a pyrotechnical train with or without booster. An overview of the test program is available in Table 2-2.

Table 2-2: Preliminary testing.

UHP (g)	ID (mm)	OD (mm)	L (mm)	Confinement	Initiation	# firings
2-5	10	14	50	Steel 316L	Deto N°8	3
100	30	38	150	INOX 321	Deto N°8 + Booster	6
100	30	38	150	PE	Deto N°8 + Booster	3

We selected an initial charge length of 150 mm, corresponding to 5 inner diameters, a commonly used reference for non-ideal commercial blasting explosives (DIN EN, [2003](#)). Scaled-up UHP explosive charges (0.75 g/cm³, loose) of approximately 100 g, were initiated with a standard N°8 military detonator and C4 plastic explosive boosters of decreasing size (20 g, 10 g, 5 g, 2.5 g). Explosive charges were initiated in direct contact with a witness plate (Al 6082 T651). The indent depths on the witness plates were measured (0.01 mm accuracy) using a Helios micrometer.

2.3.2.2 Validated Setup

Anticipating on the results (see Section 2.4.2.1), 100 g UHP charges, confined in steel cylinders of INOX 321, initiated by a standard N°8 military detonator and a 7.5 g C4 booster, were used for further detonic investigations. An overview of the test program is available in Table 2-3.

Table 2-3: Validated setup test program.

	Purpose	# firings
1	Optimum loading density	12
2	Minimum charge length for stationarity	13
3	Velocity of Detonation	15

To optimise the likelihood and reproducibility of the initiation by distributing it over the entire charge diameter, we designed a bespoke conical cup (Figure 2-2) wherein a booster of constant shape and mass (7.5 g C4) can be moulded and a standard N°8 military detonator can be inserted easily.



Figure 2-2: 3D printed booster cup

In order to assess the effect of loading density on detonation parameters, 12 steel cylinders of INOX 321 were loaded at charge densities ranging from 0.75 to 1.45 g/cm³. They were filled stepwise in 4 g increments with UHP to ensure reproducibility and a constant density along the charge. Higher densities were obtained by hydraulically pressing (0.7 to 56 kN). Densities lower than 1 g/cm³ were obtained by vibration, using ballasts on top. Either pressure or vibration was exerted during one minute at each filling step. The charges were detonated in contact with a 30 mm thick aluminium (6082 T651) witness plate, itself placed on a 20 mm thick anvil, using a standard N°8 military detonator and a 7.5 g C4 booster moulded in a conical cup, producing an initial steady overdriven reaction wave. The indent depth in the witness plate was measured using a micrometer. As we were detonating UHP charges filled at various densities with all other parameters kept constant (confinement material, length, diameter, orientation, firing setup and initiator), we investigated the effect of density on the fragmentation pattern using the Fragment Weight Distribution Map (FWDM) evaluator (Oxley et al., [2001](#); Oxley et al., [2018](#)) This tool has been developed by Oxley to assess the explosive power of pipe bomb devices with a single variable, which is insensitive to percent recovery. Fragments of the steel container (Figure

2-3) were collected, sorted and weighed according to the described procedure. FWDM slopes were determined and compared to average indent depths on the witness plate as a function of the charge loading density.



Figure 2-3: Fragmentation (90% mass recovery) and indent on witness plate for a confined 90 g UHP charge at density 0.83 g/cm^3 .

In an attempt to assess the minimum charge length to allow self-sustained detonation to develop, 13 additional steel cylinders with lengths ranging from 1 inner diameter (30 mm) to 6 inner diameter (180 mm) were detonated as previously described. Detonation velocities were recorded using Optimex 64, the passive optical analyser of explosive processes from OZM Research. We filled 15 additional steel cylinders stepwise at loading densities of 0.75, 1 and 1.1 g/cm^3 (accuracy 0.01 g/cm^3). The charges were detonated as described previously, with optical probes positioned in accordance with the minimum charge length requirement (Figure 2-4), after the first 90 mm (3x ID). 8 blind (non through) holes (depth 2 mm; spacing 7.5 mm) were drilled in the lower part of the tube to insert the optical probes safely and accurately, as shown in Figure 2-5. In this way, the optical probes were protected from noise on the signal and only triggered from the light produced by the adiabatic compression of the air trapped in the blind

hole as the detonation front passed. The VoD is calculated from the recorded arrival times and the known distance between probes.



Figure 2-4: Setup for detonation of confined UHP charge with vertical initiation, witness plate, anvil, optical probes (left), protective structure to optimise fragment recovery (right).

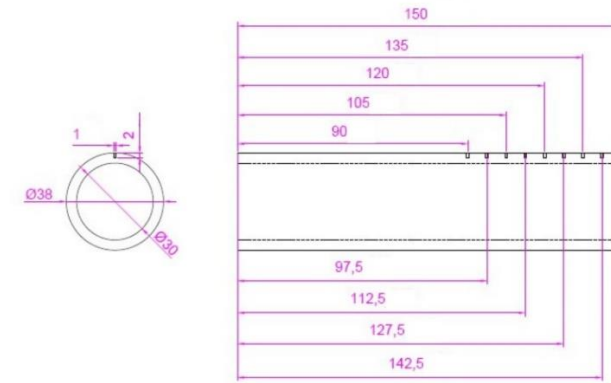


Figure 2-5: Blind holes in steel container for optical probes positioning (all dimensions in mm, tolerance 0.01 mm).

The detonation pressure can be calculated at different loading densities p_0 , using (Cooper, [1996](#)):

$$P_{det} = \frac{\rho_0 \cdot (VoD)^2}{\Gamma + 1} \quad \text{Equation 2-1}$$

Where P_{det} (GPa) is the detonation pressure, ρ_0 (g/cm³), the loading density, VoD (km/s), the detonation velocity and Γ (-), the ratio of the specific heats of the detonation product gases.

A good estimate of the detonation pressure of typical military explosives with densities ranging from 1 to 1.8 g/cm³ can be obtained using a ratio of the specific heats of the detonation product gases equal to 3. However, this value is overestimated for non-ideal explosives with lower detonation velocities, such as AN-based explosives. Detonation pressure was hence calculated from Cooper generic experimental correlation, which covers a wider range of densities:

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad \text{Equation 2-2}$$

2.3.2.3 Experimental Results Assessment

We used the following data to assess UHP detonation performance:

- 1) Visual observation and measurement of the indent depth on the witness plate.
- 2) Visual observation of the fragmentation pattern and calculation of the FWDM slope.
- 3) Measurement of detonation velocities.
- 4) Calculation of detonation pressure.

This enabled us to derive a correlation between detonation pressure and indent depth.

2.3.3 Numerical Approach

The ultimate aim of the numerical approach is to model UHP detonation prior to further large-scale experiments and risk assessment analysis. Within the scope of this paper, we simulated the setup in Ansys Autodyn V14.0 in order to model the indentation on the witness plate and compare it to experimental values. As UHP was not available in the Autodyn library, it was defined using the Chapman-

Jouguet (CJ) state ideal parameters and theoretical JWL coefficients estimated from Explo5 calculations (Section 2.3.1). Geometry was chosen as 2D, axisymmetric with mesh size 0.5 mm. We used EULER type interactions to overcome interfaces problems and two boundary conditions to fix the bottom of the witness plate (*fix*) and to allow detonation gas to escape through the top of the tube (*flowout*).

2.4 Results and Discussion

2.4.1 Theoretical Approach

The detonation parameters from the Explo5 calculations, based on a standard enthalpy of formation of -563 kJ/mol calculated from calorimeter results, are available in Table 2-4. The use of EXP-6 EoS enabled us to estimate JWL coefficients along the detonation products isentrope for explosives with low detonation temperature, when pressure quickly drops to atmospheric.

Table 2-4: Theoretical detonation parameters (CJ point).

Loading Density (g/cm ³)	0.75	0.9	1	1.1
Heat of Detonation (kJ/kg)	-2447	-2496	-2564	-2621
Detonation Pressure (GPa)	2.42	3.86	5.48	6.92
Detonation Velocity (m/s)	3657	4339	4774	5215

These values are theoretical maximum, assuming ideal detonation and infinite charge diameter, with no account of confinement, grain size or critical diameter. We used these maximum values to estimate the theoretical TNT equivalence and dimension our charges according to our firing bunker NEQ limitations, obtaining respectively 0.8 (power index) and 0.5 (hydrodynamic work) (Locking, [2013](#)).

2.4.2 Experiments

2.4.2.1 Preliminary Testing

In our setup, UHP charges (2-5 g) directly initiated by a standard N°8 military detonator failed to detonate, even under heavy confinement. Only combustion was observed, with no detonative output. These experiments did not provide any further technical information but increased our confidence to scale up UHP charges. A minimum booster charge of 5 g C4 was necessary to initiate UHP explosive charges of approximately 100 g confined in steel cylinders. However, we scaled it up to 7.5 g to avoid geometrical effects and distribute the initiation over the entire charge diameter, using a bespoke booster cup. 100 g UHP charges confined in thick polyethylene cylinders initiated by a standard N°8 military detonator and a 7.5 g C4 booster failed to sustain detonation (Figure 2-6). The upper part of the PE tube was shattered due to the detonation of the C4 booster. The UHP charge could not further sustain the detonation in a light confinement material such as plastic. A heavy confinement is required to achieve self-sustained detonation in UHP. This is consistent with literature (Matyas et al., [2017](#)) where failed detonation and explosion decay have been observed for similar UHP charges under intermediate confinement (copper, ID 36 mm).



Figure 2-6: Light confinement – failed detonation: absence of indentation in the plate, presence of unreacted UHP and fragmentation pattern, including petalling of the bottom of the tube.

Scaled-up charges of around 100 g UHP, confined in steel cylinders of INOX 321, initiated by a standard N°8 military detonator and a 7.5 g C4 booster, sustained detonation with indent depth around 5 mm in the witness plate (Figure 2-7). This latter setup was validated and selected for further experiment and modelling.



Figure 2-7: Small-scale detonation of UHP under heavy confinement.

2.4.2.2 Validated Setup

The effect of UHP loading density was first investigated, using our validated setup. The average measured indent depth increases almost linearly with growing loading densities, between 0.75 g/cm^3 (loose) and 1.1 g/cm^3 (pressed), as illustrated in Figure 2-8. Indentation then drops rapidly and less reproducible responses are observed in the interval $1.1\text{-}1.2 \text{ g/cm}^3$. This is probably explained by a decrease in shock sensitivity of pressed UHP due to pressurisation, which decreases the density of potential hotspots that play a key role in detonation propagation in heterogeneous explosives (Clark Souers and Vitello, [2007](#); Mader, [2008](#)).

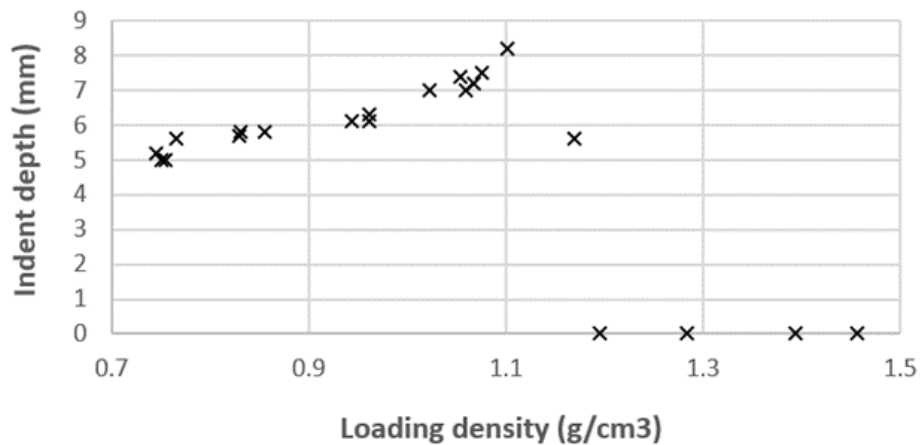


Figure 2-8: Indentation of witness plate as a function of loading density for charge lengths equal to 5 x ID.

Evidence of deflagration is recorded in the density range of 1.2 -1.3 g/cm³ (Figure 2-9). In our charge diameter, confinement and initiation conditions (C4 booster incident steady detonation), indications of dead-pressing are observed at densities above 1.3 g/cm³, including further compaction of the UHP by the shock wave, with spalling in the charge at the back of the tube, absence of fragmentation and limited dispersal of unreacted UHP. Further investigations would be necessary to statistically study UHP dead-pressing density and dying-out distance (Nie et al., [1993](#)). In our setup and geometry, we could not record sustained detonations at densities closer to 1.43 g/ cm³ Theoretical Maximum Density (TMD) (Matyas et al., [2017](#)), and maximum performance was observed at a density of 1.1 g/cm³, which we further used for theoretical predictions and modelling.

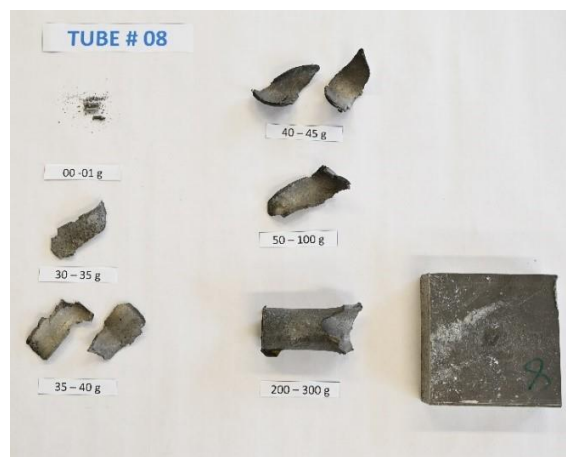


Figure 2-9: Typical deflagration fragmentation pattern (98% recovery), observed at densities above 1.2 g/cm³ with a small number of large, bent and torn fragments, with 90° fracture edges.

A good correlation was found between the indentation of the witness plates and the slopes of the FWDM plots. Both parameters are deemed complementary to assess the brisance of a confined explosive charge, i.e. its destructive fragmentation effect on its immediate vicinity (Meyer et al., [2007](#)). As expected, the brisance increases at higher densities, with maximum FWDM slope and indent depth at 1.1 g/cm³ density (Figure 2-10), while deflagrations are recorded at densities above 1.2 g/cm³.

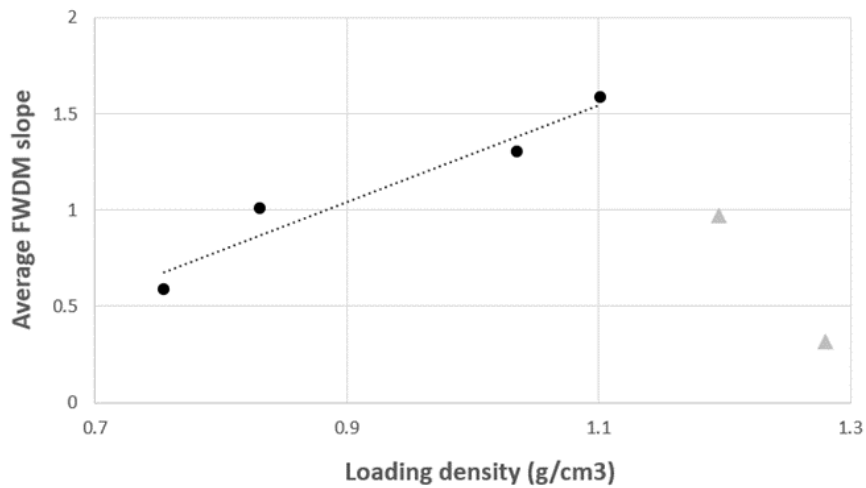


Figure 2-10: Maximum FWDM slope calculated at a density of 1.1 g/cm³. Difference between detonations (black) and deflagrations (grey) are highlighted.

In the configuration we tested and depending on loading density, stationarity is already observed at charge lengths ranging from 2 to 3 inner diameters as shown in Figure 2-11.

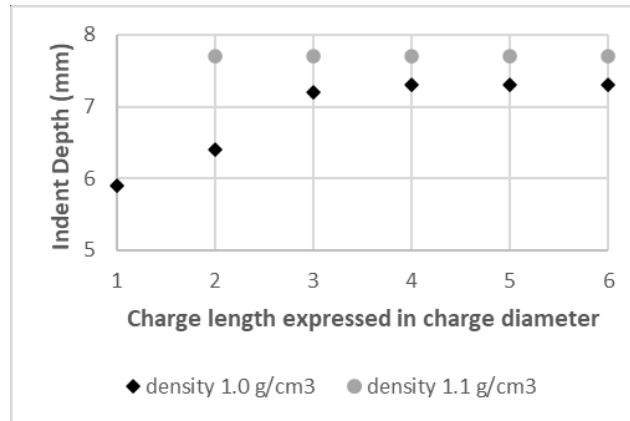


Figure 2-11: Indentation as a function of charge length.

The experimental VoD values (Table 2-5) are only about 80% of the CJ ideal theoretical predictions from Explo5. On the one hand, this could suggest that side effects affect the VoD value and that higher VoD could be recorded at higher charge diameter for a given loading density (Lewczuk et al., [2020](#)). On the other hand, non-ideal behaviour can also be intrinsic and our experimental values could be close to the maximum achievable VoD for UHP. These questions could be answered by carrying out a comprehensive large-scale parametric study focused on the influence of density, diameter and confinement. However the consistency of our small-scale results with literature values from large-scale experiments (Matyas et al., [2017](#)) shows that our study efficiently reflects the detonation property of UHP, allowing lab-scale studies to be performed.

Table 2-5: Performances of UHP charges ($L = 5 \times ID$), with standard deviations.

Loading Density (g/cm ³)	0.75	0.9	1	1.1
Average Indent depth (mm)	5.1 ±0.1	6.2 ±0.1	7.1 ±0.1	7.8 ±0.1
FWDM slope	0.59	/	1.30	1.58
Average VoD (m/s)	2897 ±34	<u>3517^a</u>	3647 ±26	3860 ±38
Calculated P_{det} (GPa)	1.86	3.06	3.82	4.67

^a : value taken from Matyas et al., 2017, VoD for a 8 kg UHP charge confined in a 8 mm thick steel container (ID = 124 mm)

2.4.2.3 Experimental Results Assessment

An overview of the performance parameters of UHP is available in Table 2-5. We derived an experimental linear correlation between the calculated detonation pressure and measured indent depth. This correlation was further compared to ideal values obtained from Explo5 and Autodyn simulation (Section 2.4.3). Figure 2-12 further compares witness plate indentation for different UHP loading densities.

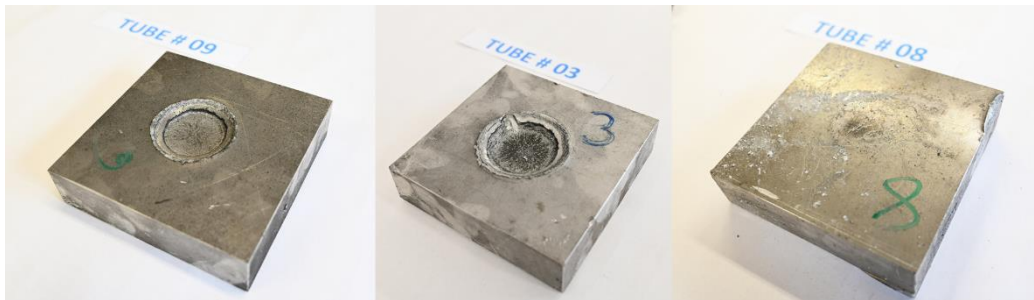


Figure 2-12: Detonation and indentation at respectively 0.75 g/cm³ (left), 1.1 g/cm³ (middle). Deflagration with no indentation at 1.2 g/cm³ (right).

2.4.3 Numerical Approach

Table 2-6 gives an overview of the UHP JWL coefficients from Explo5 (Suceska, [2018](#)), required to feed the numerical modelling (Two-Dimensional Euler – 2DE). Indentations on the witness plate are summarised in Table 2-7 and pictured in Figure 2-13.

Table 2-6: JWL coefficients (Explo5).

Loading Density (g/cm ³)	0.75	0.9	1.1
A (GPa)	102.8273	203.2893	470.6499
B (GPa)	1.4169	2.5687	5.5299
R1	5.5826	5.6525	5.921
R2	1.4846	1.5474	1.7225
w	0.3102	0.3081	0.3001

Table 2-7: Indentation values from numerical simulation.

Loading Density (g/cm ³)	0.75	0.9	1.1
Indentation (mm)	5.5	7.0	9.5

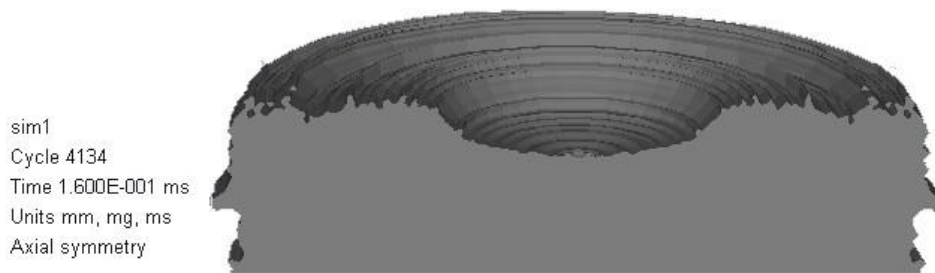


Figure 2-13: 2DE simulation – indentation witness plate.

The experimental linear correlation between the calculated detonation pressure and measured indent depth is here further compared to ideal values, obtained from Explo5 and Autodyn simulation (Figure 2-14). Even if they are within the same order of magnitude, the experimental detonation pressure is up to 33% lower and the resulting indentation of the witness plate up to 20% lower than the simulated ones, especially at growing densities. This can be explained by the fact that our numerical model was fed with theoretically ideal performance parameters, i.e. detonation velocity and pressure.

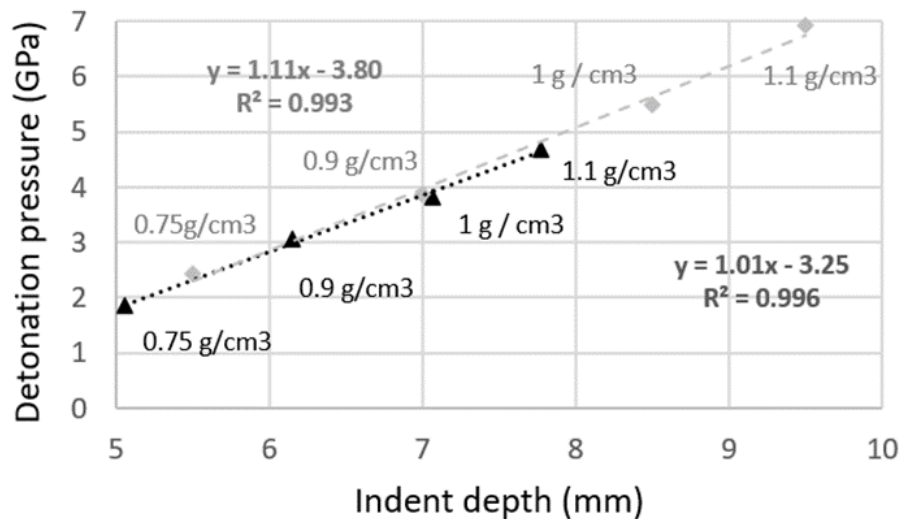


Figure 2-14: Experimental (black) and simulated (grey) linear correlations between detonation pressure and indent depth.

However, both correlations are in good agreement, suggesting that a ratio of the specific heats of the detonation product gases equal to 2.5 is more suitable to estimate the detonation pressure of UHP charges.

Our model used CJ state ideal parameters from Explo5, making it more suitable for conventional explosives (Mader, [2008](#)). We may speculate that the use of reactive flow models to simulate the detonation behaviour of confined non-ideal explosives would better match experimental data (Price and Ang, [2009](#)). However, current UHP characterisation in Autodyn is deemed satisfactory and will be further used to model future larger-scale experiment, including underwater firings.

2.5 Conclusion

In this paper, we have shown that commercial lab grade UHP (97%) is detonable at small scale. We studied the effect of initiation, charge length, charge diameter, confinement material and loading density and validated a geometry and a bespoke pyrotechnical train. In this configuration, we succeeded in accurately recording self-sustained detonation at relatively small scale under heavy confinement. Optimex 64 has proven reliable for lab-scale VoD measurements,

even for non-ideal explosives. Our small-scale results are consistent with literature VoD values from large-scale experiments. Maximum detonation performances were measured at an optimum 1.1 g/cm^3 loading density. In our setup, deflagration or dead-pressing are observed at higher loading densities. Maximum calculated detonation pressures are below 10 GPa, the order of magnitude for commercial blasting explosives. To estimate the detonation pressure of UHP charges, a value of 2.5 for the ratio of the specific heats of the detonation product gases was found more suitable. Our numerical model, including UHP characterisation with JWL coefficients from Explo5 built-in algorithm was deemed satisfactory and will be further used to model future larger-scale experiment, including underwater firings, and related risk assessment analysis. The proposed experimental method can be used to quantify the detonability and performance of other industrial materials that may have energetic properties, or small samples of homemade explosive compositions, avoiding time-consuming, expensive and potentially hazardous large-scale experiments.

3 Detonation performance of urea-hydrogen peroxide

3.1 Abstract

Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide, is commonly used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. However, it exhibits explosive properties and can be easily manufactured from readily available household chemicals, making it a potential emerging threat. We carried out a detailed performance assessment, combining experiments, thermochemical calculations and numerical simulations and highlighted a good level of agreement between experimental data from lab, field and underwater firings. A maximum detonation velocity of 3.65 km/s was recorded for unconfined 25 kg UHP charges at 0.85 g/cm³ (200 mm charge diameter). We determined in these conditions an infinite diameter detonation velocity of 3.94 km/s. These results are also consistent with previous results obtained at small scale under heavy confinement. Airblast measurements highlighted an average 40% TNT equivalence for impulse and 55% for peak overpressure at short distance, which are in good agreement with the 57% (Power Index) calculated from Explo5, while 50% for bubble energy (explosive power) and 20% for shock pressure (brisance) were obtained from underwater experiments. The use of different experimental approaches has proven useful to characterise the performances parameters of a non-ideal explosive for risk assessment purposes.

3.2 Introduction

Carbamide Peroxide or Urea Hydrogen Peroxide (UHP) is commonly used in the dental, cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. This adduct can also be easily manufactured from readily available household chemicals. Like other oxidisers such as ammonium perchlorate (Koch et al., [2022](#)) or ammonium nitrate (Stennett et al., [2020](#)), UHP exhibits explosive properties (Hussein et al., [2016](#); Matyas et al., [2017](#)) and could represent a potential emerging threat. Determining UHP detonation performance parameters is hence important for safety purposes. Because there is a need to predict large-

scale explosive behaviour from small-scale experiments (Hunter et al., [2022](#)), our previous work demonstrated UHP detonability at small scale under heavy confinement, providing an initial lab-scale characterisation of detonation performance parameters, including velocity of detonation records consistent with literature values from large-scale experiments (Halleux et al., [2022a](#)) UHP charges non-ideality was further studied by VoD dependence on charge diameter and confinement (Cooper, [1996](#)), a behaviour typically observed for charge diameters in the 10 cm range with explosives detonating at a lower regime, such as ANFO explosives, and particularly emphasised by recent research at small scale (Bohanek et al., [2022a](#), [2022b](#)). As extensive experimental data is particularly desirable to accurately evaluate the detonation parameters of non-ideal explosives (Mader, [2008](#)), we present in this paper a detailed performance assessment supported by thermochemical calculations and numerical simulations. Initial lab characterisation is completed and complemented by field and underwater instrumented firings using scaled-up charges (Figure 3-1).

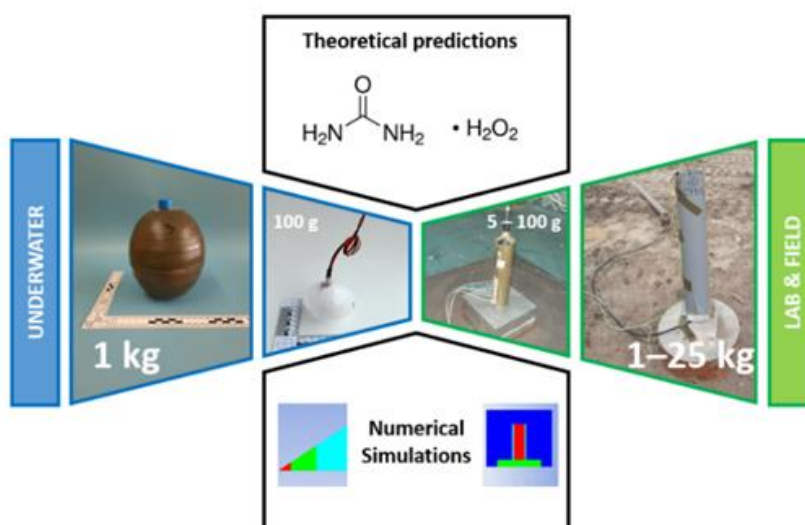


Figure 3-1: UHP Detonation Performance Assessment.

The level of agreement between small-scale and large-scale, between field and underwater experimental performance parameters and between experiment and numerical simulation has been investigated. To that end and for each performance parameter under consideration, we made use of experimental TNT equivalences (Pachman et al., [2014](#); Xiao et al., [2019](#); Collet et al., [2020](#)),

knowing the limitation of the concept (Cooper, [1994](#); Simoens et al., [2011](#); Locking, [2013](#)), especially when comparing non-ideal and ideal explosives (Maienschein, [2012](#)). However, for both academic and safety purposes, we found necessary to compare UHP detonation performance with well-known and documented standards, TNT or plastic explosives such as C4 (91% RDX), which were, for direct comparison, detonated in identical experimental conditions, with particular care for charge configuration (shape, initiation, confinement) and (scaled) distances.

3.3 Experimental Section

We used commercial lab grade Urea Hydrogen Peroxide - UHP (97%) purchased from ALFA AESAR. Average particle size was determined by dry sieving with 85% of the particles larger than 600 μm and 15% larger than 1000 μm . The standard enthalpy of formation of UHP was calculated from calorimetric measurements and we used the thermodynamic code Explo5 (V6.06.02) to determine UHP ideal detonation parameters. Following our previous work (Halleux et al., [2022a](#)), the theoretically based equation of state molecular fluid EXP-6 was selected to calculate UHP VoD and P_{det} , together with its JWL coefficients, required for further modelling of our experimental firing setups in Ansys Autodyn V14.0. For comparison purposes, we also calculated VoD and P_{det} , using the Modified Becker-Kistiakowski-Wilson (M-BKW) EoS, as this equation of state is known to lead to a better accuracy when dealing with explosives showing a high dipolar molecules content in the detonation products and a low detonation temperature (Suceska et al., [2022](#)). In the following subsections, we successively present the respective experimental methods and setups used for the lab, field and underwater firings.

3.3.1 Lab firings

The firing setup basically consists of 80-120 g UHP cylindrical charges at loading densities ranging from 0.75 to 1.1 g/cm^3 , under heavy confinement (stainless steel walls), with an outer diameter of 38 mm, an inner diameter of 30 mm and a length equal to 5 inner diameters. 40 UHP charges were initiated by a standard N°8 military detonator and an 8 g C4 booster. Initial performance assessment

(Halleux et al., [2022a](#)) included Al 6082 T651 witness plate dent and detonation velocity measurements (Optimex 64 – OZM research). VoDs were determined using arrays of passive optical fibre probes to record arrival times and a known distance between probes. P_{det} was further estimated from VoD and loading density (ρ_0) using the following empirical correlation (Cooper, [1996](#)):

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad \text{Equation 3-1}$$

Complementary firings were carried out in the lab. The confinement sleeves were filled by 4 g UHP increments to obtain the following charge densities (theoretical maximum density 1.43 g/cm³) (Matyas et al., [2017](#)), calculated from mass and volume UHP: 0.75 (loose) and 0.85 g/cm³, i.e. slightly compacted by vibration to achieve more uniform loading and homogeneity. The VoD setup (Halleux et al., [2022a](#)) was duplicated (Figure 3-2) and included a total of 16 optical fibre probes, divided in two rows of 8 probes, with 7.5 mm between probes, and the first probe of each row located 90 mm (3 x ID) from the booster charge. The setup was also slightly adapted in an attempt to capture improved signals by reducing the thickness of confinement material between the optical probes and the energetic material under investigation, while avoiding any early triggering from the light preceding the detonation wave due to translucency of the explosive. Instead of inserting the probes in 2 mm deep, non-through (blind) holes drilled in the confinement sleeve, like in previous work, we used all-through holes sealed by a piece of 30 µm thick aluminium tape glued inside the sleeve. Finally, we recorded the VoD and measured witness plate indentation from two 120 g pressed TNT charges (1.61 g/cm³) prepared and detonated in the same conditions in an attempt to assess UHP relative brisance (%) based on plate dent depth (Smith, [1963](#)).



Figure 3-2: 100 g UHP – heavy confinement: (1) N°8 detonator; (2) C4 booster in bespoke holder, (3) Confinement sleeve, (4) UHP charge, (5) 2x8 Optical probes, (6) Al witness plate.

3.3.2 Field firings

The field firings consisted of two separated experimental campaigns in order to (i) measure the VoD to determine a nominal charge diameter for studying UHP performances and (ii) record the airblast characteristics in a selected setup, for which non-ideal effects are considered as limited enough to not significantly influence the performance of the charge, in an attempt to provide a performance characterisation independent of the setup and valid for very large charges. Both experimental setups are depicted in Figure 3-3, while Table 3-1 describes the test program. Upscaled kg-size UHP charges without confinement (PVC casing) were filled in 25 increments and vibrated at each step to achieve a reproducible $0.85 \pm 0.02 \text{ g/cm}^3$ loading density at large scale, avoiding self-compaction phenomenon and density gradient observed at loose density (0.75 g/cm^3) for large charges.

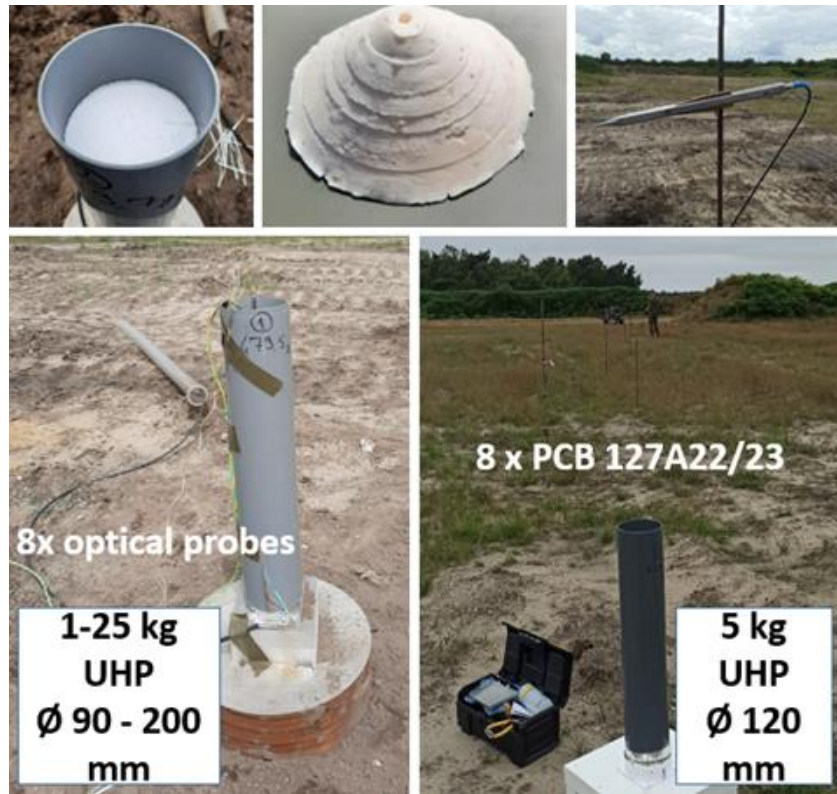


Figure 3-3: 1 to 25 kg UHP: VoD (left) and blast (right).

Table 3-1: Field Firings – UHP (0.85 g/cm³; L=5xID).

OD (mm)	ID (mm)	Mass UHP (kg)	Mass Bstr C4 (kg)	Target data	# shots
90	86.4	1.97	0.10	VoD	2
110	105	3.72	0.22	VoD	2
125	120	5.45	0.35	VoD	2
160	153.6	11.50	0.73	VoD	2
200	193	22.73	1.42	VoD	1
125	120	4.89	0.35	Blast	10

First, in order to determine the nominal charge diameter, 9 UHP charges (average loading density 0.85 g/cm³) in PVC tubes of outer diameters ranging from 90 to 200 mm, were initiated using a standard N°8 military detonator and a bespoke

moulded C4 booster (Figure 3-3, top middle) to fit the inner diameter of the tube and distribute the initiation wave over the entire charge diameter. VoD were measured using passive optical probes inserted in holes drilled in the PVC casing and sealed from inside the pipe by aluminium tape, as previously described (Section 3.3.1). The recorded experimental detonation velocities were then plotted against reciprocal diameter in order to determine unconfined VoD at infinite charge diameter.

Secondly, building upon previous results on nominal diameter, we selected a charge diameter of 120 mm for airblast measurements, a trade-off between the impact of the diameter on the performance characterisation and the practical charge size. With regard to atmospheric conditions, the test site was located 77 m above the sea level, the ambient pressure on the day of the tests was 102.35 kPa (according to the Meteorological Wing of the Belgian Defence). The temperature was 23°C and the relative humidity 60%. We recorded the pressure history and determined incident overpressure and positive phase impulse as a function of scaled distance ($Z=R/W^{1/3}$, with R the radial distance from the charge, and W the charge weight), using 8 blast pencils PCB 127A22/23 respectively positioned at 4.5 ($Z > 2 \text{ m/kg}^{1/3}$, to avoid short distance effects), 10, 15, 21, 26, 32, 37 and 43 meters distances, and compared them to a TNT reference to determine equivalences, using the airblast parameters from TNT surface burst by Kingery & Bulmash (Kingery and Bulmash, [1984](#)). We fired 10 cylindrical charges containing approximately 5 kg UHP and initiated by a 350 g C4 booster and a standard N°8 military detonator. To limit energy dissipation due to cratering and ground shock, the charge was placed on a 45 cm high wood support. As the height of burst was higher than 3 times the charge diameter, the energy loss to crater formation was considered as negligible (Cooper, [1996](#)). This was further supported by the fact that no significant crater formation was observed after detonation. In these conditions and assuming that the ground was a perfect reflector, an ideal hemispherical burst was considered with an effective yield of 200%.

3.3.3 Underwater firings

The underwater test campaign was conducted at Braboplas range, a military underwater demolition site (available depth 9 m), and consisted of two phases, 25 shots at small scale (Halleux et al., [2022b](#)) and 15 shots at larger scale, using respectively 100 g and 1 kg UHP charges. The experimental setup is depicted in Figure 3-4.

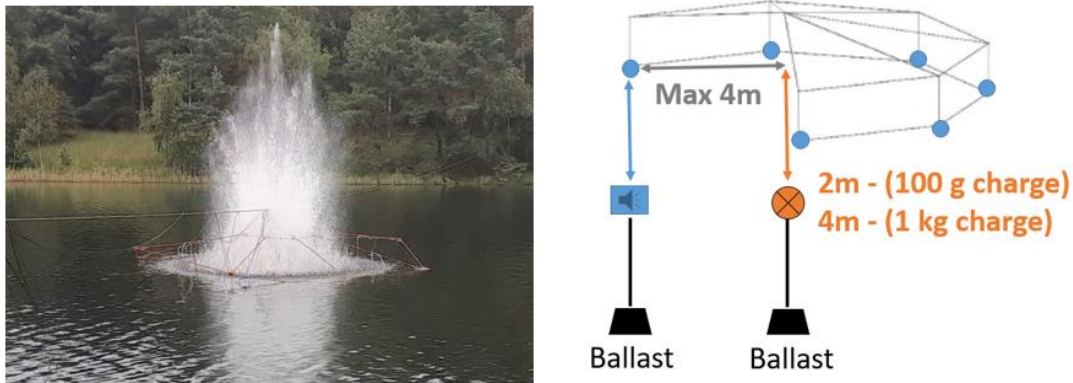


Figure 3-4: 100 g to 1 kg UHP – floating structure.

Explosive charges were suspended in the centre of a floating structure at a depth (d) of 2 m for the 100 g charges and 4 m for the 1 kg charges. Eight voltage mode tourmaline pressure sensors type PCB 138A05 were placed at the same depth, respectively at 1 m, 1.50 m, 2 m and 2.5 m range (R) for 100 g charges and 2 m, 3 m and 4 m for 1 kg charges. According to recommendations in (Milne et al., [2021](#)), pressure sensors were positioned at the depth of the centre of the charge and respectively outside the calculated maximum bubble radii of 0.75 m for a 100 g C4 explosive charge and 1.5 m for a 1 kg (DRDC, [2010](#)), considered as maximum dimensioning charges for the design of our experimental setup. Unconfined spherical charges of 100 g loose UHP (0.75 g/cm^3) in plastic casing (1 mm thick, 70 mm OD), as shown on Figure 3-5, were initiated by an explosive train comparable to the one used in the lab (Section 3.3.1), i.e. a standard N°8 military detonator and a central spherical 8 g C4 booster. We also fired, in the same conditions, spherical 100 g C4 charges for reference and comparison purposes. In an attempt to better assess the influence of the booster (Cao et al.,

[2017](#)) on UHP detonation performance (equivalent shock pressure and bubble energy), we finally fired 8 g C4 booster charges alone.



Figure 3-5: 100 g UHP charge configuration.

Upscaled unconfined spherical charges of 1 kg UHP (loading density 0.80 g/cm^3 , slightly compacted to improve homogeneity) in plastic casing (1 mm thick, 140 mm OD) were initiated by a standard N°8 military detonator, inserted in a bespoke channel to detonate a central spherical 60 g C4 booster (Figure 3-6). Additionally and similarly to the small-scale campaign, the performance of the C4 booster alone was separately investigated. Finally, we fired 1 kg spherical C4 for reference and comparison purposes.



Figure 3-6: 1 kg UHP charge configuration.

Using the procedure described in (Bjarnholt, [1980](#); DIN EN, [2004](#); Klapotke et al., [2016](#)), we recorded the pressure history to determine underwater shock pressure and first pulsation period (t_b). Because the firings were standardised (same

explosive masses, depth, range, water properties) for comparison purposes in order to assess UHP underwater performance, we made use of the so-called shock energy ($E_{s, equ}$) and bubble energy ($E_{b, equ}$) equivalents:

$$E_{s, equ} = \int_{t_0}^{t_0 + \theta} P^2(t) dt \quad \text{Equation 3-2}$$

$$E_{b, equ} = t_b^3 \quad \text{Equation 3-3}$$

where:

t_0 (ms): time of arrival of the shock wave

θ (ms): time at which the pressure has decreased to P_θ (MPa) = $P_{max} \cdot e^{-1}$

t_b (ms): first pulsation period

We simulated both setups in Ansys Autodyn V14.0 in order to model and compare peak overpressure (P_{max}) and equivalent shock energy of the different charges to experimental values. A 1D Euler multi-material model was used, representing a spherical geometry. For UHP, the JWL parameters previously calculated with Explo5 (Halleux et al., [2022a](#)) were fed into Autodyn. Models from Autodyn's standard library were used for C4 and water.

3.4 Results and Discussion

3.4.1 Lab firings

Complementary lab campaign results are available in Table 3-2, while theoretical calculations from Explo5 are presented in Table 3-3. As expected, VoD and indent depth measurements are in excellent agreement with previous measurements (Halleux et al., [2022a](#)). For our reference TNT charges pressed at 1.61 g/cm³, we recorded a detonation velocity of 6.90 km/s, a value in very good agreement with the 6.91 km/s predicted from LASL explosive properties data (Gibbs and Popolato, [1980](#)) and very close to the theoretical maximum 6.95 km/s at 1.64 g/cm³ (Cooper, [1996](#)). Using experimental VoD recorded at small scale under heavy confinement to estimate P_{det} , we determine a relative brisance

(based on P_{det}) of 9% for loose UHP (0.75 g/cm³) and 14% at 0.85 g/cm³ loading density with respect to TNT.

Table 3-2: UHP – 30 mm ID, 4 mm steel confinement, with standard deviations.

UHP Loading Density (g/cm ³)	0.75	0.85
Average VoD (km/s)	2.954 ±0.013	3.454 ±0.004
Estimated P_{det} (GPa)	1.93	2.96
Relative brisance (%) vs TNT* from P_{det}	9	14
Average indent depth (mm)	5 ±0.1	6 ±0.1
Relative brisance (%) vs TNT* from indent depth	30	35

* TNT at 1.61 g/cm³ loading density

Table 3-3: UHP – Explo5 calculations with EXP-6 and M-BKW EoS.

	EXP-6	M-BKW	EXP-6	M-BKW
Loading density (g/cm ³)	0.75	0.75	0.85	0.85
VoD (km/s)	3.66	3.96	4.11	4.37
P_{det} (GPa)	2.43	2.95	3.31	3.98
T_{det} (K)	1600	1467	1606	1483
Q_{det} (kJ/kg)	1588	1548	1624	1582
V_{gas} STP (l/g)	1.06	1.07	1.05	1.06

We measured a maximum indentation of 17.3 mm for the TNT charges and determined a 30-35% relative brisance from indent depth measurements for UHP. This value should however be treated with care. Even if the correlation between the result of a plate dent experiment and the experimentally determined detonation pressure (Smith, [1963](#)) is generally accepted and widely used to assess relative brisance of high explosives (Suceska, [1995](#)), this correlation was actually only demonstrated for conventional military explosives (Smith, [1963](#)). It was later pointed out that this correlation was a consequence of similar expansion of the detonation products of most conventional military explosives down to about 1 GPa, the pressure range of interest of the test, making the peak detonation pressure the major difference between them and leading to the observed linear

correlation (Mader, [2008](#)). However, UHP ($\text{CH}_6\text{N}_2\text{O}_3$) differs from conventional CHON explosives, like TNT, by a high water content in the detonation products and a very low detonation temperature (1500 K, calculated, Table 3-3). Noting that water is a triatomic polar molecule, a significant impact on the isentrope slope between the detonation pressure and 1 GPa is expected. In these conditions, the linear correlation observed between the plate dent result and the detonation pressure of conventional CHON explosives should not be extrapolated to UHP without additional external validation based on the measurement of the UHP detonation pressure, which will be part of future work. As shown in Table 3-3, the choice of EoS influences the calculation of the detonation parameters, such as VoD or P_{det} , and consequently the Autodyn numerical model. Due to the relatively low detonation pressure, it was only possible to achieve a fitting of the JWL equation parameters based on the calculated detonation gases isentrope with the EXP-6 EoS of the Explo5 software. Calculating the Q_{det} (4349 kJ/kg) and V_{gas} (0.67 l/g) values from M-BKW for TNT (1.63 g/cm³), we derived a 57% TNT equivalence by Power Index (PI) (Locking, [2013](#)) for UHP (0.85 g/cm³). Table 3-3 also emphasises the surprisingly low detonation temperatures of UHP as previously mentioned, potentially out of the EoS validation ranges (Suceska et al., [2022](#)) and hereby questioning the overall accuracy of the calculation.

3.4.2 Field firings

Looking at field firings (no confinement), the recorded UHP VoD value in the field are summarised in Figure 3-7, with a maximum of 3.65 km/s at 200 mm charge diameter and the possible beginning of a plateau observed from 160 mm charge diameter. The observed deviation is likely due to density variations, the charge preparation method being only accurate to ± 0.02 g/cm³ at this scale. Based on the recorded data, VoD at infinite charge diameter is about 3.94 km/s, namely 96% and 90% of the ideal VoD predicted from Explo5 using EXP-6 and M-BKW EoS, respectively, indicating a non-ideal character (Mader, [2008](#)) typically observed with explosives detonating at a comparable regime (Cooper, [1996](#)). This result is also consistent with the 3.78 km/s recorded by Matyas (Matyas et

al., [2017](#)) in comparable charge diameter (206 mm) but higher loading densities (0.93 g/cm^3) and heavier (steel) confinement.

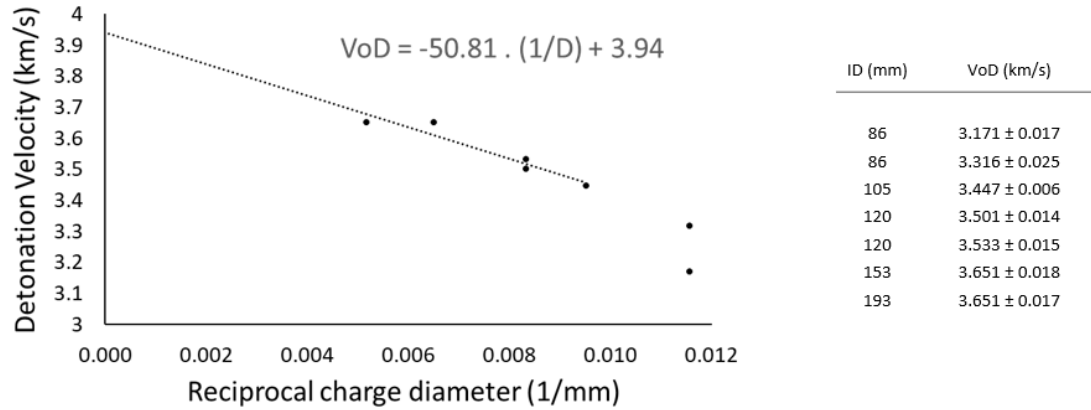


Figure 3-7: UHP Detonation Velocity vs reciprocal diameter ($0.83 \leq$ loading density (g/cm^3) ≤ 0.87) (left). 95% Confidence Interval (CI) on VoD measurements are provided in the table (right), highlighting the uncertainty within each individual firing.

As far as airblast parameters are concerned, reproducible pressure-time histories were recorded (as illustrated on Figure 3-8), enabling side-on peak overpressure and positive impulse to be determined and compared to TNT data.

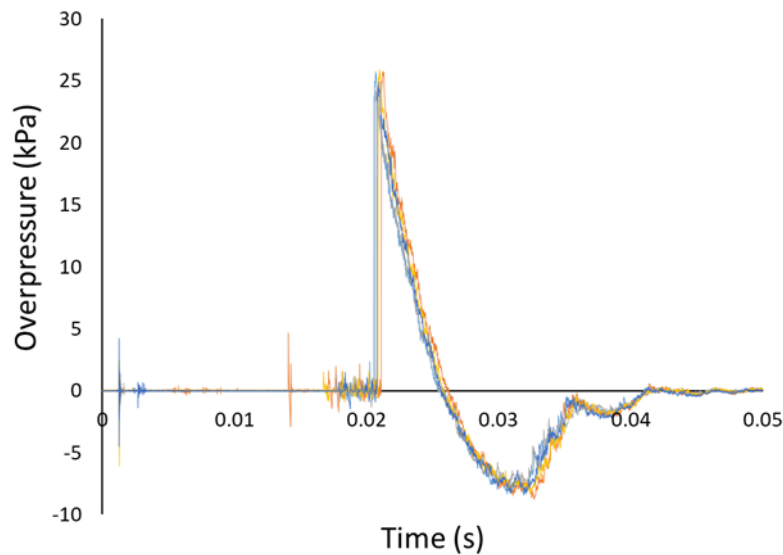


Figure 3-8: 5 kg UHP (0.85 g/cm^3) – 10 m standoff (5 shots).

Figure 3-9 summarises the TNT equivalences for overpressure and impulse as a function of UHP scaled distance. As expected, TNT equivalences are dependent on scaled distances (Pachman et al., [2014](#); Xiao et al., [2019](#)), which could be explained by the rather large distance interval considered (Simoens et al., [2011](#)) and the significant difference between the composition of TNT and UHP detonation products, as previously discussed. An influence of the charge shape at a lower scaled distance cannot be excluded (Simoens et al., [2011](#)). Even if the same trend is observed, TNT equivalences from overpressure are higher than those from impulse. The order of magnitude is however comparable to commercial blasting explosives detonating at a similar regime (Bonhoux, [1980](#); Wharton et al., [2000](#); Bourdeaux and Mory, [2003](#)) and in good agreement with the 57% TNT equivalence (PI) calculated from Explo5 (Section 3.4.1).

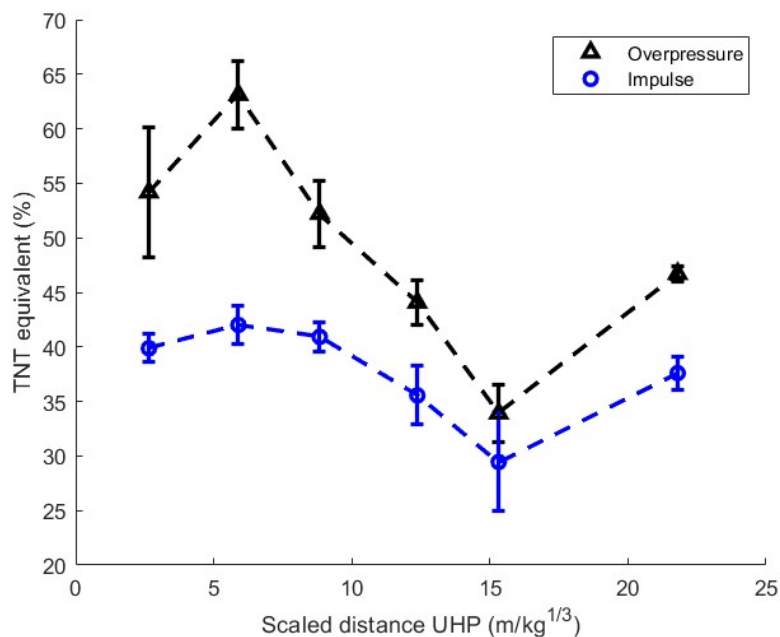


Figure 3-9: TNT equivalences for UHP airblast parameters at 0.85 g/cm^3 (line with average values as a visual guide), with error bars representing standard deviation.

3.4.3 Underwater firings

The experimental average shock wave parameters and calculated equivalent shock ($E_{s, \text{equ}}$) and bubble ($E_{b, \text{equ}}$) energies from the underwater firings are summarised in Table 3-4. As far as UHP is concerned, these values include the contribution of the respective C4 boosters (Bstr). Additionally, predictions based on numerical simulations with Autodyn (using Explo5 parameters calculated with EXP-6 EoS) for peak overpressure and equivalent shock energy are mentioned.

Table 3-4: Underwater Firings – Small and large scale – mass (M), depth (d), range (R), peak overpressure (P_{max}) and first pulsation period (t_b) with standard deviations, equivalent shock ($E_{s, \text{equ}}$) and bubble ($E_{b, \text{equ}}$) energies.

	M (g)	d (m)	R (m)	P_{max} (MPa)	t_b (ms)	$E_{s, \text{equ}}$ (kPa ² s)	$E_{b, \text{equ}}$ (10 ⁻³ s ³)
UHP ^a	100	2	1.5	5.67 ± 0.7 8.12 ^c	81 ± 2	450 2360 ^c	0.5
C4 ^b	8	2	1.5	4.07 ± 0.4	48 ± 1	162	0.1
C4	100	2	1.5	12.93 ± 0.9 12.97 ^c	121 ± 1	4590 4670 ^c	1.8
UHP ^a	1000	4	3	8.21 ± 0.7 8.70 ^c	178 ± 4	2192 4660 ^c	5.6
C4 ^b	60	4	3	4.87 ± 0.4	90 ± 2	587	0.7
C4	1000	4	3	14.22 ± 1.4 14.06 ^c	220 ± 2	11381 10930 ^c	10.6

^a main charge with C4 booster; ^b booster charge; ^c Autodyn

On the one hand, C4 has proven a good reference explosive for underwater experiments. Experimental results and simulations for C4 are in good agreement for both small-scale and large-scale campaigns, and consistent with literature data related to underwater performance of RDX-based compositions (Stromsoe and Eriksen, [1990](#); Kowsarinia et al., [2012](#)), giving us confidence in the experimental setup and the recorded results. As expected, P_{max} for the 100 g and 1 kg, respectively at 1.5 m and 3 m standoffs, are within the same order of magnitude as they have been measured at comparable scaled distances (3.23 vs 3 m/kg^{1/3}). Considering the 8 to 150 g C4 charges fired at 2 m depth, the linear regression (Figure 3-10) of experimental first pulsation periods against the cubic

root of the explosive mass is in good agreement with (Lin et al., [2014](#)) where 95% RDX charges (6 to 10 g) were detonated at the same depth.

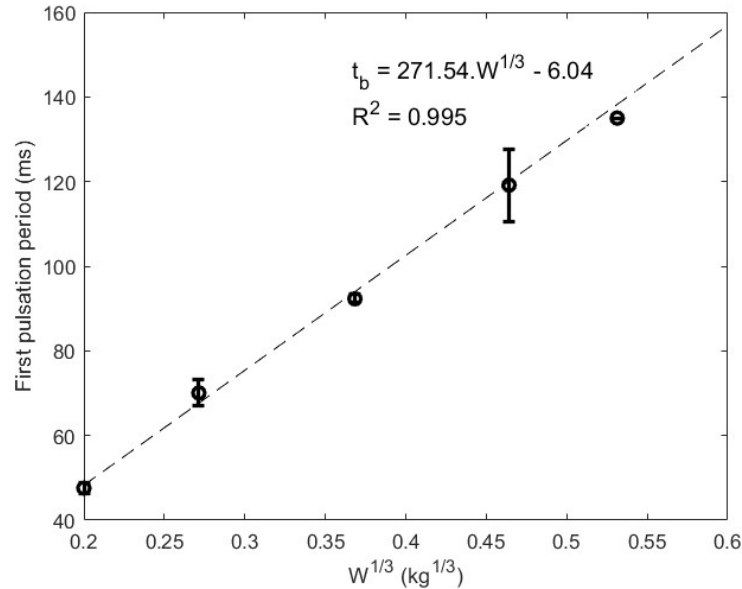


Figure 3-10: 8 to 150 g C4 (1.63 g/cm³) – experimental first pulsation period at 2 m depth, with error bars representing standard deviation.

On the other hand, UHP experimental data for equivalent shock energy ($E_{s, equ}$) differ significantly from the Autodyn simulation, particularly at small scale (Table 3-4). Even if the numerical predictions for P_{max} for the 100 g (8.12 MPa) and 1 kg charges (8.70 MPa) are in good agreement as they are calculated at comparable scaled distances, this scaling is not observed experimentally (5.67 MPa vs 8.21 MPa) and suggests that strong non-ideal effects affect the detonation of the 100 g charge. However, the numerical values from Autodyn for UHP should also be treated with care, as the JWL coefficients used in the model and calculated from Explo5 have not been validated experimentally, which would require large-scale cylinder expansion testing (Esen et al., [2005](#)). Further investigations would also be required to first characterise the actual detonation regime of UHP at small scale and assess its non-ideality. Considering the rather small charge radius (35 mm) and the absence of confinement, the detonation of the 100 g UHP charges in this configuration may have not achieved a steady state. UHP experimental performance parameters are however somehow closer to numerical predictions when considering the 1 kg charges, especially for P_{max} . The experimental

equivalent shock energy is about 50% of the numerical prediction. This difference between experiments and simulation could hence be attributed to the non-ideal behaviour of UHP in these conditions, to the limited accuracy of the model, taking into account UHP specific detonation products discussed in Section 3.4.1, or to a combination of both.

The 1 kg charge with a larger charge radius (70 mm), the mass being limited by the actual experimental setup, is therefore considered as more suitable to characterise the UHP detonation performances, which could be compared to C4. However, the equivalent shock and bubble energies of UHP available in Table 3-4 have been calculated for a 1 kg UHP charge and a 60 g C4 booster, while the 1 kg C4 did not require any booster. Assuming additivity effect (Cao et al., [2017](#)), we subtracted the relative contribution of the 60 g C4 booster from the equivalent shock ($E_{s, \text{equ}}$) and bubble ($E_{b, \text{equ}}$) energies of UHP (Table 3-4) in order to compare identical explosive quantities and derive TNT equivalences (Table 3-5). Using literature data (Kicinski and Szturomski, [2020](#)) for TNT first pulsation period, we obtain a 50% TNT equivalence for bubble energy (explosive power). When it comes to shock pressure, we eliminate the contribution of the booster and calculate a 14% equivalence with respect to C4. Using a 1.3 TNT equivalence for C4, consistent with literature data related to underwater shock performance of RDX-based compositions (Stromsoe and Eriksen, [1990](#); Kowsarinia et al., [2012](#)) and calculated from the ratio of the respective estimated detonation pressures (Cooper, [1996](#)) (Section 3.3.1), which best characterise the shattering effects (Cooper, [1994](#)) of explosives, we derive an estimated maximum 20% TNT equivalence for brisance for UHP. As expected for explosives detonating at a lower regime, the TNT equivalence of UHP for brisance is rather low.

Table 3-5: Underwater Firings – TNT equivalences (%).

Charge	Brisance	Explosive Power
1kg UHP	20	50

3.4.4 Performance assessment

Integrating all the results obtained from different experimental approaches presented above, we were able to characterise the detonation performance of UHP:

1. As expected for an energetic material detonating at a rather low regime, the brisance of UHP, its destructive fragmentation effect on its immediate vicinity (Meyer et al., [2007](#)), has proven weak (20%) when compared to conventional explosives. A good level of agreement was found between TNT equivalence from underwater shock energy and TNT equivalence based on detonation pressure calculated from VoD, either in the lab or in the field. Future work should enable us to further correlate these results to the brisance determined by indirect measurement of the detonation pressure (**Chapter 4**).
2. UHP explosive power is rather limited (50%) as demonstrated by TNT equivalence based on underwater bubble energy or TNT equivalence based on airblast characteristics (long distance blast wave), which have proven consistent and in good agreement with the 57% (PI) calculated from Explo5.

The validity of the small-scale setups used to characterise detonation parameters has been investigated. VoD measurements carried out in the lab are consistent with results from the field (95%). Further improvements might include optimisation of charge geometry and reproducibility of loading densities. When it comes to explosive power, the airblast data from the field are in good agreement with results from the kg-size underwater campaign, while smaller charges could not adequately describe large-scale steady behaviour.

3.5 Conclusion

We carried out a detailed performance assessment, combining experiments, thermochemical calculations and numerical simulations and highlighted a good level of agreement between experimental data from lab, field and underwater firings. A maximum detonation velocity of 3.65 km/s was recorded for unconfined

25 kg UHP charges at 0.85 g/cm^3 (200 mm charge diameter). We determined in these conditions an infinite diameter detonation velocity of 3.94 km/s. These results are also consistent with previous results obtained at small scale under heavy confinement. Airblast measurements highlighted an average 40% TNT equivalence for impulse and 55% for peak overpressure at short (scaled) distance ($Z=2$), which are in good agreement with the 57% (PI) calculated from *Explo5*, while 50% for bubble energy (explosive power) and 20% for shock pressure (brisance) were obtained from underwater experiments. The use of different experimental approaches has proven useful to characterise the performances parameters of a non-ideal explosive for risk assessment purposes. Future work includes experimental measurement of UHP P_{det} (**Chapter 4**) to better assess its non-ideal character and a detailed analysis of the accuracy of the related thermodynamic calculations.

4 Urea-hydrogen peroxide: comparative study on the experimental detonation pressure of a non-ideal explosive

4.1 Abstract

Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide (UHP) industrially used as a solid source of hydrogen peroxide, exhibits the behaviour of a tertiary explosive but a detailed performance characterisation is still lacking in the literature. In this work, we calculated a 20% experimental TNT equivalence for brisance, i.e. the shattering effect from the shock wave transmitted from the detonating high explosive into adjacent materials, by experimental indirect measurement of UHP detonation pressure. We determined a 3.5 GPa detonation pressure for 5 kg unconfined UHP charges (0.87 g/cm^3 , 120 mm charge diameter) by measuring the attenuated shock wave velocity (ASV) in adjacent inert materials using passive optical probes. Particle velocity measurements at the interface of a PMMA impedance window carried out with Photonic Doppler Velocimetry on scaled-down charges of 90 g UHP under heavy confinement (0.85 g/cm^3 , 30 mm charge diameter, 4 mm thick steel) are consistent with ASV results in the PMMA acceptors but further investigations are required to determine the detonation pressure, using a small-scale experimental setup. The ASV method has proven reliable to assess the brisance of a non-ideal explosive for risk assessment purposes.

4.2 Introduction

Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide (UHP), is industrially used as a solid source of hydrogen peroxide. Like other oxidisers such as ammonium nitrate (Stennett et al., [2020](#)), or AN-based explosive compositions (Scott et al., [2023](#)), it exhibits significant non-ideal detonation properties at the 10-cm scale. To the best of our knowledge, the explosive behaviour of UHP was rather recently studied in the literature and a detailed characterisation of UHP detonation performance parameters is still lacking. Hussein carried out ballistic mortar experiments and thermochemical calculations to assess the relative

explosive strength of mixtures containing urea and/or peroxide (Hussein et al., [2016](#)). Matyas investigated UHP sensitivity, thermal properties and detonability at large scale (Matyas et al., [2017](#)), while preliminary work from the authors demonstrated UHP detonability at small scale and highlighted UHP charges non-ideality by VoD dependence on charge diameter and confinement. Additionally, UHP relative explosive strength was further assessed from experimental underwater bubble energy and airblast parameters (long distance blast wave) measurements (Halleux et al., [2022a](#), [2023a](#)). Within the scope of a performance assessment, one of the key parameters still to be addressed was the brisance, the shattering effect from the shock wave transmitted from a detonating high explosive into adjacent materials. Examples of standardised tests (Cook, [1958](#); Suceska, [1995](#)) available to assess the relative brisance of explosives include the Hess test, evaluating the compression of a lead cylinder, the Kast's method, using a copper crusher or the plate-denting test (Smith, [1963](#)). The latter has proven effective to correlate the indentation of a witness plate with the experimentally determined detonation pressure of conventional military explosives but extrapolation to a material such as UHP might be questionable taking into account (major) differences in detonation products composition, particularly water content, and very low detonation temperature (Halleux et al., [2023a](#)). Considering the non-ideal behaviour of UHP, it was decided to quantify the brisance of UHP through its predominant parameter, the detonation pressure (P_{det}) (Smith, [1963](#); Suceska, [1995](#)), as illustrated in Figure 4-1.

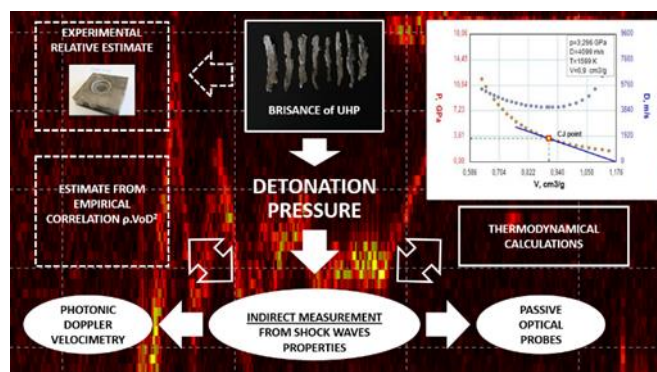


Figure 4-1: General approach – UHP brisance by indirect measurement of the detonation pressure.

The detonation pressure can be calculated from thermodynamical codes, estimated using empirical correlations from VoD and loading density (ρ) (Urtiew and Hayes, [1991](#); Cooper, [1996](#)) or determined experimentally. Considering the time-scale of the phenomenon and the severe conditions of pressure and temperature (Suceska, [1995](#)), direct measurement of the detonation pressure using in situ gauges (Fuller and Price, [1964](#)) such as Polyvinylidene fluoride (PVDF) piezoelectric (Hodges et al., [2000](#)) or Manganin piezoresistive sensors (Zhang et al., [2018](#)) is challenging and not yet widely applied or validated, especially when considering kg-scale non-ideal explosive charges. However, indirect measurement methods are also available to determine the detonation pressure, observing the shock wave properties in inert well-characterised adjacent materials (impedance matching) and not interfering with the detonation wave (Pachman et al., [2018](#)).

In this comparative study, we investigated UHP detonation pressure respectively at large and small scale using two distinct indirect methods, respectively measuring shock then particle velocities. First, at large scale, using an optical system, we looked at the Attenuated Shock Velocity (ASV) in different inert materials. Secondly, in an attempt to study large-scale behaviour from lab-scale experiments (Kunzel and Kucera, [2021](#); Hunter et al., [2022](#); Scott et al., [2023](#)) and avoid time-consuming, expensive and potentially hazardous large-scale experimental campaigns, we used Photonic Doppler Velocimetry (PDV) in combination with a Polymethylmethacrylate (PMMA) impedance window (IW). One of the key advantages of this method, compared for example to the flyer plate method (Duff and Houston, [1955](#); Pachman et al., [2018](#)), is the potential ability to capture the whole particle velocity history of an explosive/inert material interface from one single shot. It is however limited to transparent contact materials. The experimental detonation pressure is compared to the predictions from thermochemical calculations (using the ideal model) and discussed, together with the overall accuracy of the calculations and their limitations when dealing with non-ideal explosives. The experimental detonation pressure is further compared to the estimate from empirical correlations based on VoD and loading density. An experimental TNT equivalence of UHP for brisance is

proposed. We assess the reliability and accuracy of the experimental methods and the level of agreement between large-scale and small-scale results, particularly the validity of the small-scale setup for quick assessment purposes.

4.3 Experimental Section

In line with our initial work, we further used commercial lab grade UHP (97%) purchased from ALFA AESAR. We had determined the average particle size by dry sieving with 85% of the particles retained in the 600 μm mesh and 15% in the 1000 μm mesh. Using the standard enthalpy of formation of UHP calculated from calorimetric measurements, thermochemical calculations were carried out with the Explo5 code (V6.06.02) (Suceska, [2021](#)). We initially used the theoretically based equation of state molecular fluid EXP-6 (Fried et al., [2002](#)), which predicted lower detonation pressures and enabled the determination of the JWL coefficients required for the numerical modelling in Ansys Autodyn (Halleux et al., [2022a](#), [2023a](#)). However, for comparison purposes, we also performed the calculations with the M-BKW EoS, as this equation of state provides greater accuracy for explosives with a low detonation temperature and a high dipolar molecules content in the detonation products (Suceska et al., [2022](#)). UHP ideal detonation parameters, such as detonation velocity, pressure and polytropic exponent, were compared to experimental data. Building upon initial measurements carried out at loose density (0.75 g/cm^3), where self-compaction phenomenon and density gradient were observed for large charges, it was decided to increase the UHP charge loading density to 0.85 g/cm^3 ($\pm 0.02 \text{ g}/\text{cm}^3$), 59.4% of the reported 1.43 g/cm^3 TMD (Matyas et al., [2017](#)), to achieve more uniform loading and homogeneity. This density was also easily obtained, without heavy pressing equipment, which sounded realistic in a terrorist perspective, as UHP, within the scope of our research, was also studied as a potential emerging threat. In the following subsections, we present the selected indirect methods and respective experimental setups to investigate the detonation pressure at large and small scale.

4.3.1 P_{det} by ASV (large-scale campaign)

The ASV method consists of measuring the arrival time at different depths in an inert acceptor in contact with an explosive charge using optical probes and extrapolating the shock velocity at the explosive/inert interface (Kunzel et al., [2017](#)). The light signal is emitted by the ionised air at the bottom of the holes drilled to insert the probes. This method neglects the Von Neumann (VN) spike, as it does not lead to air ionisation due to its very small impulse. In this study, we selected a charge diameter of 120 mm, a trade-off between the impact of the diameter on the performance characterisation and the practical charge size. In this charge diameter (PVC casing, 2.5 mm thick), we previously recorded an average VoD of 3.520 km/s for unconfined UHP, about 90% of the VoD extrapolated at infinite charge diameter from our experimental data (Halleux et al., [2023a](#)). We fired 10 cylindrical charges (two shots for each acceptor) containing approximately 5 kg UHP ($L=5 \times D$, $\rho=0.87 \text{ g/cm}^3$, 60.8% TMD) and initiated by a bespoke moulded conical 350 g C4 booster (Figure 4-2, top left) and a standard N°8 military detonator. Building upon the results from a preliminary ASV campaign (86.4 mm charge diameter) carried out to select and design the inert acceptors, we prepared two disks (thickness 32 mm; diameter 120 mm) of five different materials with well-characterised shock properties (Marsh, [1980](#); Cooper, [1996](#)) in an attempt to cover a wide range of shock impedances and construct the (reflected) Hugoniot of the detonation reaction products of UHP: Aluminium 7075, Magnesium alloy AZ31B, Polymethylmethacrylate (PMMA), Polytetrafluoroethylene (PTFE) and Polymethylpentene (TPX). As TPX was only available in 50 mm diameter rods, we filled the outer part with 1-pentanol, a liquid with an acoustic impedance very close to that of TPX (Marsh, [1980](#)), in an attempt to mitigate the interferences with the boundaries. Figure 4-2 gives an overview of the experimental setup. Each UHP charge was in direct contact with the acceptor. Eight optical probes were inserted into the acceptor. The probes consist of a bare glass optical fiber (GOF) with a core and sleeve diameter of 50 μm and 1 mm, respectively. The fibers were stripped to the core on 1-2 mm and the cores properly cleaved with a ruby scribe. To insert the probes into the acceptor, eight holes (1 mm diameter)

were drilled at the following depths by 4 mm increments: 4, 8, 12, 16, 20, 24, 28 and 32 (all-through, isolated from the charge by a 30 μm layer of Al tape). The depth of each individual hole was re-measured after drilling (precision ± 0.01 mm) for accurate shock velocity records. All holes were located at an identical 15 mm radial distance from the charge axis to minimise the effect of the radius of curvature (ROC) of the detonation front. In fact, using the method described in Reference (Pachman et al., [2016](#)), an average experimental 180 mm relative ROC of the detonation front had been determined for 86.4 mm diameter UHP charges during the preliminary ASV campaign. The distance between probes within the acceptor disks was optimised in such a way that the arrival times were not influenced by the shock wave distortions caused by the holes. The whole measurement zone (30 mm diameter) was also chosen sufficiently small with regard to the acceptor diameter (120 mm) to limit the influence of lateral relief waves on the shock propagation.

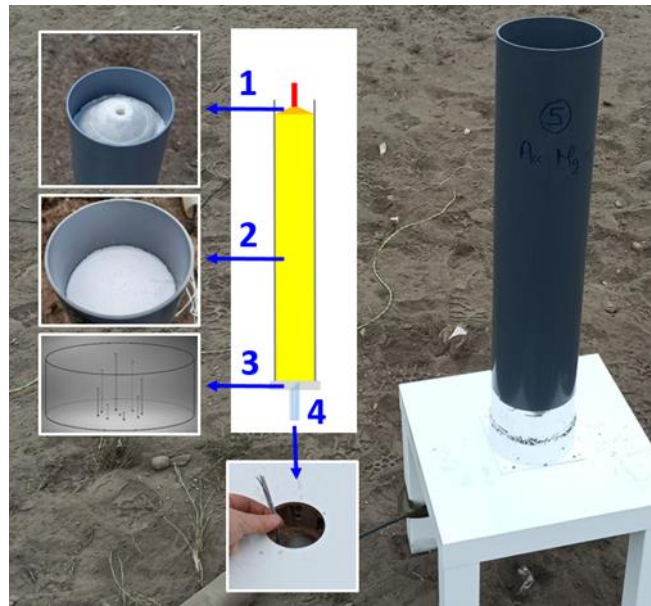


Figure 4-2: UHP (5 kg) – P_{det} by ASV – Experimental setup: (1) Initiation; (2) UHP charge; (3) Drilled inert acceptor; (4) ASV optical probes.

We used a passive light acquisition system OPTIMEX 64 (OZM research) to track the light signal (250 MHz sampling frequency) from the shock wave generated by the detonation of UHP and propagating through the inert acceptor attached to the tested explosive charge. The shock velocity in each inert material was then

calculated from distance-time records using a linear regression, which was preferred to the parabolic one suggested in (Kunzel et al., [2017](#)), taking into account significant differences between both experimental setups. In fact, Kunzel et al. made use of 40 mm diameter charges and recorded the light signal up to 20 mm deep into the acceptor, giving a charge diameter to depth ratio around 0.5. We used 120 mm diameter charges and measured up to 28 mm deep in the acceptor, which corresponds to a charge diameter to depth ratio around 0.2. We also used longer charges ($L=5xD$ compared to $1.5xD$, including booster, in Kunzel et al., [2017](#)). For those reasons, the decrease of the shock velocity due to the rarefaction wave is expected to be slower in our setup, which supports our choice for a linear regression.

For the sake of simplicity, a polytropic EoS was used to characterise the UHP detonation products and determine the detonation pressure from the ASV measurements. First, the reflected Hugoniot in the detonation gases in the pressure/particle velocity plane (P,u), is expressed as a function of the polytropic exponent (Γ), with the initial density of the charges (ρ_0) and the velocity of detonation (VoD), as input parameters:

$$P = \frac{\rho_0}{2} \cdot \left[\frac{5 \cdot (VoD)^2}{\Gamma + 1} - 4 \cdot (VoD) \cdot u + u^2 \cdot (\Gamma + 1) \right] \quad \text{Equation 4-1}$$

In this equation, Γ is the only unknown as the previously determined averaged velocity of detonation of 3.520 km/s (Halleux et al., [2023a](#)) is used. Then, we express the Hugoniot of a transmitted shock in a given acceptor material as a function of the shock velocity in the acceptor material (i) at the interface with the explosive, U_i :

$$P = \rho_{0,i} \cdot U_i \cdot u_i = \rho_{0,i} \cdot U_i \cdot \frac{U_i - C_{0,i}}{s_i} \quad \text{Equation 4-2}$$

where $\rho_{0,i}$ is the density of the acceptor material and $C_{0,i}$ and s_i the parameters of the empirical Hugoniot of the acceptor materials (Marsh, [1980](#)). By continuity, both the pressure in the acceptor material at the interface and in the detonation

gases after interaction are equal (Cooper, [1996](#)). By equating equations 4-1 and 4-2, we then obtain a model for the shock velocity in the acceptor material with Γ as only parameter. The optimal value of Γ is then determined by using a least-square methods minimising the sum of square of the errors between this model and the experimental values of the shock velocity at the interface, taking the nature of the acceptor into account. Using this optimal value of Γ , the detonation pressure is finally calculated by using the relation (Cook, [1958](#); Cooper, [1996](#)):

$$P_{det} = \frac{\rho_0 \cdot (VoD)^2}{\Gamma + 1} \quad \text{Equation 4-3}$$

4.3.2 P_{det} by IWM (small-scale campaign)

In line with our previous work on detonability and detonation performance of UHP at small scale, we further used the following charge geometry: 4 mm thick steel confinement, ID 30 mm, OD 38 mm, L 150 mm (=5xID). The initiation train consisted of an 8 g C4 (PE8 for PDV) booster in a bespoke conical cup holding a N°8 standard military detonator. At that time, the stationarity of the detonation wave after 2 to 3 charge diameters was assessed by measuring the indentation of a witness plate resulting from the detonation of 1 to 6 diameters long UHP charges (Halleux et al., [2022a](#)). In this work, we could further confirm stationarity by monitoring the VoD of UHP along the whole confinement sleeve using 19 GOF, with 7.5 mm between probes (Figure 4-3).



Figure 4-3: UHP (90 g) under heavy confinement – VoD stationarity assessment using 19 GOF.

For the PDV campaign itself, a total of 12 devices were fired. The confinement steel sleeves were filled with approximately 90 g of UHP ($\rho = 0.85 \text{ g/cm}^3$, 59.4% TMD, slightly compacted). The OPTIMEX 64 (OZM research) passive light acquisition system (250 MHz sampling frequency) already presented in Section 2.1 was further used but in another configuration to record VoD. The setup included a total of 8 GOF, with 7.5 mm between probes, and the first probe located 90 mm (3xID) from the booster charge, as explained previously. The probes were inserted in all-through holes drilled in the confinement sleeve and sealed by a piece of 30 μm thick aluminium tape.

In order to measure surface velocities, we used a first generation photonic Doppler velocimeter. This equipment included a 1550 nm laser source, emitting laser light from a fibre-coupled collimator with a 75 mm working distance and a 220 μm spot size. The reflected (Doppler-shifted) light was mixed in the interferometer, and a Thor Labs PDA-8GS photodetector amplified the intensity of the beat signal. We used a Tektronix 6 GHz bandwidth oscilloscope, sampling at 5 GHz, to record the electrical output from the photodetector. A Hamming window Fourier transform with variable window width was used to process each velocity record, producing a time-resolved power spectrum image, which was manually digitised to analyse numerical time-velocity data. We used PDV in combination with the Impedance Window Method (IWM) (Sheffield and Blomquist, [1984](#); Pachman et al., [2018](#)) in an attempt to determine the P_{det} of UHP at small scale.

Building upon preliminary results from our first attempts to determine the detonation pressure of UHP using the IWM (Halleux et al., [2023b](#)), the initial experimental setup was slightly modified (Figure 4-4). We used two separated parallel steel rod stands (10 mm diameter) and a bespoke impedance window holder to avoid any contact between the PMMA and the confinement sleeve, while ensuring good contact between the aluminium interface and the UHP granular bed. The holder (Figure 4-4, top right) was also designed to position the laser probe on a reproducible way, aligned normal to the surface to get the strongest signals, at about 2 mm standoff from the PMMA window, facing the

centre of the mirror interface. The laser probe was directed at a 100 μm thick aluminium mirror interface (28 mm diameter) placed between the end of the test specimen, directly on the granular bed (no surface preparation) without touching the steel confinement sleeve, and the 4 mm thick PMMA impedance window (28 mm diameter), to record the motion of this interface. The OPTIMEX generated the output trigger signal to start the PDV instrumentation, so that the beginning of the visible trace effectively corresponded to the detonation wave arrival to the explosive/inert interface.

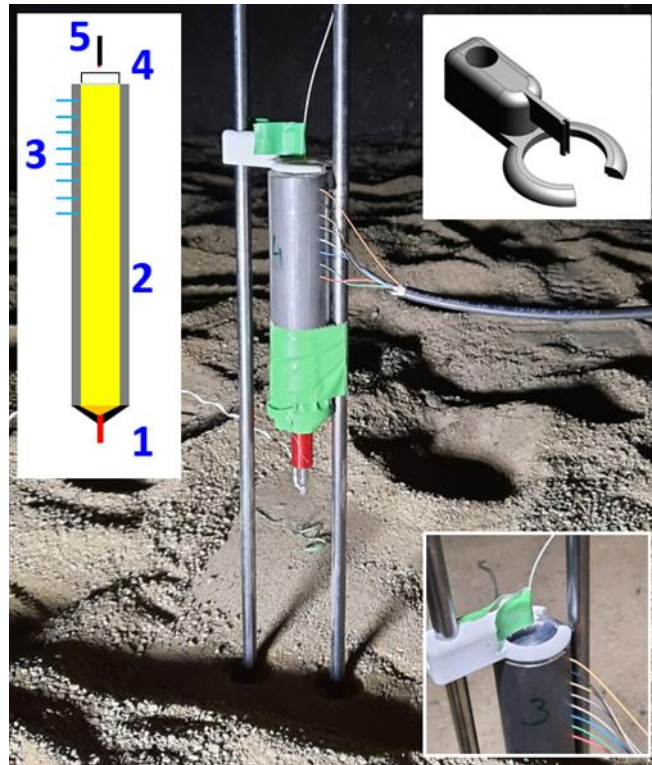


Figure 4-4: UHP (90 g) – P_{det} by IWM using PDV – Experimental setup: (1) Initiation; (2) UHP charge under heavy confinement; (3) VoD optical probes; (4) Impedance window; (5) PDV laser probe.

When it comes to the determination of P_{det} , anticipating on the results (Section 4.4.2), the intention of the authors was to apply on UHP the following method, which has proven effective for more ideal and homogeneous materials (Pachman et al., [2018](#)): identifying the CJ state on the recorded particle velocity profile (u) from two linear regressions, respectively from the initial VN spike and the following Taylor wave, then using the generalised EoS for detonation products

(Equation 4-4) (Cooper, [1996](#)) to estimate the Hugoniot of the reacted UHP and the Rayleigh line (Equation 4-5), with u_{CJ} as an input parameter for both.

$$\frac{P}{P_{CJ}} = 2.412 - 1.7315 \frac{u}{u_{CJ}} + 0.3195 \left(\frac{u}{u_{CJ}} \right)^2 \quad \text{Equation 4-4}$$

$$P = \rho_0 \cdot VoD \cdot u \quad \text{Equation 4-5}$$

Where P (GPa) is the pressure, P_{CJ} (GPa), the pressure at the CJ state, u (km/s), the particle velocity, u_{CJ} (km/s), the particle velocity at the CJ state, VoD (km/s), the detonation velocity and ρ_0 (g/cm³), the loading density.

4.4 Results

4.4.1 P_{det} by ASV (large-scale campaign)

Figure 4-5 provides an example of distance-time record with linear regression, while Table 4-1 summarises the results of the 10 ASV firings (2 per acceptor), including the measured shock velocity (U_i) determined from linear regression and calculated particle velocity (u_i) and initial pressure in inert material P_i .

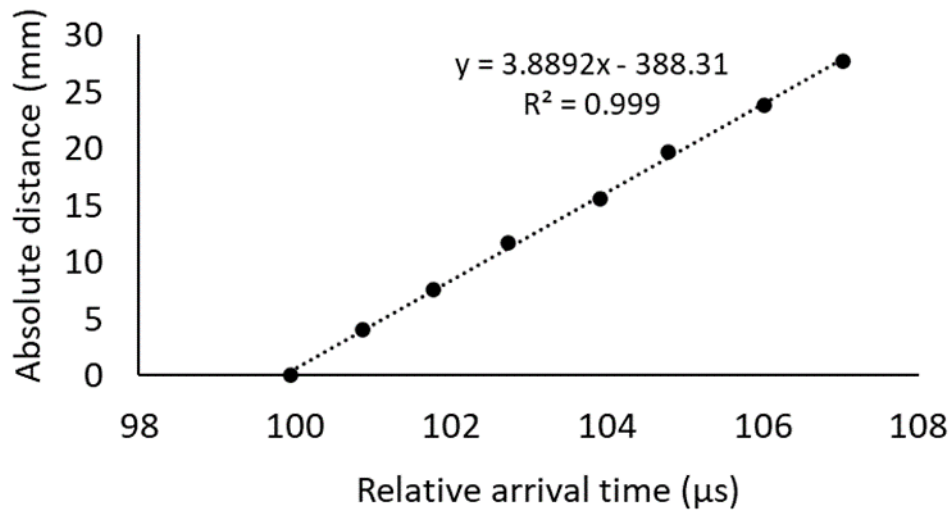


Figure 4-5: Example of distance-time record with linear regression – Shock velocity in PMMA.

Table 4-1: ASV campaign (5 kg UHP, 0.87g/cm³, charge diameter 120 mm).

Shot	Acceptor	ρ_0 (g/cm ³)	C_0 (km/s)	s (-)	U_i (km/s)	u_i (km/s)	P_i (GPa)
1	PMMA	1.186	2.598	1.516	3.971	0.906	4.266
2	PMMA	1.186	2.598	1.516	3.889	0.852	3.929
3	TPX	0.830	2.07	1.58	3.841	1.121	3.574
4	TPX	0.830	2.07	1.58	3.855	1.130	3.614
5	Mg AZ31B	1.775	4.516	1.256	5.249	0.584	5.438
6	Mg AZ31B	1.775	4.516	1.256	5.272	0.602	5.636
7	PTFE	2.153	1.841	1.707	3.056	0.712	4.684
8	PTFE	2.153	1.841	1.707	3.064	0.717	4.727
9	Al 7075	2.804	5.200	1.36	5.613	0.304	4.781
10	Al 7075	2.804	5.200	1.36	6.105	0.666	11.397

When it comes to measurement uncertainty, we calculated the particle velocity (u_i) from the measured shock velocity (U_i) in an inert acceptor and then used this value to further calculate the initial pressure P_i . For this reason, the error on P_i is proportional to the square of the measurement error on U_i . Moreover, as the Hugoniot in the U - u plane is an affine function, the error on particle velocity u_i can increase quickly, especially at low particle velocities. Due to the high shock impedance of aluminium and the rather low detonation regime, the error on pressure was too large. The shocked state (P_{Al} , u_{Al}) was disregarded and the UHP detonation products Hugoniot was then constructed from the shock states (P_i , u_i) in the four remaining inert acceptors (Figure 4-6). The steady-detonation state was found at the intersection of the experimental reflected Hugoniot and the Rayleigh line, corresponding to a P_{det} of 3.46 GPa. Despite the choice of a rather low shock impedance material such as TPX, we could not encompass the steady-detonation state and its determination required a slight extrapolation.

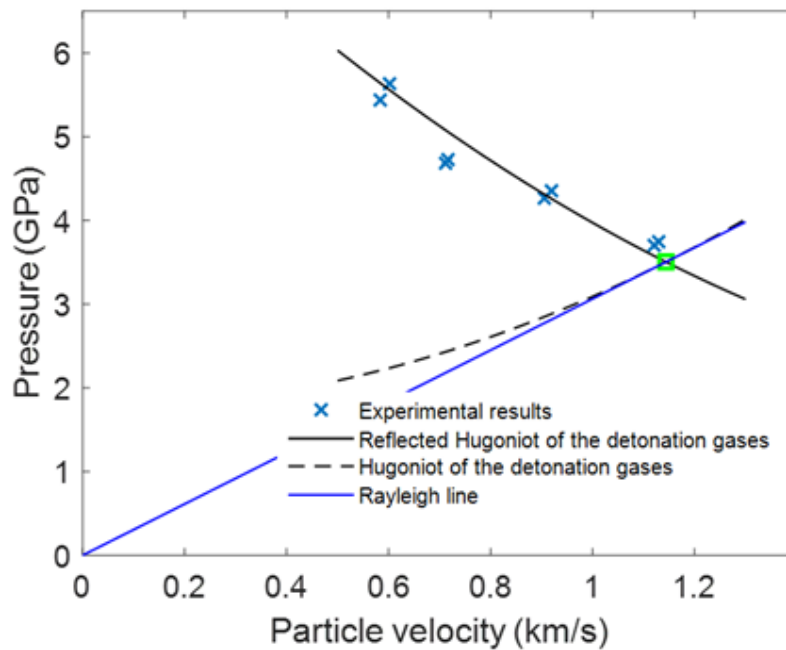


Figure 4-6: UHP steady-detonation state (green) at the intersection of the reflected Hugoniot and the Rayleigh line.

4.4.2 P_{det} by IWM (small-scale campaign)

Reproducible VoD results with an average 3.297 km/s (± 0.014 km/s for 95% CI) for 90 g UHP charges (0.85 g/cm^3 loading density) under heavy confinement were obtained. These results are consistent with previous work from the authors on small-scale detonability of UHP (Halleux et al., [2022a](#)) and the confirmatory shots carried out with 19 probes located all along the confinement sleeve to assess the stationarity of the detonation (see example on Figure 4-7). The overdriven state due to the 8 g C4 booster is obvious in the first charge diameter (30 mm), while stationarity is already observed after two charge diameters.

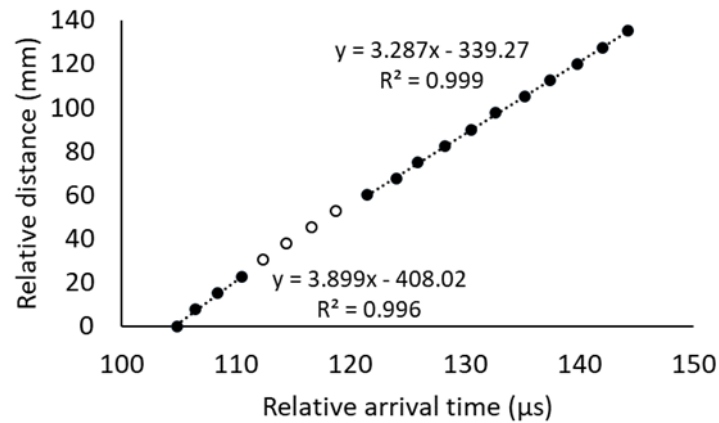


Figure 4-7: UHP VoD (0.85 g/cm³, heavy confinement) – Initial overdriven state from the 8 g C4 booster, transition and stationarity after two charge diameters.

These preliminary results confirm the consistency of our small-scale PDV setup, the output trigger signal being generated after 3 charge diameters to start the velocimeter, so that the beginning of the visible trace effectively corresponds to the arrival of a stationary detonation wave to the UHP/PMMA interface. Figure 4-8 shows an example of such a trace, typical for non-ideal explosives (Halleux et al., [2023b](#)), including the arrival of the detonation wave, the initial velocity scatter due to the heterogeneity of the explosive, the shock transit time through the PMMA, typically 1-3 μs depending on pressure, then a second trace, at approximately twice the interface velocity, which corresponds to the free surface velocity of the PMMA window.

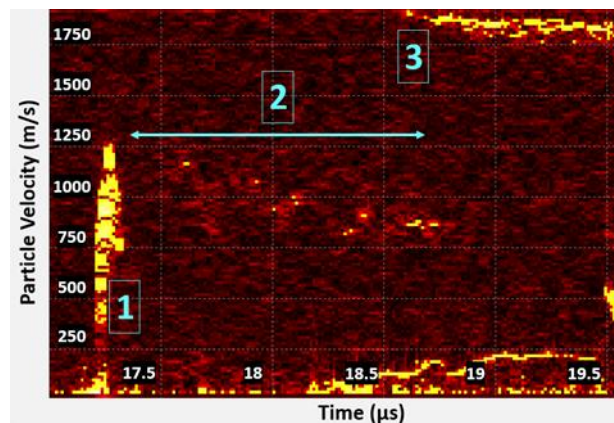


Figure 4-8: PDV – Example of time-resolved power spectrum image (1 shot): arrival of detonation wave (1), transit time through PMMA (2), free surface velocity (3).

From the 12 shots carried out in the same configuration, only 5 shots could capture the motion of the interface, the other 7 only providing the PMMA upper free surface velocity trace. Digitised time-velocity data of these 5 shots are combined in Figure 4-9. We arbitrarily selected the last 500 ns of the record in the PMMA window, when the signal seemed to stabilise after initial velocity scatter, and determined an average 877 m/s (± 18 m/s for 95% CI) particle velocity at the explosive/inert interface, a value consistent with ASV results, i.e. particle velocities calculated from shock velocities measured in PMMA (Table 4-1 in Section 4.4.1). The limited number of records of the interface motion highlights the relative difficulty to carry out IW experiments on coarse granular explosives, when compared to pressed, melt-cast, cast-cured (Pachman et al., [2018](#)) and of course homogeneous liquid explosives (Stimac et al., [2020](#)).

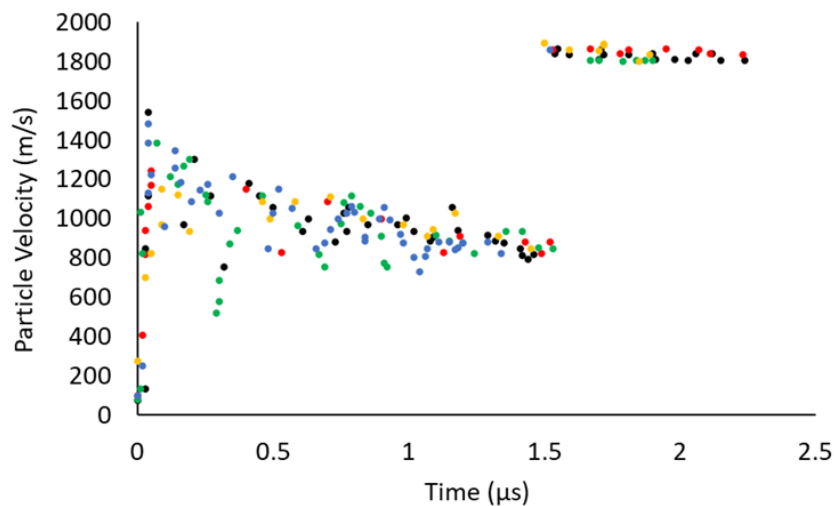


Figure 4-9: PDV – Digitised time-velocity data (5 shots) with average 877 m/s particle velocity at the UHP/PMMA interface.

The determination of P_{det} would require further investigations, as our current velocity records do not allow us to properly determine a CJ state, which is usually determined by a change of slope in the particle velocity profile (Pachman et al., [2018](#)). Due to the limited thickness of our impedance window, we cannot even confirm that we captured the whole reaction zone and, hence, the CJ point. In fact, the PMMA window thickness is clearly a limiting factor, particularly when dealing with non-ideal explosives where longer reaction zone lengths are

expected. Further experiments should hence be carried out with thicker PMMA windows, allowing for longer record, in an attempt to identify changes in slope of the velocity trace. However, in the current small-scale charge geometry, the maximum window thickness should not exceed 15 mm, about half the charge diameter, to avoid the effect of side relief waves on the velocity traces. Considering other potential improvements of the experimental setup, the contact surface between the window and the explosive specimen could be improved by filling the voids between the UHP grains at the interface. Possible preparations to fill the voids include the use of silicon grease or epoxy, surface dusting with smaller UHP particles or a combination of both. Silicon grease has proven effective to ensure a good contact between plasticised explosives and the aluminium interface of the IW (Pachman et al., [2018](#)) but, in the case of UHP, the authors speculated that its application on a coarse explosive granular bed might lead to jetting effects, producing high-velocity material (Mader, [2008](#)), and early disruption of the interface. The choice of the aluminium interface is also a key parameter. It should be reflective enough, thin enough to just act as a mirroring interface but thick enough to withstand initial shock arrival and deformation and reflect the laser beam along the path to the probe sufficiently long to provide a useful PDV record. The use of multiple measurement points could be investigated. In fact, using a single probe (point measurement) is a limiting factor, particularly when the upper part of the interface starts deforming and the laser beam is not reflected anymore along the path to the probe. The point measurement is also dependent on the position of the probe which could be an issue when dealing with a heterogeneous material, with either air gaps or UHP particles in contact with the Al interface. Finally, the sampling frequency should also be increased, shortening the Hamming window duration, giving a better time resolution and, hence, minimising the reading error on the PDV capture.

4.5 Discussion

Table 4-2 summarises and compares the ASV experimental results and the ideal thermodynamical predictions from Explo5 using the EXP-6 and M-BKW EoS. Experimental P_{det} and Γ are consistent with data available in the literature on

explosives detonating at comparable regime, such as ANFO (Cooper, [1996](#)). Using empirical correlations for comparison purposes, we first estimated detonation pressure (Equation 4-6) (Cooper, 1996), from the 3.52 km/s experimental VoD and 0.87 g/cm³ loading density (ρ_0) (Table 4-2), obtaining 3.14 GPa, a result in good agreement with our experimental data.

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad \text{Equation 4-6}$$

We further calculated a consistent 2.2 polytropic exponent, using Equation 4-7 (Keshavarz and Pouretedal, [2006](#)), a correlation which has proven effective to reliably estimate the Γ of CHNO explosives over a wide range of loading densities (0.2-2 g/cm³).

$$\Gamma = 1,819 - \frac{0,196}{\rho_0} + 0,712 \cdot \rho_0 \quad \text{Equation 4-7}$$

Table 4-2: UHP – Comparison of experimental data and thermodynamical predictions.

	ρ_0 (g/cm ³)	VoD (km/s)	u_{CJ} (km/s)	P_{CJ} (GPa)	Γ (-)
ASV large-scale*	0.87	3.52	1.13	3.46	2.1
Explo5 (EXP-6)	0.87	4.19	0.96	3.50	3.4
Explo5 (M-BKW)	0.87	4.46	1.09	4.21	3.1

* 5 kg UHP, 120 mm charge diameter, L/D = 5, no confinement

From the ratio of the experimental P_{det} of UHP and a 1.64 g/cm³ TNT reference (Cooper, [1996](#)), we derived an estimated 20% TNT equivalence for brisance, a result in good agreement with previous preliminary brisance assessment from underwater shock pressure carried out by the authors (Halleux et al., [2023a](#)). Comparing experimental P_{det} to thermodynamical predictions using the ideal model, we find an excellent level of agreement. This good fit between measured and ideally calculated detonation pressure could potentially come both from errors in measurement and errors in calculation, knowing that typical detonation

pressure measurement error is around 10-20% (Mader, [2008](#)), which is also roughly the margin error of the calculated detonation pressure of non-ideal explosives using the ideal detonation model (Stimac et al., [2021a](#)). Moreover, the calculated detonation pressure is controlled by the EoS, with value up to 20% higher using M-BKW EoS instead of EXP-6. Depending on the choice of the EoS, the predicted ideal VoDs are about 20-25 % higher than experimental value (maximum 1% expected measurement error – (Mader, [2008](#))) and higher than the 3.94 km/s extrapolated at infinite diameter from experimental data (Halleux et al., [2023a](#)). As a result, Explo5 calculates Γ higher than 3, which is rather the expected order of magnitude for typical military explosives, with 1.5 to 1.8 g/cm³ loading density (Cooper, [1996](#)), (one of) its predominant parameter (Keshavarz and Pouretedal, [2006](#)). As the polytropic exponent describes the rate of pressure release along the detonation isentrope (Fickett and Davis, [2003](#)), the difference between experimental and calculated Γ value from Explo5 suggests that the predicted isentrope shape, especially in the low pressure region, using the ideal model does not adequately model the detonation product expansion. This limited accuracy could be explained by the low detonation temperature (1500 K) and the specific detonation products of UHP, particularly a rather high water content (triatomic polar molecule), when compared to conventional CHNO explosives, such as TNT (Halleux et al., [2023a](#)). Improvement of the modelling of non-ideal detonation should include kinetics of reaction in the chemical reaction zone and radial expansion of the products (Stimac et al., [2021a](#)), which would however considerably increase the complexity of the study.

Two experimental methods, at two different charge scales, have been investigated in an attempt to assess the P_{det} of UHP.

On the one hand, the ASV method allowed for determination of the detonation pressure on the constructed experimental Hugoniot of explosive detonation products, using 5 different inert acceptors. The first advantage of this method is the fact that one single shot leads to the determination of a point on the Hugoniot of the detonation gases, which is of particular interest with non-ideal explosives for which large quantities have to be used. Moreover the method is not limited to

transparent materials as other optical techniques. The major issue with this method is the indirect determination of the parameters of interest. In fact, we calculate the particle velocity from the measured shock velocity in an inert acceptor and then use this value to further calculate the initial pressure at the interface, making the error on pressure proportional to the square of the measurement error on shock velocity.

On the other hand, for quick assessment purposes, we investigated the use of IWM using PDV for scaled-down UHP charges. Current observations are limited to a particle velocity at the UHP/PMMA interface consistent with the calculated particle velocities in PMMA acceptors from the ASV method. However, the use of the IWM at small scale on a coarse granular heavily confined low-density non-ideal explosive in small charge diameter has proven challenging, even if potential improvements have been identified. An alternative small-scale PDV-based method could be the Disc Acceleration eXperiment (DAX) (Lorenz et al., [2015](#)), which has proven effective and reliable in providing a rapid evaluation of explosive performance, i.e. detonation velocity, pressure and expansion energy. Future work will investigate the application of the method to UHP, a non-ideal material with rather low detonation regime, using a scaled-up DAX charge geometry ensuring a steady detonation.

4.6 Conclusion

Within the scope of a performance assessment, the brisance of UHP was quantified through its predominant parameter, the detonation pressure. In this comparative study, we investigated P_{det} respectively at large and small scale using two distinct indirect methods. We determined an experimental 3.5 GPa detonation pressure for 5 kg unconfined UHP charges (0.87 g/cm^3 , 120 mm charge diameter) by measuring the shock wave velocity in adjacent inert materials using passive optical probes, which corresponds to an experimental 20% TNT equivalence for brisance. This experimental detonation pressure is also consistent with the thermochemical predictions from *Explo5*, taking into account the margin error due to the use of an ideal model for the calculations. Particle velocity measurements at the interface of a PMMA impedance window carried

out with Photonic Doppler Velocimetry on scaled-down charges of 90 g UHP under heavy confinement (0.85 g/cm^3 , 30 mm charge diameter, 4 mm thick steel) are consistent with ASV results in the PMMA acceptors but further investigations are required to determine the detonation pressure, using a small-scale experimental setup. The ASV method has proven reliable to assess the brisance of a non-ideal explosive for risk assessment purposes.

5 Urea-hydrogen peroxide as an improvised explosive: a threat assessment

Due to its sensitive nature, this chapter was not included in the manuscript.

5.1 Abstract

5.2 Introduction

5.3 Materials and Methods

5.3.1 Ease of manufacture

5.3.2 Sensitivity and initiation

5.3.3 Urea Nitrate as a benchmark

5.4 Results and Discussion

5.4.1 Ease of manufacture

5.4.2 Sensitivity and initiation

5.4.3 Urea Nitrate as a benchmark

5.4.4 Discussion

5.5 Conclusion

6 Overall conclusion, research implications and recommendation for future work

6.1 Overall conclusion

The overall aim of the work presented in this thesis was to address the risk posed by dual-use industrial chemicals (Merrifield and Roberts, [1991](#)) as improvised explosives in IEDs, by characterising, as a relevant case study, the detonation properties of Urea - Hydrogen Peroxide (UHP), an oxidiser produced at large scale in the chemical industry, identified as a potential emerging threat (EU-US, [2019](#); JCAT, [2020](#)) with very limited academic literature available on its explosive properties (Matyas et al., [2017](#)). In terms of the real-world impact, the outcome of this project was hence aimed at providing relevant knowledge for both the scientific community, the industry, the law-enforcement agencies and the intelligence services. The research in this thesis included a detailed performance characterisation (**Chapter 2-3-4**), including experiments (150 instrumented firings), thermochemical calculations and numerical simulations, and a comprehensive limited release technical-operational threat assessment (**Chapter 5 – not included**) analysing the previously collected academic data in a C-IED perspective.

This combined approach has proven effective to answer the research question, “Improvised explosives, how to understand the threat and assess the risks”. On the one hand, the threat to public security was addressed by investigating UHP explosive properties at small (**Chapter 2**) and large scale (**Chapter 3-4**), its commercial availability or ease of manufacture (**Chapter 5**) and by applying a specific predictive threat analysis (**Chapter 5**). On the other hand, the risk posed by UHP as a main charge in IEDs, knowing its rather low performance (**Chapter 3-4**) and booster requirement (**Chapter 2-3**) as a tertiary explosive was studied by comparing UHP performance with Urea Nitrate, an improvised explosive with records of past terrorist use in IED attacks (**Chapter 5**), and by investigating a viable improvised explosive train to initiate UHP (**Chapter 5**). Finally, the performance characterisation of UHP provided consistent experimental TNT equivalences for brisance and explosive power (**Chapter 3-4**) to assess the risk

in terms of intentional or accidental detonation's output and potentially mitigate its effects.

To the best of our knowledge, this research project was one of the first attempts to thoroughly characterise a tertiary explosive for risk assessment purposes.

6.2 Key findings and contribution to knowledge

To address the knowledge gap described above and the related research question, the **first step** of the work described in **Chapter 2** was to **investigate the detonability at small scale**, complementing Matyas' pioneering work on UHP explosive behaviour (Matyas et al., [2017](#)), **and optimise experimental setup to closely approach large-scale behaviour**. Numerous recent and ongoing research (Kunzel and Kucera, [2021](#); Hunter et al., [2022](#)) have addressed the need to predict large-scale detonation performance parameters of energetics from small-scale tests. Large-scale experiments require specific facilities and involve kilograms of product, particularly when dealing with tertiary explosives. These campaigns can be time-consuming, difficult to organise, expensive and, depending on the sensitiveness of the energetics under investigation, potentially hazardous. This scaling requirement was particularly relevant within the scope of this threat assessment. To that end, building upon an initial comprehensive parametric study investigating initiation, loading density, charge length, diameter and confinement material, a charge geometry and an experimental setup at the 100g-scale was successfully validated, enabling further instrumentation, to characterise the detonation parameters of UHP (**Chapter 3-4**). Maximum information could hence be obtained from a limited number of reproducible small-scale firings and minimum consumption of sample, keeping a minimum number of large-scale experiments for benchmarking and validation purposes. Most of the small-scale tests recently described in the literature (Kunzel and Kucera, [2021](#)) are carried out using weak or medium confinement materials, as they are either designed to characterise more ideal material (Lorenz et al., [2015](#)) or to investigate detonation failure of non-ideal material (Hunter et al., [2022](#); Scott et al., [2023](#)). When dealing with non-ideal explosives, in terms of the actual physical-chemical processes occurring, there is competition between energy

releases as a result of exothermic reactions in the explosive and radial energy losses. In the case of tertiary explosives at small charge diameters, a heavy (high impedance) confinement is required to reduce the radial losses of energy of detonation products and allow a self-sustained detonation to propagate at small scale. In the used charge geometry, a steady detonation in UHP could not be recorded using a weak PE confinement (**Chapter 2**) and this need for heavy confinement required some changes in experimental setups, for example to measure detonation pressure (**Chapter 4**).

A heavy steel confinement (30 mm ID; 4 mm wall thickness) has proven suitable and effective to study UHP performance parameter at the 100g-scale, demonstrating brisance by indent depth measurements and recording reproducible detonation velocities corresponding to respectively 85% of the infinite diameter value extrapolated from large-scale experiments and 80% of the ideal prediction from Explo5 (M-BKW EoS) (**Chapter 3**). Increasing the wall thickness would likely have allowed for further optimisation, in line with current research on ANFO and a confinement model required for reliable numerical modelling of nonideal explosives (Bohanek et al., [2022a](#), [2022b](#)), but this fell outside the scope of the current study. In addition to lab grade UHP, the experimental method presented in **Chapter 2** has been successfully applied to quantify the performance of homemade UHP and Urea Nitrate (**Chapter 5**), recording again detonation velocities about 80% of the ideal prediction from Explo5. This small-scale experimental setup was also chosen to investigate the initiation of UHP using an improvised explosive train (**Chapter 5**), as the use of large charge of homemade explosive could represent a showstopper in terms of laboratory safety. Generally speaking, the proposed method has proven applicable to study other industrial materials that may have energetic properties, or small samples of homemade explosive compositions, avoiding time-consuming, expensive and potentially hazardous large-scale experiments.

Building upon the results from **Chapter 2**, i.e. the validation of a suitable geometry and small-scale experimental setup, the **second step** of the research described in **Chapter 3** was to **determine UHP detonation performance parameters** at

large and small scale. A detailed performance assessment was carried out, combining experiments, thermochemical calculations and numerical simulations. An excellent level of agreement was obtained between experimental data from lab, field and underwater firings, confirming the validity of the small-scale setup for quick assessment purposes (**Chapter 2**). A maximum experimental detonation velocity of 3.65 km/s was recorded for unconfined 25 kg charges at 0.85 g/cm³ (200 mm charge diameter). In these conditions, an infinite diameter detonation velocity of 3.94 km/s was determined, further highlighting UHP charges non-ideality by detonation velocity dependence on charge diameter. The use of alternative and complementary approaches, such as small-scale, free field and underwater experiments, has proven effective and reliable to target and characterise each specific detonation performance parameter of UHP and provide relevant knowledge to the scientific community, supporting and extending the rather limited existing literature about UHP explosive properties. To assess the risk in terms of intentional or accidental detonation's output, experimental TNT equivalences (Collet et al., [2020](#)) were used, taking into account the limitation of the concept reported in the literature (Cooper, [1994](#); Simoens, [2011](#); Locking, [2013](#)). To that end, well-characterised reference explosives were tested in the same experimental conditions and charge geometries to calibrate the setups (triggering, sensitivity of the measurements) and successfully provide a documented benchmark (dent in the witness plate, detonation velocities, underwater first pulsation period, etc.). Additional tests were dedicated to quantify the detonative output from the booster to better assess the effect of the UHP charges. This method enabled us to derive representative and valuable experimental TNT equivalences for explosive power (50%) (**Chapter 3**) and brisance (20%) (**Chapter 3-4**) for risk assessment purposes.

In the two first steps of the research, the detonation pressure had been either calculated by thermodynamical code or estimated from an empirical correlation (**Chapter 2**), while underwater shock energy measurements enabled us to provisionally derive a relative brisance (**Chapter 3**). Within the scope of a comprehensive performance assessment, the **third step** of the research, described in **Chapter 4**, was to directly quantify the brisance of UHP through its

predominant parameter, the detonation pressure, and to compare previous results with **detonation performance parameters obtained from advanced characterisation methods**. To that end, UHP detonation pressure was investigated respectively at large and small scale using two distinct indirect methods, respectively measuring shock then particle velocities. First, at large scale, using an optical system, the attenuated shock velocity (ASV) in different inert materials (Kunzel et al., [2017](#)) was studied. Then, at small scale, photonic Doppler velocimetry was used in combination with a PMMA impedance window (Sheffield and Blomquist, [1984](#); Pachman et al., [2018](#); Stimac et al., [2020](#)). To the best of our knowledge, the application of these two methods to non-ideal material was not documented in the literature, further contributing to the novelty of the work. On the one hand, a 3.5 GPa detonation pressure for 5 kg unconfined UHP charges (0.87 g/cm^3 , 120 mm charge diameter) was successfully determined by measuring the attenuated shock wave velocity in adjacent inert materials using passive optical probes. Conclusions drawn from this work support the use of ASV to assess the brisance of a non-ideal explosive for risk assessment purposes, deriving a 20% experimental TNT equivalence, a value consistent with underwater shock energy measurements (**Chapter 3**). On the other hand, particle velocity measurements at the interface of a PMMA impedance window carried out with photonic Doppler velocimetry on scaled-down charges of 90 g UHP under heavy confinement (0.85 g/cm^3 , 30 mm charge diameter, 4 mm thick steel) are consistent with large-scale ASV results in the PMMA acceptors but further investigations are required to determine the detonation pressure, using either the designed small-scale experimental setup (**Chapter 4**) or an alternative, such as a modified DAX (Lorenz et al., [2015](#)) to make it suitable for a non-ideal material like UHP.

Overall, the results presented in the **three first steps** of the research (**Chapter 2-3-4**) offer unique insights into the detonation performance of UHP, as very little work on its explosive behaviour is available in the literature. To assess the validity of every single result, the methodology combined three complementary pillars, theoretical predictions, modelling and experiments, the latter being the main and primary focus of the work (150 instrumented firings), as extensive experimental

data is particularly desirable to accurately evaluate the detonation parameters of non-ideal explosives (Mader, [2008](#)). The innovative character of the work was also to study the non-ideality of explosives through a rather newish case-study, UHP, as AN-based compositions, particularly ANFOs, have been extensively studied in the literature, considering their worldwide use in the mining industry and their scientific interest, taking into account the number of parameters affecting their non-ideal behaviour (Bohanek et al., [2022a](#)). The experimental phase of the project significantly demonstrated the non-ideality of UHP charges. The detonation velocity dependences on confinement and charge diameter were respectively highlighted in **Chapter 2** and **Chapter 3**. The detonation front curvature was also determined in 90 mm charge diameter during preliminary ASV campaign (**Chapter 4**), a very important result when studying non-ideality of explosives as this curvature directly relates to the rate of detonation products radial expansion in the detonation driving zone and the rate of the chemical reactions (Stimac et al., [2021b](#)). As far as metrology is concerned, most of the existing methods are obviously tailored to study the properties of interest of nearly ideal military explosives and are not directly suitable for characterising strongly non-ideal explosives as tertiary explosives. It is hence of utmost importance to adapt the experimental setups to prevent non-ideal effects from significantly affecting the measurement. It was hence essential to first investigate the nominal diameter of unconfined UHP before selecting a charge diameter of 120 mm for airblast measurements, a trade-off between the impact of the diameter on the performance characterisation and the practical charge size (**Chapter 3**). The accuracy of experimental characterisation methods using high impedance acceptors can also be questionable when studying explosives with rather low detonation regime such as UHP. This was particularly highlighted in **Chapter 4** when the shocked state obtained from the aluminium acceptor was discarded to construct the UHP detonation products Hugoniot using the ASV method. The application of the DAX method (Lorenz et al., [2015](#)), suggested as a potential small-scale alternative to study UHP, could face the same accuracy issue, as it uses aluminium or copper witness discs to determine detonation pressure. When it comes to theoretical predictions, the thermodynamical code Explo5 and the

ideal detonation model were used for quick assessment purposes to calculate maximum theoretical TNT equivalences for brisance and explosive power and dimension the NEQ of UHP charges for the small and large-scale experiments according to both the firing bunkers' limitations (**Chapter 2**) and the safety distances available on the proving grounds (**Chapter 3**). As expected, the non-ideal behaviour of UHP in the tested configurations was highlighted by a difference higher than 750 m/s (Mader, [2008](#)) between the ideal prediction from M-BKW EoS (4.37 km/s) and the experimental VoD recorded in 120 mm charge diameter (3.52 km/s) at 0.85 g/cm³, selected for blast (**Chapter 3**) and detonation pressure (**Chapter 4**) measurements. In fact, the ideal model calculates detonation parameters according to the steady state detonation theory which does not take into account a reaction zone, assumes a one-dimensional flow and chemical and thermodynamic equilibrium of the reaction-products gases leaving the detonation front. It is hence inaccurate to describe non-ideal detonations, in inhomogeneous materials such as tertiary explosives, where limited chemistry occurs in the reaction zone. Non-ideal detonation performance parameters cannot be predicted a-priori as the kinetics of reaction in chemical reaction zone and the radial expansion of the products (due to slower reactions) must be considered, which significantly increases the complexity of the models and requires specific experimental data for calibration and validation purposes. This fell outside the scope of the current project but could stimulate dedicated future research in the field. Experimental observations and thermodynamical calculations using the ideal model were further compared in **Chapter 3**, while modelling the underwater shock pressure experiments. On the one hand, C4, the (near-) ideal baseline explosive, could successfully be modelled in Autodyn and the calculated shock energy from the pressure profile was very close to experimental observations. On the other hand, the Autodyn model using the JWL coefficients calculated from the Explo5 built-in algorithm for UHP could not adequately reflect underwater measurements, highlighting the need for experimental determination and validation of these JWL coefficients, typically through large-scale cylinder expansion testing. The detonation behaviour of non-ideal explosives, such as energy release, detonation front curvature, reaction

zone, can be better predicted in Autodyn with reactive flow models and reaction rate equations, as suggested in **Chapter 2**, when modelling small-scale UHP charges under heavy confinement. Such models are complicated and require calibration data (rate stick, diameter effect) but could represent a cost-effective tool to simulate shock sensitivity and detonation propagation in tertiary explosives at a large to very large scale.

The **fourth and final step** of the research, described in **Chapter 5 (not included)**, was to **assess the risk, from previous academic characterisation (Chapter 2-3-4) and complementary operational testing**. Two critical criteria from a terrorist perspective were considered, i.e. the availability of raw materials, using a specific predictive threat analysis (Collett et al., [2021](#)), and the potential use as a main charge in IEDs, building upon previous academic work on UHP. Analysis of the results and key findings are available in the related chapter, prepared as a separate document, and will not be further discussed here. Although tertiary explosives should be considered as a major threat in a C-IED context along with homemade explosives, they are not addressed in a generic way by the international regulation, which is mainly based on the UN orange book (UN, [2009](#)). This manual describes the procedure which lead to the acceptance of a material in the hazard class 1 (explosives). In this procedure, the test series 2, similar to test series 1 but with less stringent criteria, is usually performed first for clarification purposes. If the results are negative, the substances will not further be tested and will be considered too insensitive to be included in class 1. The UN Gap Test is particularly relevant to identify tertiary explosives. In the test series 1, the focus is the ability of the substance to propagate a detonation and there is no gap between donor and acceptor. This is actually comparable to the setup (**Chapter 2**), which was used to demonstrate UHP detonability at small scale. In the less stringent test series 2, the focus is rather the sensitivity under confinement to detonative shock and the setup includes a 50 mm PMMA spacer between donor and acceptor. However, generalising the conclusions based on tests designed for the transport of dangerous goods to a C-IED context should be avoided. A detonable substance could be excluded from the hazard class 1 because it is not likely to detonate accidentally, while being used purposely as a

tertiary explosive detonated with a bespoke booster in an explosive device. This concern was here typically exemplified with the study of UHP. The latter has proven detonable but belongs to the hazard class 5 (oxidisers), which is likely to result from a trade-off between economical and safety considerations.

In terms of real-world impact, the results published in this body of work will provide relevant knowledge to the scientific community, complementing the rather limited available academic literature with a comprehensive characterisation of UHP detonation performance. The outcome is also of great interest for the industrial risk management or process safety, as UHP is produced at large scale as an oxidising agent. This work was equally important to understand the threat and assess the risk posed by tertiary explosives in a C-IED context and address relevant recommendations to the worldwide intelligence services and the law-enforcement agencies.

6.3 Further work

To the best of our knowledge, this research project was one of the first attempts to thoroughly characterise a tertiary explosive for risk assessment purposes. UHP has been addressed but there is still no general approach to the threat posed by tertiary explosives. Shortcomings have been highlighted, particularly regarding the existing metrology, the thermodynamical calculations and the numerical modelling, stimulating future work in the area.

Specific time- and cost-effective methods, combining experiments and modelling, should be developed and validated to allow a specific risk assessment to be performed and, whenever applicable, regulations on a particular energetic to be enforced in time.

These methods should:

- 1) Include efficient **screening tests at small scale** to improve current regulation on explosive material. The scale should be comparable to that of the generic UN dangerous goods tests, namely with a maximal diameter of 40 mm.
- 2) Characterise the **detonation performance** of tertiary explosives in terms of brisance and explosive power to assess the risk in terms of intentional or accidental detonation's output and potentially mitigate its effects.
- 3) Determine the **shock sensitivity** of tertiary explosives, including with homemade explosive boosters.

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APPENDICES

Appendix A: Poster presented at the 6th Defence and Security Doctoral Symposium (2020).

Home Made Explosives (HME) How to understand the threats and model the risk?

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Home Made Explosives (HME)

How to understand the threats and model the risk ?

1. Context

- HME = major public security concern, requiring specific risk assessments for first responders
- Current Threat worldwide:
 - Mixing of highly energetic pyrotechnics
 - Synthesis of peroxide explosives
- 1st investigated HME: **Urea Hydrogen Peroxide (UHP)**
 - Availability of ingredients + Ease of manufacture
 - Lacking research data



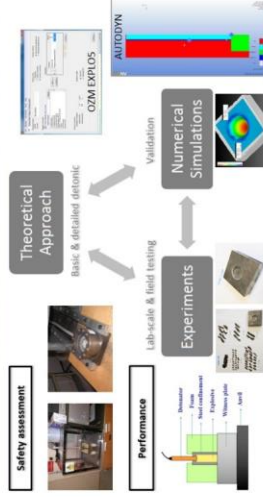
2. Challenges and objectives

- HME vs Explosive performance and safety standards
→ Extend the knowledge → **understand the threat**
- HME vs standard (ideal) detonation theory
→ Predicting the effects → **model the risk**



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3. General approach



4. Preliminary results

- Safety assessment
 - Lab scale sensitivity testing (impact, friction, ESD)
 - Thermal characterization (DSC, TGA-MS, ToI)
- Performance
 - Bomb calorimetry and Explo5 predictions
 - Preliminary detonation testing (brisance)
- Preliminary testings highlight that UHP is fairly **insensitive to handle** and has **non-ideal tertiary explosive** behaviour. Brisance has been demonstrated. A steady-state detonation regime will strongly depend on confinement, booster size and charge diameter.

5. What's next

- Detailed Detonic investigation & numerical validation
 - Detonation velocity, Detonation pressure
 - Shock sensitivity
 - Blast measurements
 - Fragmentation analysis and Post-blast residues
 - UHP with additional energetics
 - Cylinder expansion testing – JWL Equation of state



Acknowledgements

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Appendix B: Published Research Article.

Small-Scale Detonation of Industrial Urea-Hydrogen Peroxide (UHP)

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Full Paper

Small-scale detonation of industrial Urea-Hydrogen Peroxide (UHP)

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Michel Lefebvre ^[b]

Abstract: The adduct of Urea and Hydrogen Peroxide (UHP), also called Carbamide Peroxide, is industrially produced as a solid source of hydrogen peroxide for bleaching, disinfection, and oxidation reactions. As a chemical combination of fuel and oxidiser, UHP has explosive potential but it is unclear whether it could sustain a detonation at small scale. In the configuration we tested, we succeeded in recording self-sustained detonation at relatively small scale under heavy confinement, measuring a maximum experimental velocity of detonation of 3860 m/s at an optimum 1.1 g/cm³ loading density. UHP can sustain a detonation, even at the 100 g scale, but this is strongly dependant on booster size, confinement material, loading density, charge length and diameter. According to our performance assessment, pure UHP exhibits the behaviour of a non-ideal tertiary explosive. Maximum calculated detonation pressures are below 10 GPa, the order of magnitude for commercial blasting explosives. Small-scale results are consistent with literature values from large-scale experiments, although literature on the matter is quite limited. The proposed experimental method can be used to quantify the detonability and performance of other industrial materials that may have energetic properties, or small samples of homemade explosive compositions, avoiding time-consuming, expensive and potentially hazardous large-scale experiments.

Keywords: Urea hydrogen peroxide, Detonation, Non ideal explosive, Performance

1 Introduction

The 2020 Beirut explosion of an estimated 2750 tons of Ammonium Nitrate (AN) was one more tragic illustration of the explosive potential of industrial oxidising chemicals [1-2], which are strictly regulated against illicit use and require specific industrial risk control processes. Hydrogen Peroxide (HP) is another typical example of an oxidiser, widely misused by terrorists over the last 20 years for the synthesis of TATP and HMTD [3-6] or in mixture with organic material (HPOM) [7]. HP can also be explosive on its own at high concentrations [8], which also stimulates current research on novel, green, nitrogen-free, peroxide-based explosives for the mining industry [9-10].

Urea can be directly added to hydrogen peroxide to form an adduct (UHP), which is industrially produced as a solid and stable source of hydrogen peroxide for bleaching, disinfection, and oxidation reactions. As a chemical combination of fuel and oxidiser [11], UHP has explosive potential but the available academic literature about its explosive properties is surprisingly limited.

To the best of our knowledge, the explosive potential of UHP was first reported in 2016 by Hussein [12] and Matyas [13]. Hussein studied the relative explosive strength of mixtures containing urea and/or peroxide, using ballistic mortar techniques and thermochemical calculations. Matyas characterised comprehensively the explosive and thermal properties of UHP. He demonstrated its detonability, recording an experimental velocity of detonation (VoD) of 3778 m/s for a 30 kg charge. However it is unclear whether UHP could sustain a detonation at the 100 g scale.

In this paper, we investigated the detonability of commercial lab grade UHP (97%) at small scale. We studied the effect of parameters such as charge diameter, charge length, loading density and confinement material, together with initiation and boosting material in order to confirm the possibility of detonation at common commercial scales and below, extending previous large-scale publications. Further UHP performance assessment includes witness plate indentation [14-15] and VoD measurements using Optimex 64 [16].

2 Experimental Section

Our methodology (Fig 1) combined theoretical calculation, numerical simulation and a comprehensive experimental campaign, consisting of 40 firings. Theoretical predictions and numerical simulation results were compared with experimental data, obtained at small-scale.

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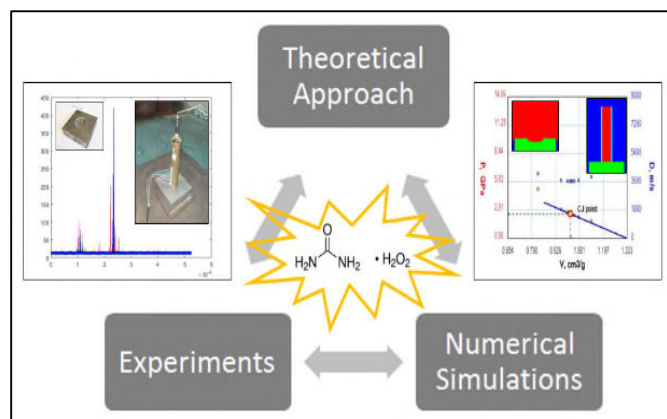


Figure 1. Research methodology.

The experimental approach preceded the numerical approach in order to experimentally validate a set-up that enabled self-sustained detonations to be recorded. This geometry was then numerically simulated in Ansys Autodyn.

We used commercial lab grade UHP (97%) from a single lot purchased from ALFA AESAR – L13940.36. The particle size distribution was determined by dry sieving (Table 1).

Table 1. Particle size distribution.

Mesh size (μm)	Sample retained (%)
1000	15.5
800	41.4
600	28.1
400	14.5
200	0.5

In accordance with Matyas' recommendations regarding thermal stability [13], UHP was stored at 5 °C when not in use and left in ambient conditions for one hour prior to the preparation of each charge.

2.1 Theoretical approach

We used thermodynamic code Explo5 (V6.05) calculations [17] in order to determine the ideal detonation parameters, based on the chemical equilibrium steady state detonation model, and compare them with the values obtained experimentally.

The standard enthalpy of formation of UHP was calculated from calorimetry measurements. A Parr 6200 isoperibol calorimeter (operated under 3 MPa O₂) was calibrated with Benzoic Acid (BA) reference and 10 single measurements were carried out on 1.75 g pellet samples (80% UHP - 20% BA as combustion aid), with no combustion residues observed. The standard enthalpy of formation at 298.15 K was calculated by applying the manufacturer standard methods for thermodynamic calculations.

The theoretically based equation of state (EoS) molecular fluid EXP-6 [18] was selected instead of Becker – Kistiakowski – Wilson (BKW) EoS to give better predictions of detonation velocity and pressure at densities below 1.2 g/cm³. We also used the Explo5

built-in algorithm [19-21] with 2250 K freezing temperature to estimate the Jones-Wilkins-Lee (JWL) coefficients and feed our hydrocode simulation (section 2.3).

2.2 Experiments

2.2.1 Preliminary testing

The objective of the preliminary testing was to define and validate a set-up that enabled self-sustained detonation to be achieved. We used charge masses ranging from 2 g up to 100 g UHP, under light or heavy confinement material, initiated by a pyrotechnical train with or without booster. An overview of the test program is available in Table 2.

Table 2. Preliminary testing.

UHP (g)	ID (mm)	OD (mm)	L (mm)	Confinement	Initiation	# firings
2-5	10	14	50	Steel 316L	Deto N°8	3
100	30	38	150	INOX 321	Deto N°8 + Booster	6
100	30	38	150	PE	Deto N°8 + Booster	3

We selected an initial charge length of 150 mm, corresponding to 5 inner diameters, a commonly used reference for non-ideal commercial blasting explosives [22]. Scaled-up UHP explosive charges (0.75 g/cm³, loose) of approximately 100 g, were initiated with a standard N°8 military detonator and C4 plastic explosive boosters of decreasing size (20 g, 10 g, 5 g, 2.5 g). Explosive charges were initiated in direct contact with a witness plate (Al 6082 T651). The indent depths on the witness plates were measured (0.01 mm accuracy) using a Helios micrometer.

2.2.2 Validated set-up

Anticipating on the results (see section 3.2.1), 100 g UHP charges, confined in steel cylinders of INOX 321, initiated by a standard N°8 military detonator and a 7.5 g C4 booster, were used for further detonation investigations. An overview of the test program is available in Table 3.

Table 3. Validated set-up test program.

	Purpose	# firings
1	Optimum loading density	12
2	Minimum charge length for stationarity	13
3	Velocity of Detonation	15

To optimise the likelihood and reproducibility of the initiation by distributing it over the entire charge diameter, we designed a bespoke conical cup (Fig 2) wherein a booster of constant shape and mass (7.5 g C4) can be moulded and a standard N°8 military detonator can be inserted easily.



Figure 2. 3D printed booster cup.

In order to assess the effect of loading density on detonation parameters, 12 steel cylinders of INOX 321 were loaded at charge densities ranging from 0.75 to 1.45 g/cm³. They were filled stepwise in 4 g increments with UHP to ensure reproducibility and a constant density along the charge. Higher densities were obtained by hydraulically pressing (0.7 to 56 kN). Densities lower than 1 g/cm³ were obtained by vibration, using ballasts on top. Either pressure or vibration was exerted during one minute at each filling step.

The charges were detonated in contact with a 30 mm thick aluminium (6082 T651) witness plate, itself placed on a 20 mm thick anvil, using a standard N°8 military detonator and a 7.5 g C4 booster moulded in a conical cup, producing an initial steady overdriven reaction wave. The indent depth in the witness plate was measured using a micrometer.

As we were detonating UHP charges filled at various densities with all other parameters kept constant (confinement material, length, diameter, orientation, firing set-up and initiator), we investigated the effect of density on the fragmentation pattern using the *Fragment Weight Distribution Map* (FWDM) evaluator [23-24]. This tool has been developed by Oxley to assess the explosive power of pipe bomb devices with a single variable, which is insensitive to percent recovery. Fragments of the steel container (Fig 3) were collected, sorted and weighed according to the described procedure. FWDM slopes were determined and compared to average indent depths on the witness plate as a function of the charge loading density.

In an attempt to assess the minimum charge length to allow self-sustained detonation to develop, 13 additional steel cylinders with lengths ranging from 1 inner diameter (30 mm) to 6 inner diameter (180 mm) were detonated as previously described.



Figure 3. Fragmentation (90% mass recovery) and indent on witness plate for a confined 90 g UHP charge at density 0.83 g/cm³.

Detonation velocities (VoD) were recorded using Optimex 64, the passive optical analyser of explosive processes from OZM Research. We filled 15 additional steel cylinders stepwise at loading densities of 0.75, 1 and 1.1 g/cm³ (accuracy 0.01 g/cm³). The charges were detonated as described previously, with optical probes positioned in accordance with the minimum charge length requirement (Fig 4), after the first 90 mm (3x ID). 8 blind (non through) holes (depth 2 mm; spacing 7.5 mm) were drilled in the lower part of the tube to insert the optical probes safely and accurately, as shown in Figure 5. In this way, the optical probes were protected from noise on the signal and only triggered from the light produced by the adiabatic compression of the air trapped in the blind hole as the detonation front passed. The VoD is calculated from the recorded arrival times and the known distance between probes.

The detonation pressure can be calculated at different loading densities ρ_0 , using [25]:

$$P_{det} = \frac{\rho_0 \cdot (VoD)^2}{\gamma + 1} \quad (1)$$

A good estimate of the detonation pressure of typical military explosives with densities ranging from 1 to 1.8 g/cm³ can be obtained using a ratio of the specific heats of the detonation product gases equal to 3. However, this value is overestimated for non-ideal explosives with lower detonation velocities, such as AN-based explosives. Detonation pressure was hence calculated from Cooper generic experimental correlation, which covers a wider range of densities:

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad (2)$$

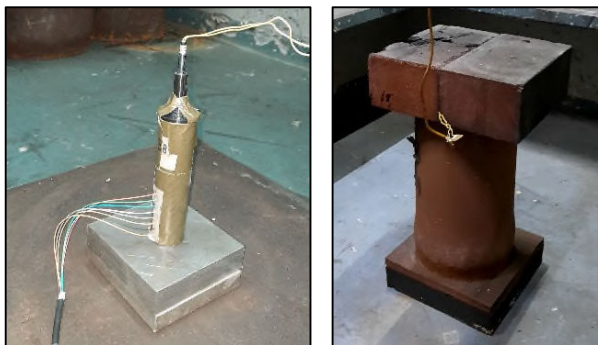


Figure 4. Set-up for detonation of confined UHP charge with vertical initiation, witness plate, anvil, optical probes (left), protective structure to optimise fragment recovery (right).

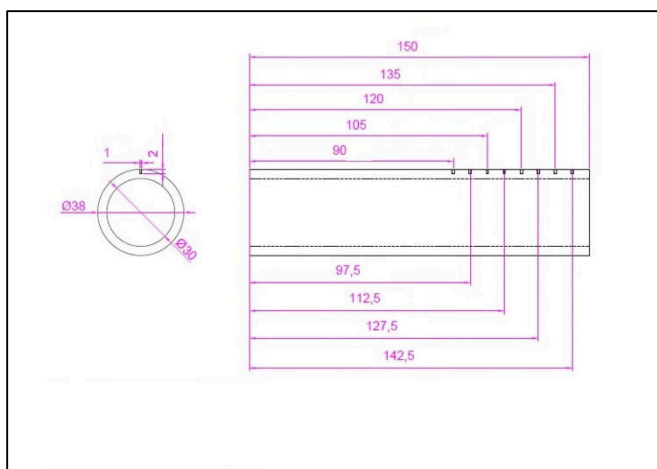


Figure 5. Blind holes in steel container for optical probes positioning (all dimensions in mm, tolerance 0.01 mm).

2.2.3 Experimental results assessment

We used the following data to assess UHP detonation performance:

- Visual observation and measurement of the indent depth on the witness plate.
- Visual observation of the fragmentation pattern and calculation of the FWDM slope.
- Measurement of detonation velocities.
- Calculation of detonation pressure.

This enabled us to derive a correlation between detonation pressure and indent depth.

2.3 Numerical approach

The ultimate aim of the numerical approach is to model UHP detonation prior to further large-scale experiments and risk assessment analysis. Within the scope of this paper, we simulated the set-up in Ansys Autodyn V14.0 in order to model the indentation on the witness plate and compare it to experimental values. As UHP was not

available in the Autodyn library, it was defined using the Chapman-Jouguet (CJ) state ideal parameters and theoretical JWL coefficients estimated from Explo5 calculations (section 2.1). Geometry was chosen as 2D, axisymmetric with mesh size 0.5mm. We used EULER type interactions to overcome interfaces problems and two boundary conditions to fix the bottom of the witness plate (*fix*) and to allow detonation gas to escape through the top of the tube (*flowout*).

3 Results and Discussion

3.1 Theoretical approach

The detonation parameters from the Explo5 calculations, based on a standard enthalpy of formation of -563 kJ/mol calculated from calorimeter results, are available in Table 4. The use of EXP-6 EoS enabled us to estimate JWL coefficients along the detonation products isentrope for explosives with low detonation temperature, when pressure quickly drops to atmospheric.

Table 4. Theoretical detonation parameters (CJ point).

Loading Density (g/cm ³)	0.75	0.9	1	1.1
Heat of Detonation (kJ/kg)	-2447	-2496	-2564	-2621
Detonation Pressure (GPa)	2.42	3.86	5.48	6.92
Detonation Velocity (m/s)	3657	4339	4774	5215

These values are theoretical maximum, assuming ideal detonation and infinite charge diameter, with no account of confinement, grain size or critical diameter. We used these maximum values to estimate the theoretical TNT equivalence and dimension our charges according to our firing bunker NEQ limitations, obtaining respectively 0.8 (power index) and 0.5 (hydrodynamic work) [26].

3.2 Experiments

3.2.1 Preliminary testing

In our set-up, UHP charges (2-5 g) directly initiated by a standard N°8 military detonator failed to detonate, even under heavy confinement. Only combustion was observed, with no detonative output. These experiments did not provide any further technical information but increased our confidence to scale up UHP charges. A minimum booster charge of 5 g C4 was necessary to initiate UHP explosive charges of approximately 100 g confined in steel cylinders. However, we scaled it up to 7.5 g to avoid geometrical effects and distribute the initiation over the entire charge diameter, using a bespoke booster cup. 100 g UHP charges confined in thick polyethylene cylinders initiated by a standard N°8 military detonator and a 7.5 g C4 booster failed to sustain detonation (Fig 6). The

upper part of the PE tube was shattered due to the detonation of the C4 booster. The UHP charge could not further sustain the detonation in a light confinement material such as plastic. A heavy confinement is required to achieve self-sustained detonation in UHP. This is consistent with literature [13] where failed detonation and explosion decay have been observed for similar UHP charges under intermediate confinement (copper, ID 36 mm).



Figure 6. Light confinement – failed detonation: absence of indentation in the plate, presence of unreacted UHP and fragmentation pattern, including petalling of the bottom of the tube.

Scaled-up charges of around 100 g UHP, confined in steel cylinders of INOX 321, initiated by a standard N°8 military detonator and a 7.5 g C4 booster, sustained detonation with indent depth around 5 mm in the witness plate (Fig 7). This latter set-up was validated and selected for further experiment and modelling.

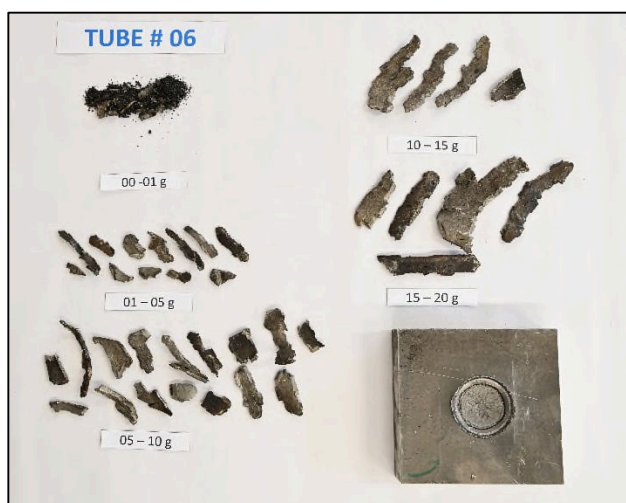


Figure 7. Small-scale detonation of UHP under heavy confinement.

3.2.2 Validated set-up

The effect of UHP loading density was first investigated, using our validated set-up. The average measured indent depth increases almost linearly with growing loading densities, between 0.75 g/cm³ (loose) and 1.1 g/cm³ (pressed), as illustrated in Figure 8. Indentation then drops rapidly and less reproducible responses are observed in the interval 1.1-1.2 g/cm³. This is probably explained by a decrease in shock sensitivity of pressed UHP due to pressurisation, which decreases the density of potential hotspots that play a key role in detonation propagation in heterogeneous explosives [15, 27].

Evidence of deflagration is recorded in the density range of 1.2 -1.3 g/cm³ (Fig 9). In our charge diameter, confinement and initiation conditions (C4 booster incident steady detonation), indications of dead-pressing are observed at densities above 1.3 g/cm³, including further compaction of the UHP by the shock wave, with spalling in the charge at the back of the tube, absence of fragmentation and limited dispersal of unreacted UHP. Further investigations would be necessary to statistically study UHP dead-pressing density and dying-out distance [28]. In our set-up geometry, we could not record sustained detonations at densities closer to 1.43 g/cm³ TMD [13], and maximum performance was observed at a density of 1.1 g/cm³, which we further used for theoretical predictions and modelling.

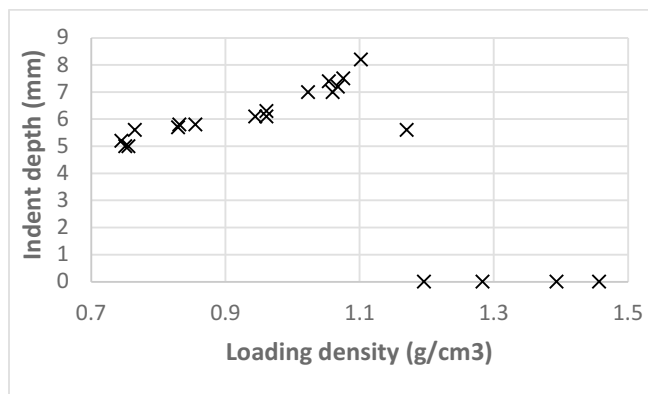


Figure 8. Indentation of witness plate as a function of loading densities for charge lengths equal to 5 x ID.

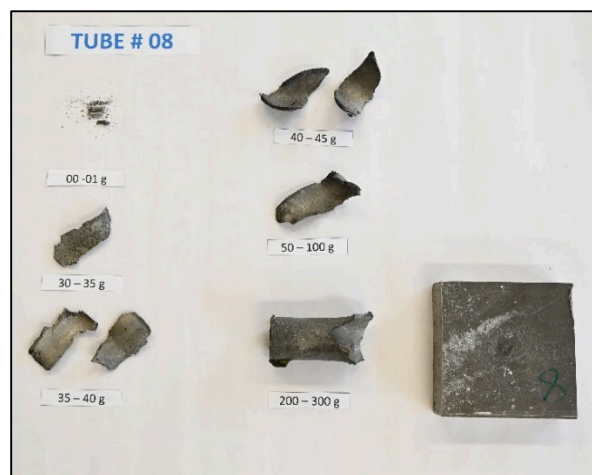


Figure 9. Typical deflagration fragmentation pattern (98% recovery), observed at densities above 1.2 g/cm³ with a small number of large, bent and torn fragments, with 90° fracture edges.

A good correlation was found between the indentation of the witness plates and the slopes of the FWDM plots. Both parameters are deemed complementary to assess the brisance of a confined explosive charge, i.e. its destructive fragmentation effect on its immediate vicinity [29]. As expected, the brisance increases at higher densities, with maximum FWDM slope and indent depth at 1.1 g/cm³ density (Fig 10), while deflagrations are recorded at densities above 1.2 g/cm³.

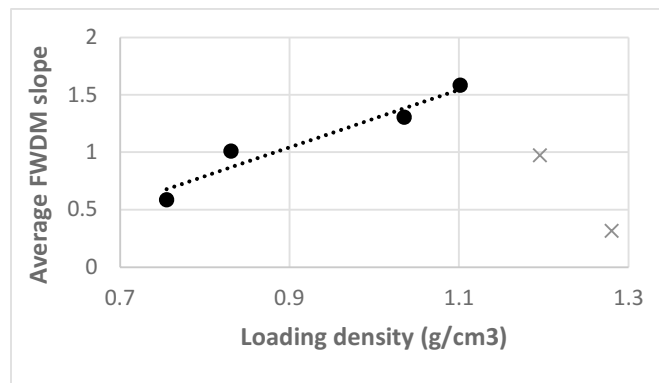


Figure 10. Maximum FWDM slope calculated at a density of 1.1 g/cm³. Difference between detonations (black) and deflagrations (grey) are highlighted.

In the configuration we tested and depending on loading density, stationarity is already observed at charge lengths ranging from 2 to 3 inner diameters as shown in Figure 11.

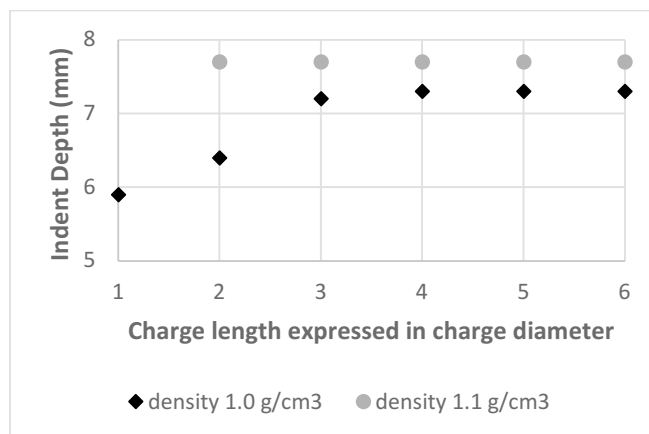


Figure 11. Indentation as a function of charge length.

The experimental VoD values (Table 5) are only about 80% of the CJ ideal theoretical predictions from Explo5. On the one hand, this could suggest that side effects affect the VoD value and that higher VoD could be recorded at higher charge diameter for a given loading density [30]. On the other hand, non-ideal behaviour can also be intrinsic and our experimental values could be close to the maximum achievable VoD for UHP. These questions could be answered by carrying out a comprehensive large-scale parametric study focused on the influence of density, diameter and confinement. However the consistency of our small-scale results with literature values from large-scale experiments [13] shows that our study efficiently reflects the detonation property of UHP, allowing lab-scale studies to be performed.

3.2.3 Experimental result assessment

An overview of the performance parameters of UHP is available in Table 5. We derived an experimental linear correlation between the calculated detonation pressure and measured indent depth. This correlation was further compared to ideal values obtained from Explo5 and Autodyn simulation (section 3.3). Figure 12 further compares witness plate indentation for different UHP loading densities.

Table 5. Performances of UHP charges (L = 5 x ID).

Loading Density (g/cm ³)	0.75	0.9	1	1.1
Average Indent depth (mm)	5.1	6.2	7.1	7.8
Average FWDM slope	0.59	/	1.30	1.58
Average VoD (m/s)	2897	<u>3517</u> ^a	3647	3860
Calculated P _{det} (GPa)	1.86	3.06	3.82	4.67

^a : value taken from Matyas [13], VoD for a 8 kg UHP charge confined in a 8 mm thick steel container (ID = 124 mm)

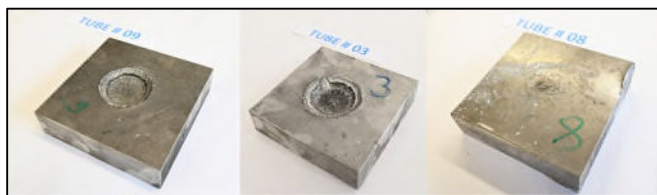


Figure 12. Detonation and indentation at respectively 0.75 g/cm³ (left), 1.1 g/cm³ (middle). Deflagration with no indentation at 1.2 g/cm³ (right).

3.3 Numerical approach

Table 6 gives an overview of the UHP JWL coefficients from Explo5 [17], required to feed the numerical modelling. Indentations on the witness plate are summarised in Table 7 and pictured in Figure 13.

Table 6. JWL coefficients (Explo5).

Loading Density (g/cm3)	0.75	0.9	1.1
A (GPa)	102.8273	203.2893	470.6499
B (GPa)	1.4169	2.5687	5.5299
R1	5.5826	5.6525	5.921
R2	1.4846	1.5474	1.7225
w	0.3102	0.3081	0.3001

Table 7. Indentation values from numerical simulation.

Loading Density (g/cm3)	0.75	0.9	1.1
Indentation (mm)	5.5	7.0	9.5

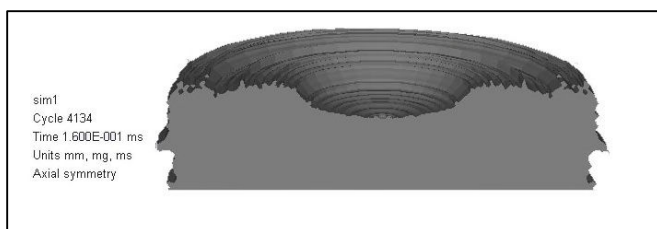


Figure 13. 2DE simulation – indentation witness plate

We previously derived an experimental linear correlation between the calculated detonation pressure and measured indent depth. This correlation is here further compared to ideal values, obtained from Explo5 and Autodyn simulation (Fig 14). Even if they are within the same order of magnitude, the experimental detonation pressure is up to 33% lower and the resulting indentation of the witness plate up to 20% lower than the simulated ones, especially at growing densities. This can be explained by the fact that our numerical model was fed with theoretically ideal performance parameters, i.e. detonation velocity and pressure.

However, both correlations are in good agreement, suggesting that a ratio of the specific heats of the detonation product gases equal to 2.5 is more suitable to estimate the detonation pressure of UHP charges.

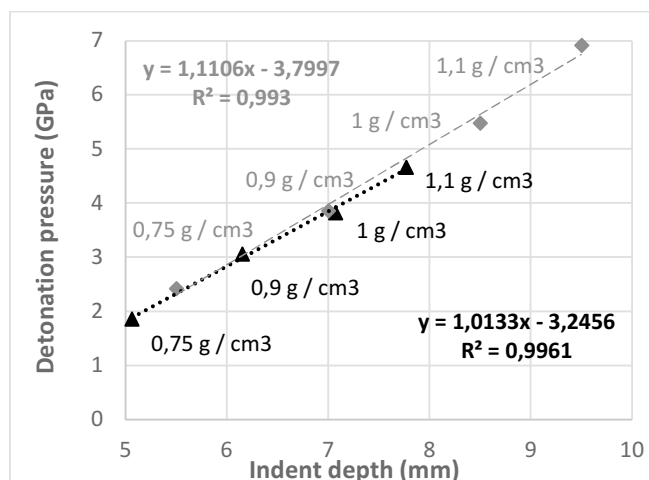


Figure 14. Experimental (black) and simulated (grey) linear correlations between detonation pressure and indent depths.

Our model used Chapman-Jouguet state ideal parameters from Explo5, making it more suitable for conventional explosives [15]. We may speculate that the use of reactive flow models to simulate the detonation behavior of confined non-ideal explosives would better match experimental data [31]. However, current UHP characterization in Autodyn is deemed satisfactory and will be further used to model future larger-scale experiment, including underwater firings.

4 Conclusion

In this paper, we have shown that commercial lab grade UHP (97%) is detonable at small scale. We studied the effect of initiation, charge length, charge diameter, confinement material and loading density and validated a geometry and a bespoke pyrotechnical train. In this configuration, we succeeded in accurately recording self-sustained detonation at relatively small scale under heavy confinement. Optimex 64 has proven reliable for lab-scale VoD measurements, even for non-ideal explosives. Our small-scale results are consistent with literature VoD values from large-scale experiments.

Maximum detonation performances were measured at an optimum 1.1 g/cm³ loading density. In our set-up, deflagration or dead-pressing are observed at higher loading densities. Maximum calculated detonation pressures are below 10 GPa, the order of magnitude for commercial blasting explosives. To estimate the detonation pressure of UHP charges, a value of 2.5 for the ratio of the specific heats of the detonation product gases was found more suitable.

Our numerical model, including UHP characterization with JWL coefficients from Explo5 built-in algorithm was deemed satisfactory and will be further used to model future larger-scale experiment, including underwater firings, and related risk assessment analysis.

The proposed experimental method can be used to quantify the detonability and performance of other industrial materials that may have energetic properties, or small samples of homemade explosive compositions, avoiding time-consuming, expensive and potentially hazardous large-scale experiments.

Symbols and Abbreviations

AN	Ammonium Nitrate
BA	Benzoic Acid
BKW	Becker Kistiakowski Wilson
CJ	Chapman-Jouguet
EoS	Equation of State
FWDM	Fragment Weight Distribution Map
HMTD	Hexamethylene Triperoxide Diamine
HP	Hydrogen Peroxide
HPOM	Hydrogen Peroxide Organic Material
ID	Inner Diameter
JWL	Jones Wilkins Lee
L	Charge Length
NEQ	Net Explosive Quantity
OD	Outer Diameter
PE	Polyethylene
TATP	Triacetone Triperoxide
TMD	Theoretical Maximum Density
TNT	Trinitrotoluene
UHP	Urea Hydrogen Peroxide
VoD	Velocity of Detonation

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Small-scale detonation of industrial Urea-Hydrogen Peroxide (UHP)

Halleux, Francis

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Appendix C: Poster presented at the 24th New Trends in Research of Energetic Materials Conference (2022).

Urea Hydrogen Peroxide Detonation Performance

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1. Introduction

Urea Hydrogen Peroxide (UHP) – Carbamide Peroxide:

- Commonly used in the cosmetic and pharmaceutical industries
- Easily manufactured from readily available household chemicals
- Explosive properties recently studied [1-2] : non-ideal, detonable at large scale

Scope of our research:

- Detonability of commercial lab grade UHP at the **100 g – scale**
- Determining detonation **performance parameters** for risk assessment purposes

2. Material and methods

- Commercial lab grade UHP** (97%); 85% particles > 600 µm
- Explo5:** Ideal detonation parameters & JWL coefficients for **Autodyn** modelling
- Need for **maximum experimental data**: lab & underwater measurements
- Detonation velocity (VoD), Detonation pressure (P_{det}), Equivalent shock (E_s) & bubble (E_b) energy

Lab firing:

- 100 g cylindrical charges
- ID 30 mm, length 5 ID
- Heavy confinement (4 mm steel)
- Initiation by a standard N°8 military detonator and an 8 g C4 booster

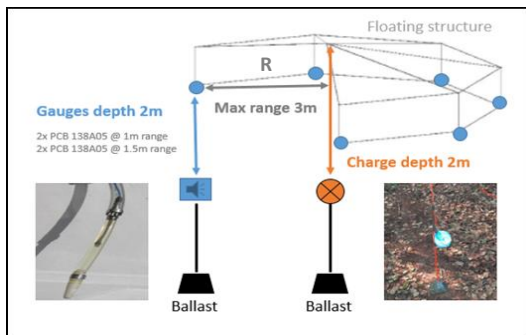


Performance assessment: witness plate indentation and VoD measurements (Optimex 64), detonation pressure calculated from Cooper [3] from VoD and loading density

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04})$$

Underwater firing:

- 100 g loose UHP spherical charges in plastic (PE) bags
- Initiation by a standard N°8 military detonator and an 8 g C4 booster
- 100 g C4 spherical charges fired for comparison



Performance assessment: brisance from underwater shock pressure and explosive power from bubble period (t_b)

3. Results and discussion

Lab firings results (theoretical predictions between brackets)

UHP loading density [g/cm³]	0.75	1	1.1
Average VoD [m/s]	2897 (3657)	3647 (4774)	3860 (5215)
Calculated P_{det} [GPa]	1.86 (2.42)	3.82 (5.48)	4.67 (6.92)
Average indent depth [mm]	5.1 (5.5)	7.1 (8.5)	7.8 (9.5)
Relative brisance vs TNT [%]	9	18	22
Relative brisance vs C4 [%]	6.5	13	16
Relative brisance vs ANFO [%]	28	58	71

- Differences between the calculated and the experimental **velocities of detonation** between 750 and 1300 m/s, highlighting the non-ideal behaviour of UHP in these conditions [4]
- Calculated **detonation pressures** up to 33% lower than the predictions from the thermodynamic code Explo5 and the resulting indentations of the witness plate up to 20% lower than the simulated ones, especially at growing densities

Underwater results at R=1m (theoretical predictions between brackets)

	ρ [g/cm³]	m [g]	P_{max} [MPa]	t_b [ms]	E_s [Pa²s]	E_{sw} [MJ/kg]	E_b [s²]	E_{bw} [MJ/kg]
C4	1.63	100	21.45 (21.47)	121.5	11097 (11090)	0.929161 (0.928603)	0.0018	1.9735
UHP	0.75	100	8 (13.02)	80.7	1170 (5450)	0.097968 (0.456347)	0.0005	0.5784

- UHP: **highly non-ideal behaviour** with experimental data significantly lower than the value from our Autodyn model (60% P_{max} , 20% shock energy equivalent)
- Autodyn model** based on CJ state ideal parameters calculated from Explo5, more suitable for military explosives, such as C4
- Calculated **equivalencies** (from TNT literature data):

Underwater explosions – TNT equivalencies [%]

Charge	Brisance	Explosive Power
UHP	13	33
C4	129	105

4. Conclusions and future work

- Detonation performance of UHP** at the 100 g-scale has been characterised.
- Lab results confirmed self-sustained detonation under heavy confinement, with observed detonation velocities consistent with literature values from large-scale field experiments.
- TNT equivalents were calculated based on experimental results and compared to those obtained by theoretical prediction.
- UHP explosive power and brisance were quantified from bubble period and underwater shock pressure, with respective TNT equivalencies of 33% and 13%. This latter shock energy equivalent from underwater explosions is consistent with UHP relative brisance calculated from lab firing.
- Performing such an **experimental campaign** has proven useful to characterise the performances of non-ideal explosives for risk assessment purposes.
- Future work** includes further assessment of booster contribution on total energy and a size-effect study, firing kg-size UHP charges underwater using the same scaled distances.

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Appendix D: Published Proceedings – 24th NTREM.

Detonation performance of urea hydrogen peroxide

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Detonation performance of urea hydrogen peroxide

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Abstract

Carbamide Peroxide is commonly used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. This adduct of Urea and Hydrogen Peroxide (UHP) has explosive properties, which have been only recently studied, highlighting its behaviour as a non-ideal tertiary explosive and its detonability at large scale. Our work focussed on investigating UHP detonability at the 100 g - scale. Our lab results confirmed self-sustained detonation under heavy confinement, with observed detonation velocities consistent with literature values from large-scale field experiments. We further fired UHP charges underwater and quantified brisance (13%) and explosive power (33%) with respect to TNT. Performing such an experimental campaign has proven useful to characterise the performances of non-ideal explosives for risk assessment purposes.

Keyword: urea hydrogen peroxide; detonation; non ideal explosive; performance

1 Introduction

Carbamide Peroxide or Urea Hydrogen Peroxide (UHP) is commonly used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. As a chemical combination of oxidiser and fuel, this adduct has explosive properties, which have been only recently studied, highlighting its behaviour as a non-ideal tertiary explosive and its detonability at large scale [1-2]. UHP can also be easily manufactured from readily available household chemicals, making it a potential emerging threat. Determining UHP detonation performance parameters is hence very important for risk assessment purposes.

Our work here focussed on investigating detonability of commercial lab grade UHP at the 100 g - scale. As a maximum of experimental data is desirable to evaluate the detonation performance of a non-ideal explosive, we carried out a detailed assessment, combining experimental results from lab and underwater firings, supported by thermochemical calculations and numerical simulations, in order to determine detonation velocity (VoD), detonation pressure (P_{det}), equivalent shock (E_s) and bubble (E_b) energy. By comparing experimental results and numerical simulations, we could assess the level of agreement between lab and underwater detonation performance parameters.

2 Material and methods

We used commercial lab grade UHP (97%) purchased from ALFA AESAR. Average particle size was determined by dry sieving with 85% of the particles retained in the 600 μm mesh and 15% in the 1000 μm mesh. The standard enthalpy of formation of UHP was calculated from calorimetric measurements and we used the thermodynamic code Explo5 (V6.05) [3] to determine UHP ideal detonation parameters (VoD, P_{det}) at the Chapman-Jouguet point, together with its Jones-Wilkins-Lee coefficients, required for further modelling of our lab and underwater firing setups in Ansys Autodyn V14.0.

2.1. Lab firings

Our validated setup (Fig 1) for lab detononic investigations is extensively described in [4]. It basically consists of 100 g UHP cylindrical charges, with an inner diameter of 30 mm and a length equal to 5 inner diameters under heavy confinement (4 mm thick stainless steel walls). The charges were initiated by a standard N°8 military detonator and an 8 g C4 booster. They were detonated in contact with a 30 mm thick aluminium (6082 T651) witness plate. Performance assessment included witness plate indentation and detonation velocity measurements using a passive optical fibre-based instrument (Optimex 64 from OZM Instrument). Detonation pressure was estimated from VoD and loading density (ρ_0), using an empirical correlation [5]:

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04})$$

From the estimated detonation pressures, we further quantified UHP relative brisance (%) with respect to TNT ($\rho_0=1.64 \text{ g/cm}^3$; VoD=6950 m/s) and C4, two military explosives which we further used in the underwater explosion experiments, and ANFO, a typical commercial blasting explosive with detonation pressure below 10 GPa [5].

We simulated the set-up in Ansys Autodyn V14.0 in order to model and compare witness plate indentation to experimental values. Geometry was chosen as 2D, axisymmetric with mesh size 0.5 mm and EULER type interactions to overcome interface problems.



Figure 1. Experimental setup for lab firings

2.2. Underwater firings

The underwater test campaign was conducted at *Braboplas* range, a military underwater demolition site with an average depth of 5 m. The experimental setup is depicted in Figure 2. Explosive charges were suspended in the centre of a floating structure at a depth of 2 m. Four voltage mode tourmaline pressure sensors type PCB 138A05 were placed at the same depth, respectively 2 gauges at 1 m and 2 gauges at 1.50 m range (R) from the charge. According to recommendations in [6], pressure sensors were aligned on the radial axis of the charge and outside a calculated maximum bubble radius of 0.75 m for a 100 g C4 explosive charge [7], considered as maximum dimensioning charge for the design of our experimental setup.

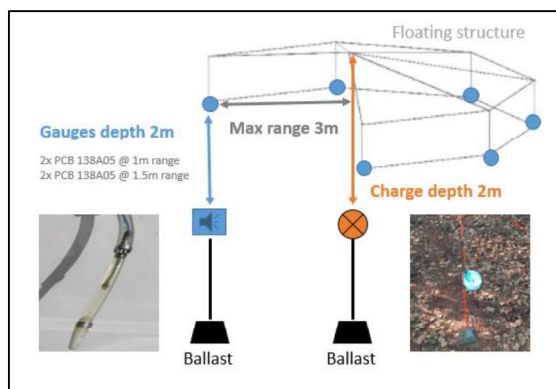


Figure 2. Experimental setup for underwater firings

Spherical charges of 100 g loose UHP in plastic (PE) bags (no confinement), were initiated by the same explosive train we used in the lab, i.e. a standard N°8 military detonator and an 8 g C4 booster. Because, to the best of our knowledge, UHP experimental data from underwater explosion are lacking in the literature, we also fired, in the same conditions, spherical 100 g C4 charges and standard military 100 g TNT cartridges (CTG) for reference and comparison purposes. Additionally, we finally fired 8 g C4 booster charges alone in an attempt to better assess the influence of the booster on UHP detonation performance. An overview of the test program (10 shots) is available in Table 1.

Table 1. Underwater firings - test program

Charge	Charge and sensors depth [m]	Number of shots
100 g UHP (+ 8 g C4)	2	3
8 g C4	2	2
100 g C4	2	3
100 g TNT CTG	2	2

Performance assessment included determination of underwater shock pressure and bubble period (t_b) in order to quantify brisance (shock wave energy) and explosive power respectively, using the procedure described in [8-11], assuming no boundary effects and using Willis formula to calculate bubble energy [8].

We simulated the set-up (Fig 2) in Ansys Autodyn V14.0 in order to model and compare the performance of the different charge types to experimental values, using a 1D spherical geometry (5000 cells) with 22 gauges located from 0.3 to 2.4 m from the charge centre.

3 Results and discussion

Detailed lab campaign results are available in [4]. Key experimental data are highlighted in Table 2 with theoretical predictions from Autodyn (using Explo5 parameters) mentioned between brackets. The differences between the calculated and the experimental velocities of detonation range between 750 and 1300 m/s, highlighting the non-ideal behaviour of UHP in these conditions [12]. Accordingly, the calculated detonation pressures are up to 33% lower than the predictions from the thermodynamic code Explo5 and the resulting indentations of the witness plate up to 20% lower than the simulated ones, especially at growing densities. We hence calculate, under heavy confinement, a relative brisance of 9% for loose UHP (0.75 g/cm^3) and a maximum relative brisance of 22% at the optimum density of our setup (1.1 g/cm^3), with respect to TNT.

Table 2. Lab firings results (theoretical predictions between brackets)

UHP loading density [g/cm^3]	0.75	1	1.1
Average VoD [m/s]	2897 (3657)	3647 (4774)	3860 (5215)
Calculated Pdet [GPa]	1.86 (2.42)	3.82 (5.48)	4.67 (6.92)
Average indent depth [mm]	5.1 (5.5)	7.1 (8.5)	7.8 (9.5)
Relative brisance vs TNT [%]	9	18	22
Relative brisance vs C4 [%]	6.5	13	16
Relative brisance vs ANFO [%]	28	58	71

The experimental shock wave parameters and calculated equivalent and specific shock (E_s , E_{sw}) and bubble (E_b , E_{bw}) energy are summarised in Table 3. Additionally, theoretical predictions from Autodyn (using Explo5 parameters) are mentioned between brackets. C4 has proven a good reference explosive for underwater experiments. Experimental results and simulation for C4 are in very good agreement, and consistent with literature data [13-15], giving us confidence in the experimental setup and the recorded results.

Table 3. Underwater results at R=1m (theoretical predictions between brackets)

	ρ [g/cm^3]	m [g]	$P_{\max}$ [MPa]	t_b [ms]	E_s [Pa^2s]	E_{sw} [MJ/kg]	E_b [s^3]	E_{bw} [MJ/kg]
C4	1.63	100	21.45 (21.47)	121.5	11097 (11090)	0.929161 (0.928603)	0.0018	1.9735
UHP	0.75	100	8 (13.02)	80.7	1170 (5450)	0.097968 (0.456347)	0.0005	0.5784

As expected, UHP exhibits a highly non-ideal behaviour and the experimental data are significantly lower than the value from our Autodyn model (60% of predicted $P_{\max}$, 20% for shock energy equivalent). Again, the Autodyn model was based on Chapman-Jouguet state ideal parameters calculated from Explo5, making it more suitable for military explosives [12], such as C4.

Unlike C4, the use of TNT CTG was unfortunately not successful for direct comparison purposes. Because of different charge geometry (cartridges) and, hence, position of the initiator, the obtained pressure histories ($P_{\max}$, E_s , t_b), especially at short distance from the charge, differed significantly from the predictions from both our Autodyn model and the empirical calculations for TNT. We hence used TNT literature data [15-16] to determine equivalencies, which are summarised in Table 4.

Table 4. Underwater explosions – TNT equivalencies [%]

Charge	Brisance	Explosive Power
UHP	13	33
C4	129	105

As far as UHP is concerned, the calculated shock and bubble energies include the contribution of the booster, which we wanted to better quantify. Looking at the performance of the 8 g C4 booster alone, we calculate a relative shock energy of 30% and relative bubble energy of 20% with respect to the respective shock and bubble energies of a 100 g UHP charge initiated by the same booster. This is of course a rough approximation assuming additivity effects. In order to better quantify the effect of the booster, one should first determine the maximum contribution in the total energy using C4 boosters of different sizes [17], which will be performed during our next underwater firing campaign. UHP relative brisance from lab firing is however consistent with its shock energy equivalent from underwater explosions, which will be refined.

4 Conclusion

Detonation performance of UHP at the 100 g -scale has been characterised. Our lab results confirmed self-sustained detonation under heavy confinement, with observed detonation velocities consistent with literature values from large-scale field experiments. TNT equivalents were calculated based on experimental results and compared to those obtained by theoretical prediction. UHP explosive power and brisance were quantified from bubble period and underwater shock pressure, with respective TNT equivalencies of 33% and 13%. This latter shock energy equivalent from underwater explosions is consistent with UHP relative brisance calculated from lab firing. Performing such an experimental campaign has proven useful to characterise the performances of non-ideal explosives for risk assessment purposes.

Future work includes further assessment of booster contribution on total energy, Autodyn simulation of the bubble effect and, ultimately, a size-effect study, firing kg-size UHP charges underwater using the same scaled-distances.

Acknowledgement

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Appendix E: Poster presented at the 8th Defence and Security Doctoral Symposium (2022).

Investigation into the detonation performance of Urea-Hydrogen Peroxide

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Investigation into the detonation performance of Urea Hydrogen Peroxide

1. Context

- Current Home Made Explosive (HME) threat worldwide:
 - Mixing of highly energetic pyrotechnics
 - Synthesis of **peroxide explosives**
- Carbamide Peroxide or **Urea Hydrogen Peroxide (UHP)**, widely used in the dental, cosmetic and pharmaceutical industries, has proven detonable at small-scale under heavy confinement [1].



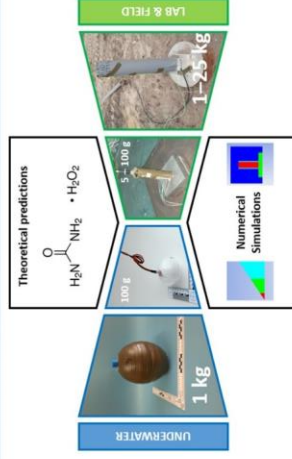
2. Objectives and challenges

- Characterise UHP detonation performance for **risk assessment** purposes [2].
- Collect **maximum experimental data**, particularly desirable for evaluating the performance of non-ideal explosives: lab, field and underwater instrumented firings, with military reference explosive, supported by thermochemical calculations and numerical simulations.
- Assess the **level of agreement** between:
 - Laboratory, field and underwater data
 - Small-scale and large-scale experiments
 - Experiments, theory and simulations



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3. General approach



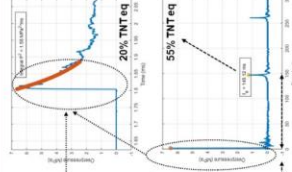
4. Preliminary results

➤ Underwater firings:

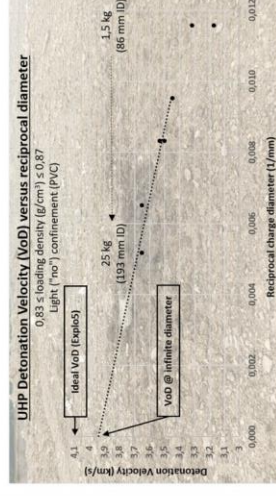
Shock pressure (Brisance)



Bubble period (Explosive Power)



➤ Field firings: Detonation velocity & Blast parameters



5. What's next

- Non-ideality vs numerical simulations
- Size effects vs validity of small-scale set-ups
- Propose and discuss TNT equivalences for UHP

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Appendix F: Published Research Article.

Detonation performance of urea-hydrogen peroxide (UHP)

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Detonation Performance of Urea-Hydrogen Peroxide (UHP)

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Romuald Van Riet ^[b], Michel Lefebvre ^[b]

Abstract: Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide, is commonly used in the cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. However, it exhibits explosive properties and can be easily manufactured from readily available household chemicals, making it a potential emerging threat. We carried out a detailed performance assessment, combining experiments, thermochemical calculations and numerical simulations and highlighted a good level of agreement between experimental data from lab, field and underwater firings. A maximum detonation velocity of 3.65 km/s was recorded for unconfined 25 kg UHP charges at 0.85 g/cm³ (200 mm charge diameter). We determined in these conditions an infinite diameter detonation velocity of 3.94 km/s. These results are also consistent with previous results obtained at small scale under heavy confinement. Airblast measurements highlighted an average 40% TNT equivalence for impulse and 55% for peak overpressure at short distance, which are in good agreement with the 57% (Power Index) calculated from Explo5, while 50% for bubble energy (explosive power) and 20% for shock pressure (brisance) were obtained from underwater experiments. The use of different experimental approaches has proven useful to characterise the performances parameters of a non-ideal explosive for risk assessment purposes.

Keywords: Urea hydrogen peroxide, Detonation, Non ideal explosive, Performance

1 Introduction

Carbamide Peroxide or Urea Hydrogen Peroxide (UHP) is commonly used in the dental, cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide. This adduct can also be easily manufactured from readily available household chemicals. Like other oxidisers such as ammonium perchlorate [1] or ammonium nitrate [2], UHP exhibits explosive properties [3, 4] and could represent a potential emerging threat. Determining UHP detonation performance parameters is hence important for safety purposes.

Because there is a need to predict large-scale explosive behaviour from small-scale experiments [5], our previous work demonstrated UHP detonability at small scale under heavy confinement, providing an initial lab-scale characterisation of detonation performance parameters, including velocity of detonation (VoD) records consistent with literature values from large-scale experiments [6]. UHP charges non-ideality was further studied by VoD dependence on charge diameter and confinement [7], a behaviour typically observed for charge diameters in the 10 cm range with explosives detonating at a lower regime, such as ANFO explosives, and particularly emphasised by recent research at small-scale [8, 9].

As extensive experimental data is particularly desirable to accurately evaluate the detonation parameters of non-ideal explosives [10], we present in this paper a detailed performance assessment supported by thermochemical calculations and numerical simulations. Initial lab characterisation is completed and complemented by field and underwater instrumented firings using scaled-up charges (Figure 1).

The level of agreement between small-scale and large-scale, between field and underwater experimental

performance parameters and between experiment and numerical simulation has been investigated. To that end and for each performance parameter under consideration, we made use of experimental TNT equivalences [11-13], knowing the limitation of the concept [14-16], especially when comparing non-ideal and ideal explosives [17]. However, for both academic and safety purposes, we found necessary to compare UHP detonation performance with well-known and documented standards, TNT or plastic explosives such as C4 (91% RDX), which were, for direct comparison, detonated in identical experimental conditions, with particular care for charge configuration (shape, initiation, confinement) and (scaled) distances.

2 Experimental Section

We used commercial lab grade Urea Hydrogen Peroxide - UHP (97%) purchased from ALFA AESAR. Average particle size was determined by dry sieving with 85% of the particles retained in the 600 µm mesh and 15% in the 1000 µm mesh. The standard enthalpy of formation of UHP was calculated from calorimetric measurements and we used the thermodynamic code Explo5 (V6.06.02) to determine UHP ideal detonation parameters. Following our previous work [6], the

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theoretically based equation of state (EoS) molecular fluid EXP-6 was selected to calculate UHP VoD and detonation pressure (P_{det}), together with its Jones-Wilkins-Lee (JWL) coefficients, required for further modelling of our experimental firing setups in Ansys Autodyn V14.0. For comparison purposes, we also calculated VoD and P_{det} using the Modified Becker-Kistiakowski-Wilson (M-BKW) EoS, as this equation of state is known to lead to a better accuracy when dealing with explosives showing a high dipolar molecules content in the detonation products and a low detonation temperature [18].

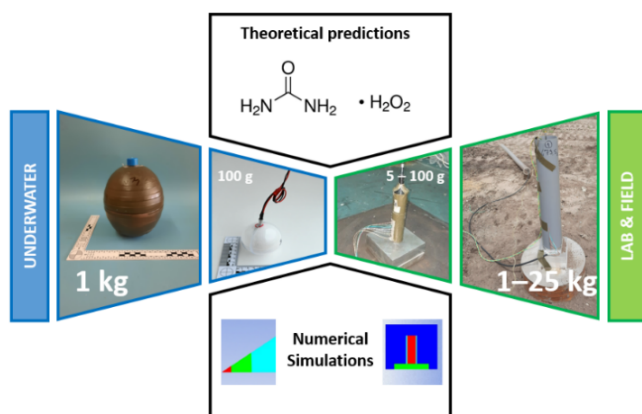


Figure 1. UHP Detonation Performance Assessment.

In the following subsections, we successively present the respective experimental methods and set-ups used for the lab, field and underwater firings.

2.1 Lab Firings

The firing setup basically consists of 80-120 g UHP cylindrical charges at loading densities ranging from 0.75 to 1.1 g/cm³, under heavy confinement (stainless steel walls), with an outer diameter (OD) of 38 mm, an inner diameter (ID) of 30 mm and a length equal to 5 inner diameters. 40 UHP charges were initiated by a standard N°8 military detonator and an 8 g C4 booster. Initial performance assessment [6] included Al 6082 T651 witness plate dent and detonation velocity measurements (Optimex 64 – OZM research). VoDs were determined using arrays of passive optical fibre probes to record arrival times and a known distance between probes. P_{det} was further estimated from VoD and loading density (ρ_0) using the following empirical correlation [7]:

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad (1)$$

Complementary firings were carried out in the lab. The confinement sleeves were filled by 4 g UHP increments to obtain the following charge densities (theoretical maximum density 1.43 g/cm³ [3]), calculated from mass and volume UHP: 0.75 (loose) and 0.85 g/cm³, i.e. slightly compacted by vibration to achieve more uniform loading and homogeneity. The VoD setup [6] was duplicated (Figure 2) and included a total of 16 optical fibre probes, divided in two rows of 8 probes, with 7.5 mm between probes, and the first

probe of each row located 90 mm (3 x ID) from the booster charge. The setup was also slightly adapted in an attempt to capture improved signals by reducing the thickness of confinement material between the optical probes and the energetic material under investigation, while avoiding any early triggering from the light preceding the detonation wave due to translucency of the explosive. Instead of inserting the probes in 2 mm deep, non-through (blind) holes drilled in the confinement sleeve, like in previous work [6], we used all-through holes sealed by a piece of 30 μ m thick aluminium tape glued inside the sleeve. Finally, we recorded the VoD and measured witness plate indentation from two 120 g pressed TNT charges (1.61 g/cm³) prepared and detonated in the same conditions in an attempt to assess UHP relative brisance (%) based on plate dent depth [19].

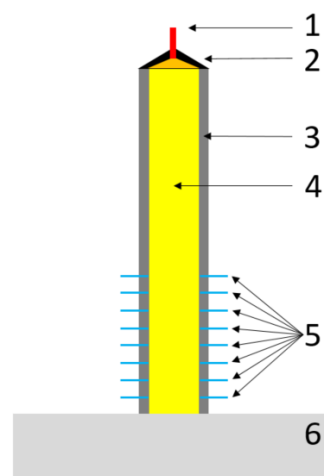
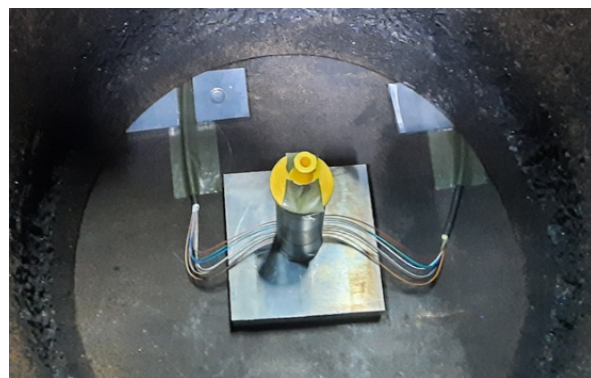


Figure 2. 100 g UHP – heavy confinement : (1) N°8 detonator; (2) C4 booster in bespoke holder, (3) Confinement sleeve, (4) UHP charge, (5) 2x8 Optical probes, (6) Al witness plate

2.2 Field Firings

The field firings consisted of two separated experimental campaigns in order to measure the VoD to determine a nominal charge diameter for studying UHP performances (1) and record the airblast characteristics in a selected setup, for which non-ideal effects are considered as limited enough to not significantly influence the performance of the charge, in

an attempt to provide a performance characterisation independent of the setup and valid for very large charges (2). Both experimental setups are depicted in Figure 3, while Table 1 describes the test program. Upscaled kg-size UHP charges without confinement (PVC casing) were filled in 25 increments and vibrated at each step to achieve a reproducible $0.85 \pm 0.02 \text{ g/cm}^3$ loading density at large scale, avoiding self-compaction phenomenon and density gradient observed at loose density (0.75 g/cm^3) for large charges.

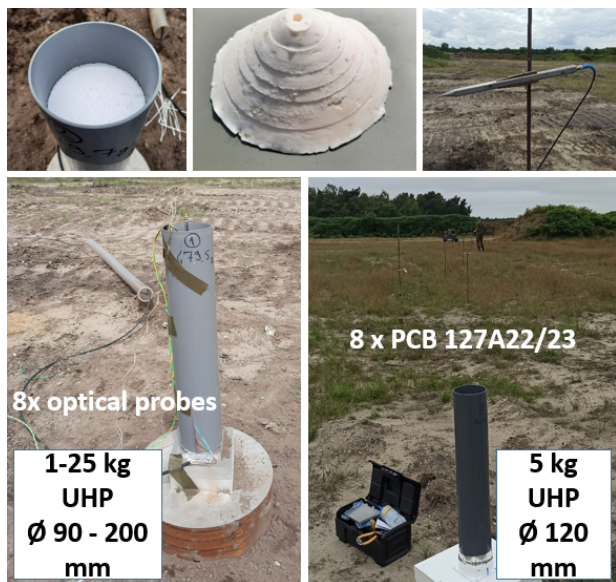


Figure 3. 1 to 25 kg UHP: VoD (left) and blast (right).

Table 1. Field Firings – UHP (0.85 g/cm^3 ; $L=5 \times ID$)

OD (mm)	ID (mm)	Mass UHP (kg)	Mass Bstr C4 (kg)	Target data	# shots
90	86.4	1.97	0.10	VoD	2
110	105	3.72	0.22	VoD	2
125	120	5.45	0.35	VoD	2
160	153.6	11.50	0.73	VoD	2
200	193	22.73	1.42	VoD	1
125	120	4.89	0.35	Blast	10

First, in order to determine the nominal charge diameter, 9 UHP charges (average loading density 0.85 g/cm^3) in PVC tubes of outer diameters ranging from 90 to 200 mm, were initiated using a standard N°8 military detonator and a bespoke moulded C4 booster (Figure 3, top middle) to fit the inner diameter of the tube and distribute the initiation wave over the entire charge diameter. VoD were measured using passive optical probes inserted in holes drilled in the PVC casing and sealed from inside the pipe by aluminium tape, as previously described (section 2.1). The recorded experimental detonation velocities were then plotted

against reciprocal diameter in order to determine unconfined VoD at infinite charge diameter.

Secondly, building upon previous results on nominal diameter, we selected a charge diameter of 120 mm for airblast measurements, a trade-off between the impact of the diameter on the performance characterisation and the practical charge size. With regard to atmospheric conditions, the test site was located 77 m above the sea level, the ambient pressure on the day of the tests was 102.35 kPa (according to the Meteorological Wing of the Belgian Defence). The temperature was 23°C and the relative humidity 60%. We recorded the pressure history and determined incident overpressure and positive phase impulse as a function of scaled distance ($Z=R/W^{1/3}$, with R the radial distance from the charge, and W the charge weight), using 8 blast pencils PCB 127A22/23 respectively positioned at 4.5 ($Z > 2 \text{ m/kg}^{1/3}$, to avoid short distance effects), 10, 15, 21, 26, 32, 37 and 43 meters distances, and compared them to a TNT reference to determine equivalences, using the airblast parameters from TNT surface burst by Kingery & Bulmash [20]. We fired 10 cylindrical charges containing approximately 5 kg UHP and initiated by a 350 g C4 booster and a standard N°8 military detonator. To limit energy dissipation due to cratering and ground shock, the charge was placed on a 45 cm high wood support. As the height of burst was higher than 3 times the charge diameter, the energy loss to crater formation was considered as negligible [7]. This was further supported by the fact that no significant crater formation was observed after detonation. In these conditions and assuming that the ground was a perfect reflector, an ideal hemispherical burst was considered with an effective yield of 200%.

2.3 Underwater Firings

The underwater test campaign was conducted at *Braboplas* range, a military underwater demolition site (available depth 9 m), and consisted of two phases, 25 shots at small scale [21] and 15 shots at larger scale, using respectively 100 g and 1 kg UHP charges. The experimental setup is depicted in Figure 4.

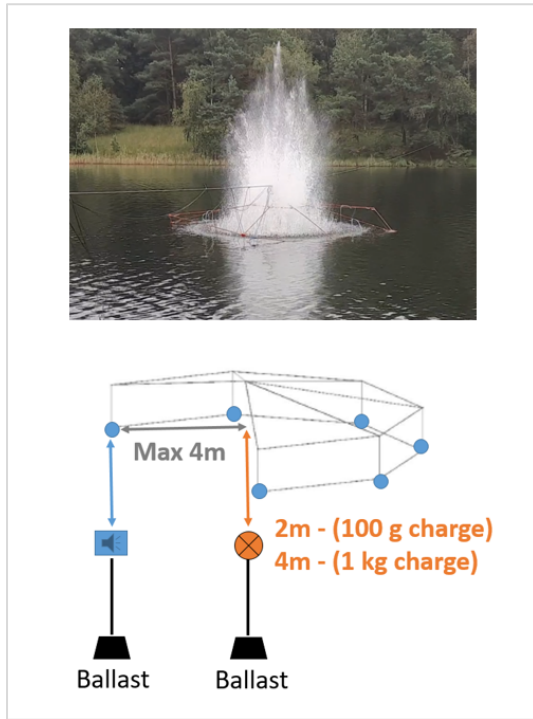


Figure 4. 100 g to 1 kg UHP – floating structure.

Explosive charges were suspended in the centre of a floating structure at a depth of 2 m for the 100 g charges and 4 m for the 1 kg charges. Eight voltage mode tourmaline pressure sensors type PCB 138A05 were placed at the same depth (D), respectively at 1 m, 1.50 m, 2 m and 2.5 m range (R) for 100 g charges and 2 m, 3 m and 4 m for 1 kg charges. According to recommendations in [22], pressure sensors were positioned at the depth of the centre of the charge and respectively outside the calculated maximum bubble radii of 0.75 m for a 100 g C4 explosive charge and 1.5 m for a 1 kg [23], considered as maximum dimensioning charges for the design of our experimental setup.

Unconfined spherical charges of 100 g loose UHP (0.75 g/cm^3) in plastic casing (1 mm thick, 70 mm OD), as shown on Figure 5, were initiated by an explosive train comparable to the one used in the lab (section 2.1), i.e. a standard N°8 military detonator and a central spherical 8 g C4 booster. We also fired, in the same conditions, spherical 100 g C4 charges for reference and comparison purposes. In an attempt to better assess the influence of the booster [24] on UHP detonation performance (equivalent shock pressure and bubble energy), we finally fired 8 g C4 booster charges alone.



Figure 5. 100 g UHP charge configuration.

Upscaled unconfined spherical charges of 1 kg UHP (loading density 0.80 g/cm^3 , slightly compacted to improve homogeneity) in plastic casing (1 mm thick, 140 mm OD) were initiated by a standard N°8 military detonator, inserted in a bespoke channel to detonate a central spherical 60 g C4 booster (Figure 6). Additionally and similarly to the small-scale campaign, the performance of the C4 booster alone was separately investigated. Finally, we fired 1 kg spherical C4 for reference and comparison purposes.

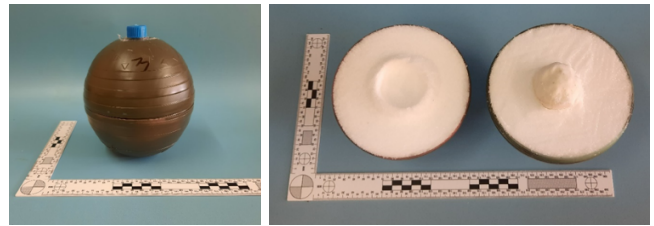


Figure 6. 1 kg UHP charge configuration.

Using the procedure described in [25-27], we recorded the pressure history to determine underwater shock pressure and first pulsation period (t_b). Because the firings were standardised (same explosive masses, depth, range, water properties) for comparison purposes in order to assess UHP underwater performance, we made use of the so-called shock energy ($E_{s, equ}$) and bubble energy ($E_{b, equ}$) equivalents:

$$E_{s, equ} = \int_{t_0}^{t_0 + \theta} P^2(t) dt \quad (2)$$

$$E_{b, equ} = t_b^3 \quad (3)$$

where:

t_0 : time of arrival of the shock wave
 θ : time at which the pressure has decreased to $P_\theta = P_{max} \cdot e^{-1}$
 t_b : first pulsation period

We simulated both set-ups in Ansys Autodyn V14.0 in order to model and compare peak overpressure (P_{max}) and equivalent shock energy of the different

charges to experimental values. A 1D Euler multi-material model was used, representing a spherical geometry. For UHP, the JWL parameters previously calculated with Explo5 [6] were fed into Autodyn. Models from Autodyn's standard library were used for C4 and water.

3 Results and Discussion

3.1 Lab Firings

Complementary lab campaign results are available in Table 2, while theoretical calculations from Explo5 are presented in Table 3. As expected, VoD and indent depth measurements are in excellent agreement with previous measurements [6]. For our reference TNT charges pressed at 1.61 g/cm³, we recorded a detonation velocity of 6.90 km/s, a value in very good agreement with the 6.91 km/s predicted from LASL explosive properties data [28] and very close to the theoretical maximum 6.95 km/s at 1.64 g/cm³ [7]. Using experimental VoD recorded at small scale under heavy confinement to estimate P_{det} , we determine a relative brisance (based on P_{det}) of 9% for loose UHP (0.75 g/cm³) and 14% at 0.85 g/cm³ loading density with respect to TNT.

Table 2. UHP – 30 mm ID, 4 mm steel confinement (VoD $\pm$ max 0.026 km/s for 95% confidence interval)

UHP Loading Density (g/cm ³)	0.75	0.85
Average VoD (km/s)	2.954	3.454
Estimated P_{det} (GPa)	1.93	2.96
Relative brisance (%) vs TNT* from P_{det}	9	14
Average indent depth (mm)	5	6
Relative brisance (%) vs TNT* from indent depth	30	35

*TNT at 1.61 g/cm³ loading density

We measured a maximum indentation of 17.3 mm for the TNT charges and determined a 30-35% relative brisance from indent depth measurements for UHP. This value should however be treated with care. Even if the correlation between the result of a plate dent experiment and the experimentally determined detonation pressure [19] is generally accepted and widely used to assess relative brisance of high explosives [29], this correlation was actually only demonstrated for conventional military explosives [19]. It was later pointed out that this correlation was a consequence of similar expansion of the detonation products of most conventional military explosives down to about 1 GPa, the pressure range of interest of the test, making the peak detonation pressure the major difference between them and leading to the observed linear correlation [10]. However, UHP (CH₆N₂O₃) differs from conventional CHON explosives, like TNT, by a high water content in the detonation products and a very low detonation temperature (1500 K, calculated, Table 3). Noting that water is a triatomic polar molecule, a significant impact on the isentrope slope between the

detonation pressure and 1 GPa is expected. In these conditions, the linear correlation observed between the plate dent result and the detonation pressure of conventional CHON explosives should not be extrapolated to UHP without additional external validation based on the measurement of the UHP detonation pressure, which will be part of future work.

Table 3. UHP – Explo5 calculations with EXP-6 and M-BKW EoS

	EXP-6	M-BKW	EXP-6	M-BKW
Loading density (g/cm ³)	0.75	0.75	0.85	0.85
VoD (km/s)	3.66	3.96	4.11	4.37
P_{det} (GPa)	2.43	2.95	3.31	3.98
T_{det} (K)	1600	1467	1606	1483
Q_{det} (kJ/kg)	1588	1548	1624	1582
V_{gas} STP (l/g)	1.06	1.07	1.05	1.06

As shown in Table 3, the choice of EoS influences the calculation of the detonation parameters, such as VoD or P_{det} , and consequently the Autodyn numerical model. Due to the relatively low detonation pressure, it was only possible to achieve a fitting of the JWL equation parameters based on the calculated detonation gases isentrope with the EXP-6 EoS of the Explo5 software. Calculating the Q_{det} (4349 kJ/kg) and V_{gas} (0.67 l/g) values from M-BKW for TNT (1.63 g/cm³), we derived a 57% TNT equivalence by Power Index (PI) [14] for UHP (0.85 g/cm³). Table 3 also emphasises the surprisingly low detonation temperatures of UHP as previously mentioned, potentially out of the EoS validation ranges [18] and hereby questioning the overall accuracy of the calculation.

3.2 Field Firings

Looking at field firings (no confinement), the recorded UHP VoD value (max $\pm$ 0.025 km/s for 95% confidence interval) in the field are summarised in Figure 7, with a maximum of 3.65 km/s at 200 mm charge diameter and the possible beginning of a plateau observed from 160 mm charge diameter. The observed deviation is likely due to density variations, the charge preparation method being only accurate to ± 0.02 g/cm³ at this scale. Based on the recorded data, VoD at infinite charge diameter is about 3.94 km/s, namely 96% and 90% of the ideal VoD predicted from Explo5 using EXP-6 and M-BKW EoS, respectively, indicating a non-ideal character [10] typically observed with explosives detonating at a comparable regime [7]. This result is also consistent with the 3.78 km/s recorded by Matyas [3] in comparable charge diameter (206 mm) but higher loading densities (0.93 g/cm³) and heavier (steel) confinement.

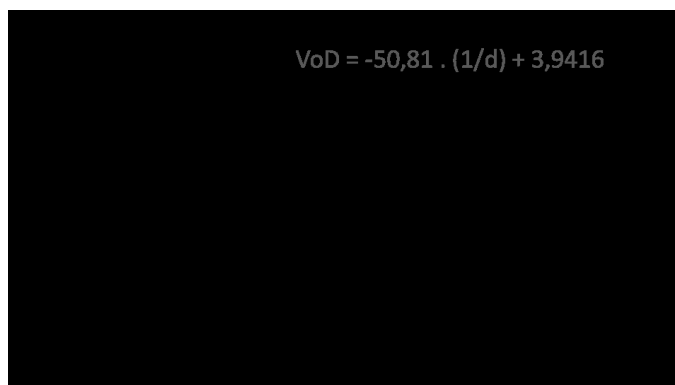


Figure 7. UHP Detonation Velocity vs reciprocal diameter ($0.83 \leq \text{loading density (g/cm}^3) \leq 0.87$).

As far as airblast parameters are concerned, reproducible pressure-time histories were recorded (as illustrated on Figure 8), enabling side-on peak overpressure and positive impulse to be determined and compared to TNT data.

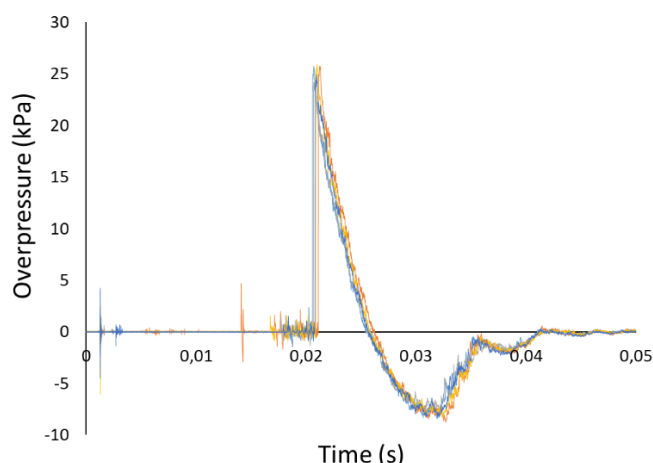


Figure 8. 5 kg UHP (0.85 g/cm^3) – 10 m standoff (5 shots).

Figure 9 summarises the TNT equivalences for overpressure and impulse as a function of UHP scaled distance. As expected, TNT equivalences are dependent on scaled distances [12, 13], which could be explained by the rather large distance interval considered [15] and the significant difference between the composition of TNT and UHP detonation products, as previously discussed. An influence of the charge shape at a lower scaled distance cannot be excluded [15].

Even if the same trend is observed, TNT equivalences from overpressure are higher than those from impulse. The order of magnitude is however comparable to commercial blasting explosives detonating at a similar regime [30-32] and in good agreement with the 57% TNT equivalence (PI) calculated from Explo5 (section 3.1).

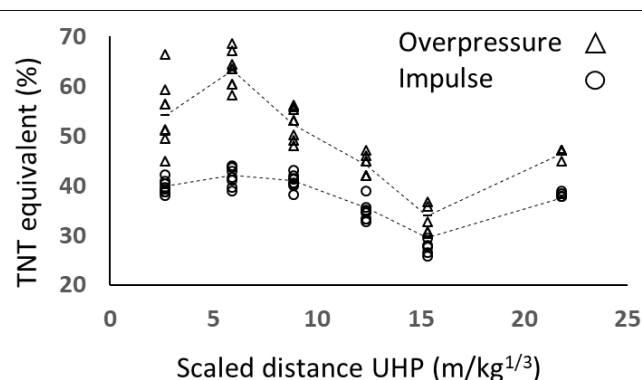


Figure 9. TNT equivalences for UHP airblast parameters at 0.85 g/cm^3 (line with average values as a visual guide).

3.3 Underwater Firings

The experimental average shock wave parameters and calculated equivalent shock ($E_{s, \text{equ}}$) and bubble ($E_{b, \text{equ}}$) energies from the underwater firings are summarised in Table 4. As far as UHP is concerned, these values include the contribution of the respective C4 boosters (bstr). Additionally, predictions based on numerical simulations with Autodyn (using Explo5 parameters calculated with EXP-6 EoS) for peak overpressure and equivalent shock energy are mentioned.

Table 4. Underwater Firings – Small and large scale – mass (M), depth (D), range (R), peak overpressure (P_{max}), first pulsation period (t_b), equivalent shock ($E_{s, \text{equ}}$) and bubble ($E_{b, \text{equ}}$) energies.

	M (g)	D (m)	R (m)	P_{max} (MPa)	t_b (ms)	$E_{s, \text{equ}}$ (kPa $\cdot$ s)	$E_{b, \text{equ}}$ (10^{-3} s 3)
UHP ^a 100	2	1.5		5.67 ± 0.7	81 ± 2	450	0.5
				8.12^c		2360 ^c	
C4 ^b 8	2	1.5		4.07 ± 0.4	48 ± 1	162	0.1
C4 100	2	1.5		12.93 ± 0.9	121 ± 1	4590	1.8
				12.97^c		4670 ^c	
UHP ^a 1000	4	3		8.21 ± 0.7	178 ± 4	2192	5.6
				8.70^c		4660 ^c	
C4 ^b 60	4	3		4.87 ± 0.4	90 ± 2	587	0.7
C4 1000	4	3		14.22 ± 1.4	220 ± 2	11381	10.6
				14.06^c		10930 ^c	

^a main charge with C4 booster; ^b booster charge; ^c Autodyn

On the one hand, C4 has proven a good reference explosive for underwater experiments. Experimental results and simulations for C4 are in good agreement for both small-scale and large-scale campaigns, and consistent with literature data related to underwater performance of RDX-based compositions [33, 34], giving us confidence in the experimental setup and the recorded results. As expected, P_{max} for the 100 g and 1 kg, respectively at 1.5 m and 3 m standoffs, are within the same order of magnitude as they have been

measured at comparable scaled distances (3.23 vs 3 m/kg^{1/3}). Considering the 8 to 150 g C4 charges fired at 2 m depth, the linear regression (Figure 10) of experimental first pulsation periods against the cubic root of the explosive mass is in good agreement with Reference [35] where 95% RDX charges (6 to 10 g) were detonated at the same depth.

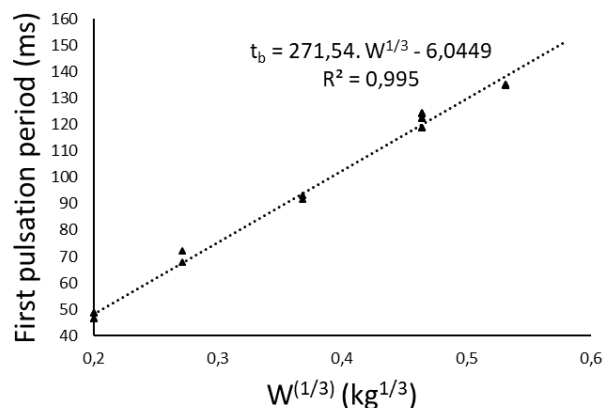


Figure 10. 8 to 150 g C4 (1.63 g/cm³) – experimental first pulsation period at 2 m depth.

On the other hand, UHP experimental data for equivalent shock energy ($E_{s, equ}$) differ significantly from the Autodyn simulation, particularly at small scale (Table 4). Even if the numerical predictions for P_{max} for the 100 g (8.12 MPa) and 1 kg charges (8.70 MPa) are in good agreement as they are calculated at comparable scaled distances, this scaling is not observed experimentally (5.67 MPa vs 8.21 MPa) and suggests that strong non-ideal effects affect the detonation of the 100 g charge. However, the numerical values from Autodyn for UHP should also be treated with care, as the JWL coefficients used in the model and calculated from Explo5 have not been validated experimentally, which would require large-scale cylinder expansion testing [36]. Further investigations would also be required to first characterise the actual detonation regime of UHP at small scale, and assess its non-ideality. Considering the rather small charge radius (35 mm) and the absence of confinement, the detonation of the 100 g UHP charges in this configuration may have not achieved a steady state. UHP experimental performance parameters are however somehow closer to numerical predictions when considering the 1 kg charges, especially for P_{max} . The experimental equivalent shock energy is about 50% of the numerical prediction. This difference between experiments and simulation could hence be attributed to the non-ideal behaviour of UHP in these conditions, to the limited accuracy of the model, taking into account UHP specific detonation products discussed in section 3.1, or to a combination of both.

The 1 kg charge with a larger charge radius (70 mm), the mass being limited by the actual experimental setup, is therefore considered as more suitable to characterise the UHP detonation performances, which could be compared to C4. However, the equivalent shock and bubble energies of UHP available in Table 4 have been calculated for a 1 kg UHP charge and a 60 g C4 booster, while the 1 kg C4 did not require any booster. Assuming additivity effect [24], we subtracted the relative contribution of the 60 g C4 booster from the equivalent shock ($E_{s, equ}$) and bubble ($E_{b, equ}$) energies of UHP (Table 4) in order to compare identical explosive quantities and derive TNT equivalences (Table 5). Using literature data [37] for TNT first pulsation period, we obtain a 50% TNT equivalence for bubble energy (explosive power). When it comes to shock pressure, we eliminate the contribution of the booster and calculate a 14% equivalence with respect to C4. Using a 1.3 TNT equivalence for C4, consistent with literature data related to underwater shock performance of RDX-based compositions [33, 34] and calculated from the ratio of the respective estimated detonation pressures [7] (section 2.1), which best characterise the shattering effects [16] of explosives, we derive an estimated maximum 20% TNT equivalence for brisance for UHP. As expected for explosives detonating at a lower regime, the TNT equivalence of UHP for brisance is rather low.

Table 5. Underwater Firings – TNT equivalences (%).

Charge	Brisance	Explosive Power
1kg UHP	20	50

3.4 Detonation Performance Assessment

Integrating all the results obtained from different experimental approaches presented above, we were able to characterise the detonation performance of UHP:

1. As expected for an energetic material detonating at a rather low regime, the brisance of UHP, its destructive fragmentation effect on its immediate vicinity [38], has proven weak (20%) when compared to conventional explosives. A good level of agreement was found between TNT equivalence from underwater shock energy and TNT equivalence based on detonation pressure calculated from VoD, either in the lab or in the field. Future work should enable us to further correlate these results to the brisance determined by indirect measurement of the detonation pressure.
2. UHP explosive power is rather limited (50%) as demonstrated by TNT equivalence based on underwater bubble energy or TNT equivalence based on airblast characteristics (long distance

blast wave), which have proven consistent and in good agreement with the 57% (PI) calculated from Explo5.

The validity of the small-scale setups used to characterise detonation parameters has been investigated. VoD measurements carried out in the lab are consistent with results from the field (95%). Further improvements might include optimisation of charge geometry and reproducibility of loading densities. When it comes to explosive power, the airblast data from the field are in good agreement with results from the kg-size underwater campaign, while smaller charges could not adequately describe large-scale steady behaviour.

4 Conclusion

We carried out a detailed performance assessment, combining experiments, thermochemical calculations and numerical simulations and highlighted a good level of agreement between experimental data from lab, field and underwater firings. A maximum detonation velocity of 3.65 km/s was recorded for unconfined 25 kg UHP charges at 0.85 g/cm³ (200 mm charge diameter). We determined in these conditions an infinite diameter detonation velocity of 3.94 km/s. These results are also consistent with previous results obtained at small scale under heavy confinement. Airblast measurements highlighted an average 40% TNT equivalence for impulse and 55% for peak overpressure at short (scaled) distance ($Z=2$), which are in good agreement with the 57% (PI) calculated from Explo5, while 50% for bubble energy (explosive power) and 20% for shock pressure (brisance) were obtained from underwater experiments. The use of different experimental approaches has proven useful to characterise the performances parameters of a non-ideal explosive for risk assessment purposes. Future work includes experimental measurement of UHP P_{det} to better assess its non ideal character and a detailed analysis of the accuracy of the related thermodynamic calculations.

Symbols and Abbreviations

ANFO	Ammonium Nitrate Fuel Oil
Bstr	Booster
D	Depth
$E_{b, equ}$	Equivalent bubble energy
EoS	Equation of State
$E_{s, equ}$	Equivalent shock energy
ID	Inner Diameter
JWL	Jones-Wilkins-Lee
L	(charge) Length
LASL	Los Alamos Scientific Laboratory
M	Mass
M-BKW	Modified Becker-Kistiakowski-Wilson
OD	Outer Diameter
PCB	PicoCoulomb
P_{det}	Detonation pressure
PI	Power Index
P_{max}	Side-on peak overpressure

PVC	Polyvinyl chloride
Q_{det}	Heat of Detonation
R	Range
RDX	Research Department Explosive
t_b	First pulsation period
T_{det}	Detonation temperature
TNT	Trinitrotoluene
UHP	Urea Hydrogen Peroxide
V_{gas}	Volume of gas
VoD	Velocity of Detonation
Z	Scaled distance

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Detonation performance of Urea-Hydrogen Peroxide (UHP)

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Appendix G: Poster presented at the 1st International Explosives Conference (2022).

Small-scale characterisation of Urea Hydrogen Peroxide Explosive performance using Heterodyne Velocimetry

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Small-scale characterisation of Urea Hydrogen Peroxide Explosive performance using Heterodyne Velocimetry

1. Context

- Current Home Made Explosive (HME) threat worldwide:
 - Mixing of highly energetic pyrotechnics
 - Synthesis of **peroxide explosives**
- Carbamide Peroxide or **Urea Hydrogen Peroxide (UHP)**, widely used in the dental, cosmetic and pharmaceutical industries, has proven detonable at small-scale under heavy confinement [1].



2. Objectives and challenges

- Further small-scale **characterisation of explosive performance** for risk assessment purposes: detonation velocity (VoD), pressure (P_{det}) and metal acceleration.
- **Heterodyne velocimetry (Het-V)**, or Photonic Doppler Velocimetry (PDV) is a powerful tool to carry out advanced detonics investigation, such as a direct measurement of particle velocity in inert materials [2].
- UHP is heterogeneous and exhibits the behaviour of a **non-ideal** (tertiary) explosive. At small scale, UHP detonation requires a strong confinement wherein the shock propagates faster than the reaction wave in UHP.

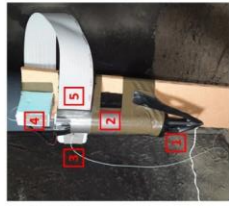


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3. General approach

- ➔ Change configuration from previous research, all target data in a single test

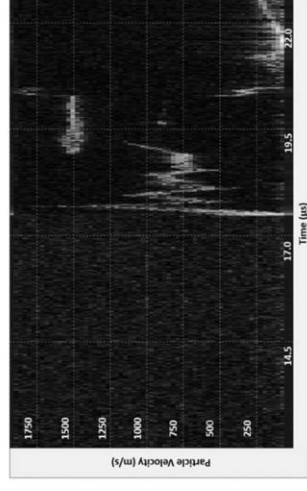


- 1) **Initiation**: N°8 detonator, 8 g PE8 booster
- 2) **Explosive charge**: 80 g loose UHP in 4 mm thick steel (ID=30 mm, length 150 mm)
- 3) **Het-V probe** for Cylinder expansion
- 4) **Het-V probe** for P_{det} measurement by IWM Impedance Window Method [2]
- 5) **Contact probes** ribbon for VoD record

- ➔ 8 shots UHP & 2 shots PE8 plastic explosive (86.5% RDX) for reference

4. Preliminary results

- Average **VoD**: 3200 m/s from contact probes, in excellent agreement with measurements using Optimetx passive optical probes [1].
- Cylinder expansion – **metal acceleration ability**:
 - Max initial acceleration $54 \times 10^6 \text{ m/s}^2$
 - Radial pressure **4 GPa**
- Best Het-V power spectrum obtained from a 2.8 mm thick PMMA impedance window. Calculation by impedance matching [2] gives an average **2.5 GPa** for P_{det} , a **13% TNT equivalence for brisance**, confirming calculations using empirical correlation [1].



5. What's next

- Improvement of the experimental setup, including hardware, to improve shot-to-shot repeatability and achieve accurate P_{det} measurement, including error estimate.

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Appendix H: Published Proceedings – 1st IEC.

Small-Scale Characterisation of Urea Hydrogen Peroxide Explosive Performance using Heterodyne Velocimetry

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SMALL-SCALE CHARACTERISATION OF UREA HYDROGEN PEROXIDE EXPLOSIVE PERFORMANCE USING HETERODYNE VELOCIMETRY

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ABSTRACT

Urea Hydrogen Peroxide (UHP) is widely available in the cosmetic and pharmaceutical industries. UHP exhibits the behaviour of a tertiary explosive and previous research from the same authors has highlighted its detonability at small-scale under heavy confinement. In this work, UHP performance parameters are further investigated by heterodyne velocimetry. A detonation pressure of 2.5 GPa for UHP at a mean density of 0.75 g/cm³ has been determined using the impedance window method, corresponding to a 13% TNT equivalence for brisance. This result is consistent with calculation from empirical correlations. An average 3200 m/s detonation velocity was recorded using contact probes, in excellent agreement with measurements from passive optical probes. This small-scale experimental campaign, which is complementary to and consistent with previous research, has proven useful to characterise the performances of non-ideal explosives for risk assessment purposes.

Keywords: *Urea Hydrogen Peroxide, Detonation, Heterodyne Velocimetry*

1. INTRODUCTION

Urea Hydrogen Peroxide (UHP), also referred to as Carbamide Peroxide, is widely available in the cosmetic and pharmaceutical industries. UHP exhibits the behaviour of a tertiary explosive and is hence investigated for risk assessment purposes within the scope of potential homemade explosives (HME) emerging threats.

Previous research from the same authors has highlighted UHP detonability at small-scale under heavy confinement (see Figure 1.1).¹ In this configuration, detonation velocities (VoD) were recorded using passive optical probes and the results were consistent with literature value from large-scale experiments.²



Figure 1.1: Experimental setup (left), witness plate indentation (middle) and fragmentation pattern (right).

The brisance of UHP, which describes its destructive shattering effect, was demonstrated by indent depth measurement on an aluminium witness plate, fragmentation pattern observation and fragments distribution analysis. Additionally, the detonation pressure (P_{det}) was estimated from an empirical correlation, using VoD and loading density (ρ_0).³

In this work, UHP P_{det} is further investigated in the same charge configuration by Heterodyne Velocimetry (Het-V), also referred to as Photonic Doppler Velocimetry (PDV). In a fact, Het-V is a powerful technique to observe materials under high dynamic pressure and carry out advanced detonics investigation, such as a direct measurement of the particle velocity at the interface between the explosive charge and an inert material whose shock properties are well documented.

2. MATERIAL AND METHODS

We used commercial lab grade UHP (97%) purchased from ALFA AESAR (85% of the particles > 600 μ m) and the validated charge geometry (Inner Diameter 30 mm, Charge Length 150 mm), initiation train (8 g PE8 booster and N°8 standard military detonator) and confinement material (4 mm thick steel), which are extensively described in Reference 1. A total of 10 devices were fired

in the containment building of the Explosives Research and Demonstration Area (ERDA) at the Defence Academy of the United Kingdom. Eight devices were filled with approximately 80 g of loose UHP ($\rho = 0.75 \text{ g/cm}^3$) and two devices contained 40 g PE8 (Chemring Energetics UK, VoD nominal 8000 m/s, $\rho = 1.57 \text{ g/cm}^3$) for comparison.

Surface velocities were measured using a generation 1 heterodyne velocimeter. This instrument used a 1550 nm laser source, emitting laser light from a fibre-coupled collimator with a 75 mm working distance and a 220 μm spot size. The reflected (Doppler-shifted) light was mixed in the interferometer, and the intensity of the beat signal was amplified by a Thor Labs PDA-8GS photodetector. The electrical output from the photodetector was recorded using a Tektronix 6 GHz bandwidth oscilloscope, sampling at 5 GS/s. The instrument used in these firings provided two independent channels, recorded on the same time-base. Each velocity record was processed using a Hamming window Fourier transform with variable window width, to produce a time-resolved power spectrum image. This was manually digitised to produce numerical time-velocity data for analysis in Microsoft Excel.

Het-V was primarily used to measure P_{det} by the impedance window method (IWM).⁴ The first channel was directed at the interface between the end of the test specimen and the polymethylmethacrylate (PMMA) impedance window, to record the motion of this interface. Different PMMA window thicknesses (2.8 mm, 9.5 mm) and mirror interface types (first Aluminium spray painted, then reflective foil to get stronger reflection) were tested. Detonation pressure was calculated from IWM data by impedance matching across the explosive-inert interface.

The second channel was directed normal to the cylindrical surface of the confining cylinder, to record radial expansion of the cylinder driven by the reaction products from the test specimen. The metal acceleration by explosives is typically studied using the cylinder expansion test with thin pure copper cylinders. However, this confinement is unlikely to be strong enough to allow UHP detonation to develop in this charge configuration.² From the initial metal acceleration, we calculated the maximum radial pressure for comparison.

The progress of the reaction wave (VoD) was recorded by a linear array of 32 contact probes placed at a distance of 2.0 mm parallel to the surface of the cylinder. During the experiment, the collision of the grounded metal cylinder against the contact probes provided measurement of the position of the confining cylinder as a function of time. The contact probes were spaced 1.27 mm apart, measuring the wave progress over a distance of 40 mm; the last probe was positioned approximately 10 mm from the end of the cylinder closest to the impedance window. Probe contacts were recorded on an Intronix 32-channels logic analyser, sampling at 200 MHz, and hence giving a contact time resolution of 5 ns. Probe data were tabulated in Microsoft Excel, to produce a plot of probe distance as a function of contact arrival time. The slope of a linear best fit line through the data provided a measurement of the steady propagation

velocity of the reaction wave. The results were compared to previous measurements with passive optical probes.

Figure 2.1 gives an overview of the experimental setup.

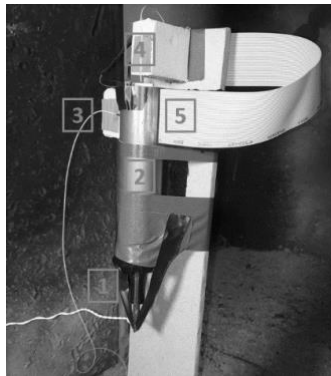


Figure 2.1: Experimental setup – Initiation (1), Explosive charge in steel sleeve (2), Het-V probe for cylinder expansion (3), Het-V probe for impedance window (4), VoD ribbon cable probes (5).

3. RESULTS AND DISCUSSION

An overview of the measured explosive performance data is available in Table 3.1.

Table 3.1: Measured explosive performance data.

Detonation Velocity (average)	m/s	3200
Detonation Pressure	GPa	2.5
Maximum Radial Pressure	GPa	4

In this charge configuration, we could record an average 3200 m/s VoD for UHP at a 0.75 g/cm^3 density, which is consistent with previous measurements using passive optical probes.

As far as P_{det} measurement is concerned, the first five shots with PMMA impedance windows glued to the steel sleeve were unsuccessful. Because the shock propagates faster in the steel confinement than the detonation front in UHP, the PMMA plate was already moving, disrupting the setup, which gave unusable power spectrum. The use of a PMMA impedance window (10 mm by 10 mm) placed on the UHP particles bed, avoiding any contact with the steel sleeve, provided improved signals.

This was particularly true for the particle velocity profile at the interface UHP/PMMA, obtained from a 2.8 mm thick PMMA window (Figure 3.1). The obtained signal shows, as expected, some velocity scatter due to the heterogeneity of the explosive. The duration of the signal is similar to the shock transition time through the PMMA, which is dependent on the pressure, typically

1-3 μs . After the shock transit, a second velocity trace appears which corresponds to the free surface velocity of the PMMA window, approximately twice the interface velocity.

Calculation of P_{det} by impedance matching across the explosive-inert interface provided an average 2.5 GPa (13% TNT equivalent for brisance), a value consistent with our previous work.

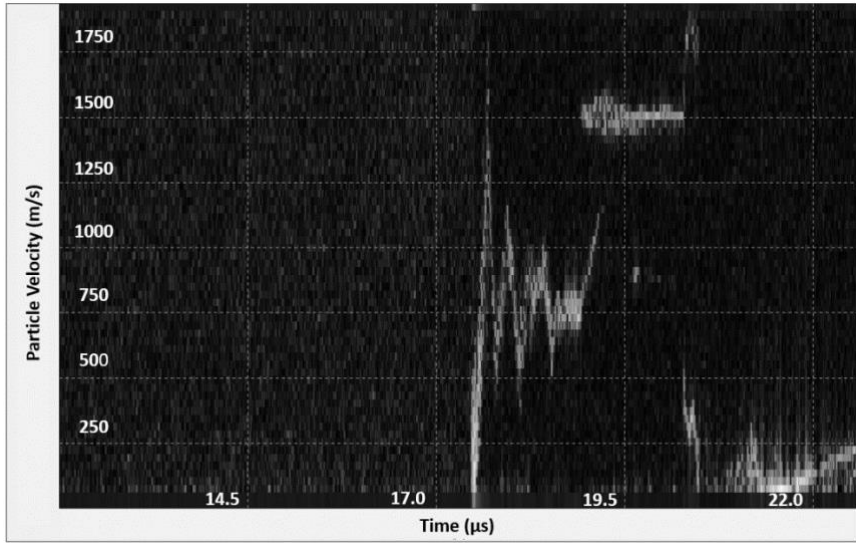


Figure 3.1: Power spectrum obtained for a single shot using a 2.8 mm thick PMMA window and reflective foil, giving an average 750 m/s at the interface with UHP.

Only one of three UHP tests with similar setups provided such a record, while the remaining tests only provided the PMMA upper free surface velocity trace. Impedance window experiments often fail with granular or coarse crystalline explosives, as highlighted by similar experiment⁵ carried out on ANFO, especially if there is only a thin aluminium foil as a reflective layer. A 0.3 mm thick aluminium plate would be required to get at least some signal. Moreover, contact between UHP and the impedance window has to be improved, given the granular nature of the charge.

From the cylinder expansion records (see Figure 3.2), we determined an average maximum initial metal acceleration of $54 \times 10^6 \text{ m/s}^2$, corresponding to a maximum radial pressure of 4 GPa.

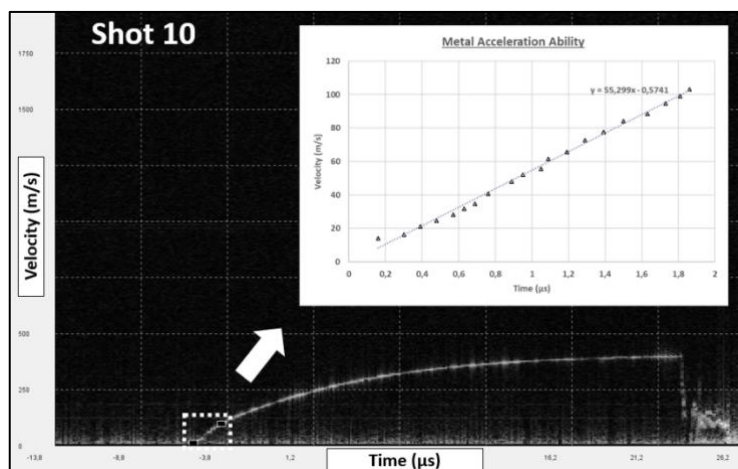


Figure 3.2: Initial metal acceleration from cylinder expansion – example shot 10.

4. CONCLUSION

A detonation pressure of 2.5 GPa for UHP has been measured using heterodyne velocimetry and applying the impedance window method. This value (13% TNT equivalent for brisance) is consistent with calculation from empirical correlation.

These are only preliminary results and future work includes improvements of the experimental setup, including hardware, in order to achieve accurate and reproducible measurement of detonation pressure, including error estimate.

This small-scale experimental campaign, which is complementary and consistent with previous research, has proven useful to characterise the performances of non-ideal explosives for risk assessment purposes.

ACKNOWLEDGEMENT

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Small-scale characterisation of urea hydrogen peroxide explosive performance using heterodyne velocimetry

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<https://www.iec-2022.com/?action=main>

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Appendix I: Published Research Article.

Urea-Hydrogen Peroxide (UHP): Comparative Study on the Experimental Detonation Pressure of a Non-ideal Explosive

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Full Paper

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Urea-Hydrogen Peroxide (UHP): Comparative Study on the Experimental Detonation Pressure of a Non-ideal Explosive

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Abstract: Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide (UHP) industrially used as a solid source of hydrogen peroxide, exhibits the behaviour of a tertiary explosive but a detailed performance characterisation is still lacking in the literature. In this work, we calculated a 20% experimental TNT equivalence for brisance, i.e. the shattering effect from the shock wave transmitted from the detonating high explosive into adjacent materials, by experimental indirect measurement of UHP detonation pressure. We determined a 3.5 GPa detonation pressure for 5 kg unconfined UHP charges (0.87 g/cm³, 120 mm charge diameter) by measuring the attenuated shock wave velocity (ASV) in adjacent inert materials using passive optical probes. Particle velocity measurements at the interface of a PMMA impedance window carried out with Photonic Doppler Velocimetry on scaled-down charges of 90 g UHP under heavy confinement (0.85 g/cm³, 30 mm charge diameter, 4 mm thick steel) are consistent with ASV results in the PMMA acceptors but further investigations are required to determine the detonation pressure, using a small-scale experimental set-up. The ASV method has proven reliable to assess the brisance of a non-ideal explosive for risk assessment purposes.

Keywords: Urea hydrogen peroxide, Non ideal explosive, Detonation pressure, Passive optical probes, Photonic Doppler Velocimetry

1 Introduction

Carbamide Peroxide, an adduct of Urea and Hydrogen Peroxide (UHP), is industrially used as a solid source of hydrogen peroxide. Like other oxidisers such as ammonium nitrate (AN) [1], or AN-based explosive compositions [2], it exhibits significant non-ideal detonation properties at the 10-cm scale. To the best of our knowledge, the explosive behaviour of UHP was rather recently studied in the literature and a detailed characterisation of UHP detonation performance parameters is still lacking. Hussein carried out ballistic mortar experiments and thermochemical calculations to assess the relative explosive strength of mixtures containing urea and/or peroxide [3]. Matyas investigated UHP sensitivity, thermal properties and detonability at large-scale [4], while preliminary work from the authors demonstrated UHP detonability at small-scale and highlighted UHP charges non-ideality by Velocity of Detonation (VoD) dependence on charge diameter and confinement. Additionally, UHP relative explosive strength was further assessed from experimental underwater bubble energy and airblast parameters (long distance blast wave) measurements [5-6].

Within the scope of a performance assessment, one of the key parameters still to be addressed was the brisance, the shattering effect from the shock wave transmitted from a detonating high explosive into adjacent materials. Examples of standardised tests [7-8] available to assess the relative brisance of explosives include the Hess test, evaluating the compression of a lead cylinder, the Kast's method, using a copper crusher

or the plate-denting test [9]. The latter has proven effective to correlate the indentation of a witness plate with the experimentally determined detonation pressure of conventional military explosives but extrapolation to a material such as UHP might be questionable taking into account (major) differences in detonation products composition, particularly water content, and very low detonation temperature [6]. Considering the non-ideal behaviour of UHP, it was decided to quantify the brisance of UHP through its predominant parameter, the detonation pressure (P_{det}) [8-9], as illustrated in Figure 1.

The detonation pressure can be calculated from thermodynamical codes, estimated using empirical correlations from VoD and loading density (ρ) [10-11] or determined experimentally. Considering the time-scale of the phenomenon and the severe conditions of pressure and temperature [8], direct measurement of the detonation pressure using in situ gauges [12] such as Polyvinylidene fluoride (PVDF) piezoelectric [13] or Manganin piezoresistive sensors [14] is challenging and not yet widely applied or validated, especially when considering kg-scale non-ideal explosive charges.

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However, indirect measurement methods are also available to determine the detonation pressure, observing the shock wave properties in inert well-characterised adjacent materials (impedance matching) and not interfering with the detonation wave [15].

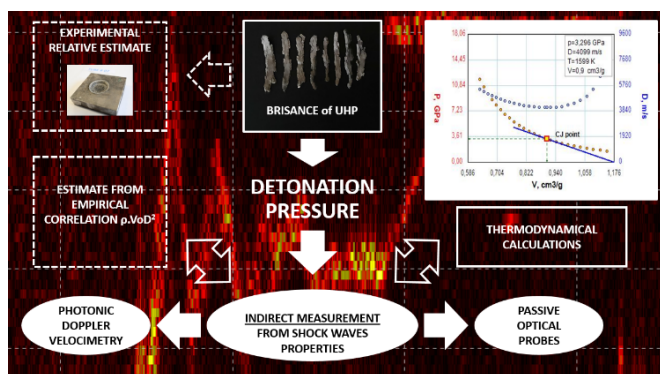


Figure 1. General approach – UHP brisance by indirect measurement of the detonation pressure.

In this comparative study, we investigated UHP detonation pressure respectively at large and small scale using two distinct indirect methods, respectively measuring shock then particle velocities. First, at large-scale, using an optical system, we looked at the Attenuated Shock Velocity (ASV) in different inert materials. Secondly, in an attempt to study large-scale behaviour from lab-scale experiments [2, 16, 17] and avoid time-consuming, expensive and potentially hazardous large-scale experimental campaigns, we used Photonic Doppler Velocimetry (PDV) in combination with a Polymethylmethacrylate (PMMA) impedance window (IW). One of the key advantages of this method, compared for example to the flyer plate method [15, 18], is the potential ability to capture the whole particle velocity history of an explosive/inert material interface from one single shot. It is however limited to transparent contact materials. The experimental detonation pressure is compared to the predictions from thermochemical calculations (using the ideal model) and discussed, together with the overall accuracy of the calculations and their limitations when dealing with non-ideal explosives. The experimental detonation pressure is further compared to the estimate from empirical correlations based on VoD and loading density. An experimental TNT equivalence of UHP for brisance is proposed. We assess the reliability and accuracy of the experimental methods and the level of agreement between large-scale and small-scale results, particularly the validity of the small-scale setup for quick assessment purposes.

2 Experimental Section

In line with our initial work, we further used commercial lab grade UHP (97%) purchased from ALFA AESAR. We had determined the average particle size by dry sieving with 85% of the particles retained in the 600 μm mesh and 15% in the 1000 μm mesh. Using the

standard enthalpy of formation of UHP calculated from calorimetric measurements, thermochemical calculations were carried out with the Explo5 code (V6.06.02) [19]. We initially used the theoretically based equation of state (EoS) molecular fluid EXP-6 [20], which predicted lower detonation pressures and enabled the determination of the Jones-Wilkins-Lee (JWL) coefficients required for the numerical modelling in Ansys Autodyn [5-6]. However, for comparison purposes, we also performed the calculations with the Modified Becker-Kistiakowski-Wilson (M-BKW) EoS, as this equation of state provides greater accuracy for explosives with a low detonation temperature and a high dipolar molecules content in the detonation products [21]. UHP ideal detonation parameters, such as detonation velocity, pressure and polytropic exponent, were compared to experimental data.

Building upon initial measurements carried out at loose density (0.75 g/cm^3), where self-compaction phenomenon and density gradient were observed for large charges, it was decided to increase the UHP charge loading density to 0.85 g/cm^3 ($\pm 0.02 \text{ g/cm}^3$), 59.4% of the reported 1.43 g/cm^3 [4] Theoretical Maximum Density (TMD), to achieve more uniform loading and homogeneity. This density was also easily obtained, without heavy pressing equipment, which sounded realistic in a terrorist perspective, as UHP, within the scope of our research, was also studied as a potential emerging threat.

In the following subsections, we present the selected indirect methods and respective experimental set-ups to investigate the detonation pressure at large and small scale.

2.1 P_{det} by ASV (large-scale campaign)

The ASV method consists of measuring the arrival time at different depths in an inert acceptor in contact with an explosive charge using optical probes, and extrapolating the shock velocity at the explosive/inert interface [22]. The light signal is emitted by the ionised air at the bottom of the holes drilled to insert the probes. This method neglects the Von Neumann (VN) spike, as it does not lead to air ionisation due to its very small impulse. In this study, we selected a charge diameter of 120 mm, a trade-off between the impact of the diameter on the performance characterisation and the practical charge size. In this charge diameter (PVC casing, 2.5 mm thick), we previously recorded an average VoD of 3.520 km/s for unconfined UHP, about 90% of the VoD extrapolated at infinite charge diameter from our experimental data [6]. We fired 10 cylindrical charges (two shots for each acceptor) containing approximately 5 kg UHP ($L=5xD$, $\rho=0.87 \text{ g/cm}^3$, 60.8% TMD) and initiated by a bespoke moulded conical 350 g C4 booster (Figure 2, top left) and a standard N°8 military detonator. Building upon the results from a preliminary ASV campaign (86.4 mm charge diameter) carried out to select and design the inert acceptors, we prepared two disks (thickness 32 mm; diameter 120 mm) of five different materials with well-characterised shock properties [10, 23] in an attempt to cover a wide range of shock impedances and construct the (reflected)

Hugoniot of the detonation reaction products of UHP: Aluminium 7075, Magnesium alloy AZ31B, Polymethylmethacrylate (PMMA), Polytetrafluoroethylene (PTFE) and Polymethylpentene (TPX). As TPX was only available in 50 mm diameter rods, we filled the outer part with 1-pentanol, a liquid with an acoustic impedance very close to that of TPX [23], in an attempt to mitigate the interferences with the boundaries. Figure 2 gives an overview of the experimental setup. Each UHP charge was in direct contact with the acceptor. Eight optical probes were inserted into the acceptor. The probes consist of a bare glass optical fiber with a core and sleeve diameter of 50 μm and 1 mm, respectively. The fibers were stripped to the core on 1-2 mm and the cores properly cleaved with a ruby scribe. To insert the probes into the acceptor, eight holes (1 mm diameter) were drilled at the following depths by 4 mm increments: 4, 8, 12, 16, 20, 24, 28 and 32 (all-through, isolated from the charge by a 30 μm layer of Al tape). The depth of each individual hole was re-measured after drilling (precision ± 0.01 mm) for accurate shock velocity records. All holes were located at an identical 15 mm radial distance from the charge axis to minimise the effect of the radius of curvature (ROC) of the detonation front. In fact, using the method described in Reference [24], an average experimental 180 mm relative ROC of the detonation front had been determined for 86.4 mm diameter UHP charges during the preliminary ASV campaign. The distance between probes within the acceptor disks was optimised in such a way that the arrival times were not influenced by the shock wave distortions caused by the holes. The whole measurement zone (30 mm diameter) was also chosen sufficiently small with regard to the acceptor diameter (120 mm) to limit the influence of lateral relief waves on the shock propagation.

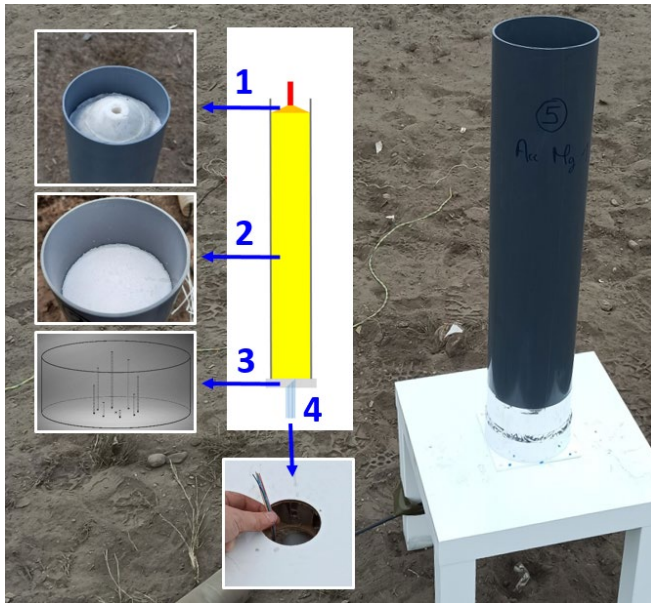


Figure 2. UHP (5 kg) – P_{det} by ASV – Experimental setup: (1) Initiation; (2) UHP charge; (3) Drilled inert acceptor; (4) ASV optical probes.

We used a passive light acquisition system OPTIMEX 64 (OZM research) to track the light signal (250 MHz sampling frequency) from the shock wave generated by the detonation of UHP and propagating through the inert acceptor attached to the tested explosive charge. The shock velocity in each inert material was then calculated from distance-time records using a linear regression, which was preferred to the parabolic one suggested in [22], taking into account significant differences between both experimental setups. In fact, Künzel et al. made use of 40 mm diameter charges and recorded the light signal up to 20 mm deep into the acceptor, giving a charge diameter to depth ratio around 0.5. We used 120 mm diameter charges and measured up to 28 mm deep in the acceptor, which corresponds to a charge diameter to depth ratio around 0.2. We also used longer charges ($L=5xD$ compared to $1.5xD$, including booster, in [22]). For those reasons, the decrease of the shock velocity due to the rarefaction wave is expected to be slower in our setup, which supports our choice for a linear regression.

For the sake of simplicity, a polytropic EoS was used to characterise the UHP detonation products and determine the detonation pressure from the ASV measurements. First, the reflected Hugoniot in the pressure/particle velocity plane (P, u), is expressed as a function of the polytropic exponent (Γ), with the initial density of the charges (ρ_0) and the velocity of detonation (VoD), as input parameters:

$$P = \frac{\rho_0}{2} \cdot \left[\frac{5 \cdot (VoD)^2}{\Gamma + 1} - 4 \cdot (VoD) \cdot u + u^2 \cdot (\Gamma + 1) \right] \quad (1)$$

In this equation, Γ is the only unknown as the previously determined averaged velocity of detonation of 3.520 km/s [6] is used. Then, we express the Hugoniot of a transmitted shock in a given acceptor material as a function of the shock velocity in the acceptor material (i) at the interface with the explosive, U_i :

$$P = \rho_{0,i} \cdot U_i \cdot u_i = \rho_{0,i} \cdot U_i \cdot \frac{U_i - C_{0,i}}{s_i} \quad (2)$$

where $\rho_{0,i}$ is the density of the acceptor material and $C_{0,i}$ and s_i the parameters of the empirical Hugoniot of the acceptor materials [23]. By continuity, both the pressure in the acceptor material at the interface and in the detonation gases after interaction are equal [10]. By equating equations (1) and (2), we then obtain a model for the shock velocity in the acceptor material with Γ as only parameter. The optimal value of Γ is then determined by using a least-square methods minimising the sum of square of the errors between this model and the experimental values of the shock velocity at the interface, taking the nature of the acceptor into account. Using this optimal value of Γ , the detonation pressure is finally calculated by using the relation [7, 10]:

$$P_{\text{det}} = \frac{\rho_0 \cdot (VoD)^2}{\Gamma + 1} \quad (3)$$

2.2 P_{det} by IWM (small-scale campaign)

In line with our previous work on detonability and detonation performance of UHP at small scale, we further used the following charge geometry: 4 mm thick steel confinement, Inner Diameter (ID) 30 mm, Outer Diameter (OD) 38 mm, Charge Length (L) 150 mm ($=5 \times ID$). The initiation train consisted of an 8 g C4 (PE8 for PDV) booster in a bespoke conical cup holding a N°8 standard military detonator. At that time, the stationarity of the detonation wave after 2 to 3 charge diameters was assessed by measuring the indentation of a witness plate resulting from the detonation of 1 to 6 diameters long UHP charges [5]. In this work, we could further confirm stationarity by monitoring the VoD of UHP along the whole confinement sleeve using 19 GOF, with 7.5 mm between probes (Figure 3).



Figure 3. UHP (90 g) under heavy confinement – VoD stationarity assessment using 19 GOF.

For the PDV campaign itself, a total of 12 devices were fired. The confinement steel sleeves were filled with approximately 90 g of UHP ($\rho = 0.85 \text{ g/cm}^3$, 59.4% TMD, slightly compacted). The OPTIMEX 64 (OZM research) passive light acquisition system (250 MHz sampling frequency) already presented in Section 2.1 was further used but in another configuration to record VoD. The setup included a total of 8 GOF, with 7.5 mm between probes, and the first probe located 90 mm ($3 \times ID$) from the booster charge, as explained previously. The probes were inserted in all-through holes drilled in the confinement sleeve and sealed by a piece of 30 μm thick aluminium tape.

In order to measure surface velocities, we used a first generation photonic Doppler velocimeter. This equipment included a 1550 nm laser source, emitting laser light from a fibre-coupled collimator with a 75 mm working distance and a 220 μm spot size. The reflected (Doppler-shifted) light was mixed in the interferometer, and a Thor Labs PDA-8GS photodetector amplified the intensity of the beat signal. We used a Tektronix 6 GHz bandwidth oscilloscope, sampling at 5 GHz, to record the electrical output from the photodetector. A Hamming window Fourier transform with variable window width was used to process each velocity record, producing a time-resolved power spectrum image, which was manually digitised to analyse numerical time-velocity

data. We used PDV in combination with the Impedance Window Method (IWM) [15, 25] in an attempt to determine the P_{det} of UHP at small scale.

Building upon preliminary results from our first attempts to determine the detonation pressure of UHP using the IWM [26], the initial experimental setup was slightly modified (Figure 4). We used two separated parallel steel rod stands (10 mm diameter) and a bespoke impedance window holder to avoid any contact between the PMMA and the confinement sleeve, while ensuring good contact between the aluminium interface and the UHP granular bed. The holder (Figure 4, top right) was also designed to position the laser probe on a reproducible way, aligned normal to the surface to get the strongest signals, at about 2 mm standoff from the PMMA window, facing the centre of the mirror interface. The laser probe was directed at a 100 μm thick aluminium mirror interface (28 mm diameter) placed between the end of the test specimen, directly on the granular bed (no surface preparation) without touching the steel confinement sleeve, and the 4 mm thick PMMA impedance window (28 mm diameter), to record the motion of this interface. The OPTIMEX generated the output trigger signal to start the PDV instrumentation, so that the beginning of the visible trace effectively corresponded to the detonation wave arrival to the explosive/inert interface.

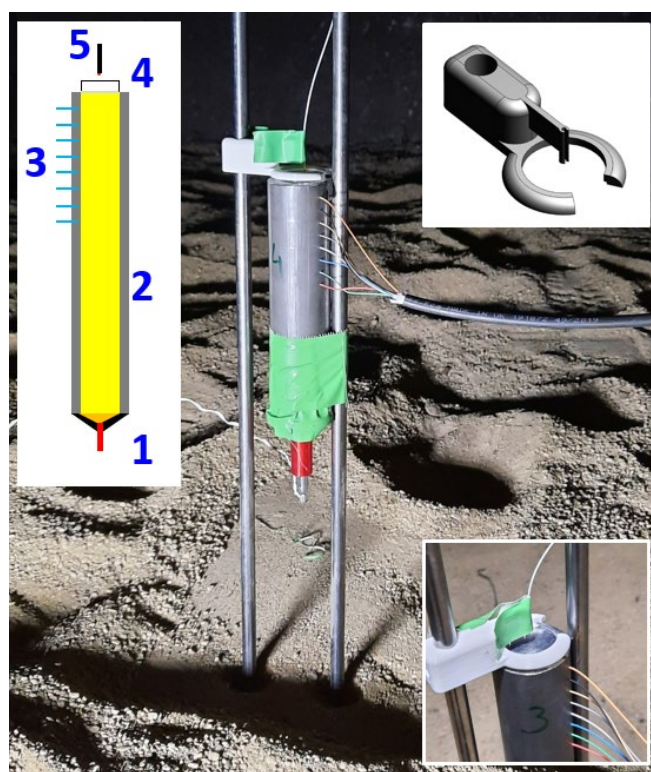


Figure 4. UHP (90 g) – P_{det} by IWM using PDV – Experimental setup: (1) Initiation; (2) UHP charge under heavy confinement; (3) VoD optical probes; (4) Impedance window; (5) PDV laser probe.

When it comes to the determination of P_{det} , anticipating on the results (Section 3.2), the intention of the authors was to apply on UHP the following method, which has proven effective for more ideal and homogeneous materials [15]: identifying the Chapman-Jouguet (CJ) state on the recorded particle velocity profile (u) from two linear regressions, respectively from the initial VN spike and the following Taylor wave, then using the generalised EoS for detonation products (Equation 4) [10] to estimate the Hugoniot of the reacted UHP and the Rayleigh line (Equation 5), with u_{CJ} as an input parameter for both.

$$\frac{P}{P_{CJ}} = 2.412 - 1.7315 \frac{u}{u_{CJ}} + 0.3195 \left(\frac{u}{u_{CJ}} \right)^2 \quad (4)$$

$$P = \rho_0 \cdot VoD \cdot u \quad (5)$$

3 Results

3.1 P_{det} by ASV (large-scale campaign)

Figure 5 provides an example of distance-time record with linear regression, while Table 1 summarises the results of the 10 ASV firings (2 per acceptor), including the measured shock velocity (U_i) determined from linear regression and calculated particle velocity (u_i) and initial pressure in inert material P_i .

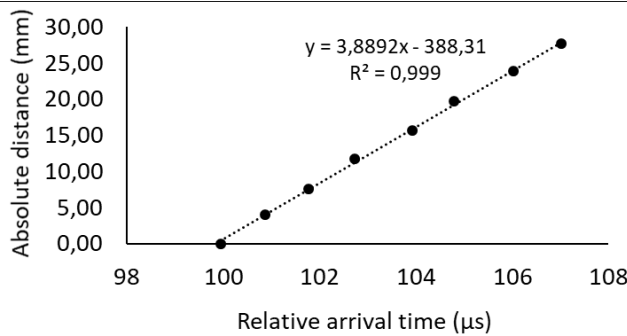


Figure 5. Example of distance-time record with linear regression – Shock velocity in PMMA.

Table 1. ASV campaign (5 kg UHP, 0.87g/cm³, charge diameter 120 mm).

Shot	Acceptor	ρ_0 (g/cm ³)	C_0 (km/s)	s (-)	U_i (km/s)	u_i (km/s)	P_i (GPa)
1	PMMA	1.186	2.598	1.516	3.971	0.906	4.266
2	PMMA	1.186	2.598	1.516	3.889	0.852	3.929
3	TPX	0.830	2.07	1.58	3.841	1.121	3.574
4	TPX	0.830	2.07	1.58	3.855	1.130	3.614
5	Mg AZ31B	1.775	4.516	1.256	5.249	0.584	5.438
6	Mg AZ31B	1.775	4.516	1.256	5.272	0.602	5.636
7	PTFE	2.153	1.841	1.707	3.056	0.712	4.684
8	PTFE	2.153	1.841	1.707	3.064	0.717	4.727
9	Al 7075	2.804	5.200	1.36	5.613	0.304	4.781
10	Al 7075	2.804	5.200	1.36	6.105	0.666	11.397

When it comes to measurement uncertainty, we calculated the particle velocity (u_i) from the measured shock velocity (U_i) in an inert acceptor and then used this value to further calculate the initial pressure P_i . For this reason, the error on P_i is proportional to the square of the measurement error on U_i . Moreover, as the Hugoniot in the U-u plane is an affine function, the error on particle velocity u_i can increase quickly, especially at low particle velocities. Due to the high shock impedance of aluminium and the rather low detonation regime, the error on pressure was too large. The shocked state (P_{Al} , u_{Al}) was disregarded and the UHP detonation products Hugoniot was then constructed from the shock states (P_i , u_i) in the four remaining inert acceptors (Figure 6). The steady-detonation state was found at the intersection of the experimental reflected Hugoniot and the Rayleigh line, corresponding to a P_{det} of 3.46 GPa. Despite the choice of a rather low shock impedance material such as TPX, we could not encompass the steady-detonation state and its determination required a slight extrapolation.

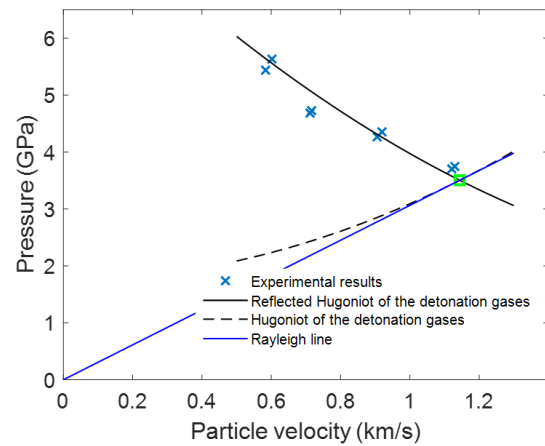


Figure 6. UHP steady-detonation state (green) at the intersection of the reflected Hugoniot and the Rayleigh line.

3.2 P_{det} by IWM (small-scale campaign)

Reproducible VoD results with an average 3.297 km/s (± 0.014 km/s for 95% confidence interval) for 90 g UHP charges (0.85 g/cm³ loading density) under heavy confinement were obtained. These results are consistent with previous work from the authors on small-scale detonability of UHP [5] and the confirmatory shots carried out with 19 probes located all along the confinement sleeve to assess the stationarity of the detonation (see example on Figure 7). The overdriven state due to the 8 g C-4 booster is obvious in the first charge diameter (30 mm), while stationarity is already observed after two charge diameters.

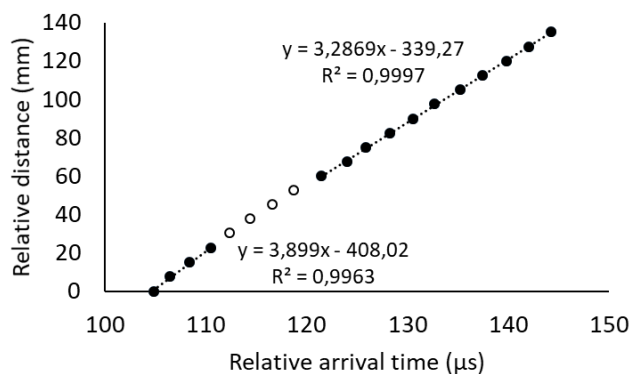


Figure 7. UHP VoD (0.85 g/cm³, heavy confinement) – Initial overdriven state from the 8 g C4 booster, transition and stationarity after two charge diameters.

These preliminary results confirm the consistency of our small-scale PDV setup, the output trigger signal being generated after 3 charge diameters to start the velocimeter, so that the beginning of the visible trace effectively corresponds to the arrival of a stationary detonation wave to the UHP/PMMA interface. Figure 8 shows an example of such a trace, typical for non-ideal explosives [26], including the arrival of the detonation wave, the initial velocity scatter due to the heterogeneity of the explosive, the shock transit time through the PMMA, typically 1-3 μs depending on pressure, then a second trace, at approximately twice the interface velocity, which corresponds to the free surface velocity of the PMMA window.

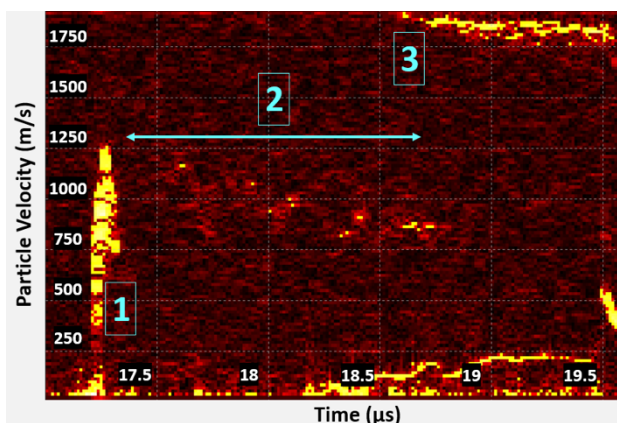


Figure 8. PDV – Example of time-resolved power spectrum image (1 shot): arrival of detonation wave (1), transit time through PMMA (2), free surface velocity (3).

From the 12 shots carried out in the same configuration, only 5 shots could capture the motion of the interface, the other 7 only providing the PMMA upper free surface velocity trace. Digitised time-velocity data of these 5 shots are combined in Figure 9. We arbitrarily selected the last 500 ns of the record in the PMMA window, when the signal seemed to stabilise after initial velocity scatter, and determined an average 877 m/s (± 18 m/s for 95% confidence interval) particle velocity at the explosive/inert interface, a value consistent with ASV results, i.e. particle velocities calculated from shock velocities measured in PMMA

(Table 1 in Section 3.1). The limited number of records of the interface motion highlights the relative difficulty to carry out IW experiments on coarse granular explosives, when compared to pressed, melt-cast, cast-cured [15] and of course homogeneous liquid explosives [27].

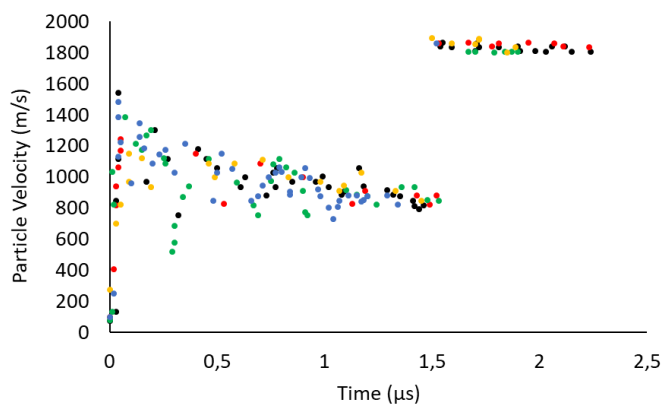


Figure 9. PDV – Digitised time-velocity data (5 shots) with average 877 m/s particle velocity at the UHP/PMMA interface.

The determination of P_{det} would require further investigations, as our current velocity records do not allow us to properly determine a CJ state, which is usually determined by a change of slope in the particle velocity profile [15]. Due to the limited thickness of our impedance window, we cannot even confirm that we captured the whole reaction zone and, hence, the CJ point. In fact, the PMMA window thickness is clearly a limiting factor, particularly when dealing with non-ideal explosives where longer reaction zone lengths are expected. Further experiments should hence be carried out with thicker PMMA windows, allowing for longer record, in an attempt to identify changes in slope of the velocity trace. However, in the current small-scale charge geometry, the maximum window thickness should not exceed 15 mm, about half the charge diameter, to avoid the effect of side relief waves on the velocity traces.

Considering other potential improvements of the experimental setup, the contact surface between the window and the explosive specimen could be improved by filling the voids between the UHP grains at the interface. Possible preparations to fill the voids include the use of silicon grease or epoxy, surface dusting with smaller UHP particles or a combination of both. Silicon grease has proven effective to ensure a good contact between plasticised explosives and the aluminium interface of the IW [15] but, in the case of UHP, the authors speculated that its application on a coarse explosive granular bed might lead to jetting effects, producing high-velocity material [28], and early disruption of the interface. The choice of the aluminium interface is also a key parameter. It should be reflective enough, thin enough to just act as a mirroring interface but thick enough to withstand initial shock arrival and deformation and reflect the laser beam along the path

to the probe sufficiently long to provide a useful PDV record. The use of multiple measurement points could be investigated. In fact, using a single probe (point measurement) is a limiting factor, particularly when the upper part of the interface starts deforming and the laser beam is not reflected anymore along the path to the probe. The point measurement is also dependent on the position of the probe which could be an issue when dealing with a heterogeneous material, with either air gaps or UHP particles in contact with the Al interface. Finally, the sampling frequency should also be increased, shortening the Hamming window duration, giving a better time resolution and, hence, minimising the reading error on the PDV capture.

4 Discussion

Table 2 summarises and compares the ASV experimental results and the ideal thermodynamical predictions from Explo5 using the EXP-6 and M-BKW EoS. Experimental P_{det} and Γ are consistent with data available in the literature on explosives detonating at comparable regime, such as ANFO [10]. Using empirical correlations for comparison purposes, we first estimated detonation pressure (Equation 6) [10], from the 3.52 km/s experimental VoD and 0.87 g/cm³ loading density (ρ_0) (Table 2), obtaining 3.14 GPa, a result in good agreement with our experimental data.

$$P_{det} = \rho_0 \cdot (VoD)^2 \cdot (1 - 0,7125 \cdot \rho_0^{0,04}) \quad (6)$$

We further calculated a consistent 2.2 polytropic exponent, using Equation 7 [29], a correlation which has proven effective to reliably estimate the Γ of CHNO explosives over a wide range of loading densities (0.2-2 g/cm³).

$$\Gamma = 1,819 - \frac{0,196}{\rho_0} + 0,712 \cdot \rho_0 \quad (7)$$

From the ratio of the experimental P_{det} of UHP and a 1.64 g/cm³ TNT reference [10], we derived an estimated 20% TNT equivalence for brisance, a result in good agreement with previous preliminary brisance assessment from underwater shock pressure carried out by the authors [6].

Table 2. UHP – Comparison of experimental data and thermodynamical predictions

	ρ_0 (g/cm ³)	VoD (km/s)	u_{CJ} (km/s)	P_{CJ} (GPa)	Γ (-)
ASV large-scale*	0.87	3.52	1.13	3.46	2.1
Explo5 (EXP-6)	0.87	4.19	0.96	3.50	3.4
Explo5 (M-BKW)	0.87	4.46	1.09	4.21	3.1

* 5 kg UHP, 120 mm charge diameter, L/D = 5, no confinement

Comparing experimental P_{det} to thermodynamical predictions using the ideal model, we find an excellent level of agreement. This good fit between measured

and ideally calculated detonation pressure could potentially come both from errors in measurement and errors in calculation, knowing that typical detonation pressure measurement error is around 10-20% [28], which is also roughly the margin error of the calculated detonation pressure of non-ideal explosives using the ideal detonation model [30]. Moreover, the calculated detonation pressure is controlled by the EoS, with value up to 20% higher using M-BKW EoS instead of EXP-6.

Depending on the choice of the EoS, the predicted ideal VoDs are about 20-25 % higher than experimental value (maximum 1% expected measurement error – [28]) and higher than the 3.94 km/s extrapolated at infinite diameter from experimental data [6]. As a result, Explo5 calculates Γ higher than 3, which is rather the expected order of magnitude for typical military explosives, with 1.5 to 1.8 g/cm³ loading density [10], (one of) its predominant parameter [29]. As the polytropic exponent describes the rate of pressure release along the detonation isentrope [31], the difference between experimental and calculated Γ value from Explo5 suggests that the predicted isentrope shape, especially in the low pressure region, using the ideal model does not adequately model the detonation product expansion. This limited accuracy could be explained by the low detonation temperature (1500 K) and the specific detonation products of UHP, particularly a rather high water content (triatomic polar molecule), when compared to conventional CHNO explosives, such as TNT [6]. Improvement of the modelling of non-ideal detonation should include kinetics of reaction in the chemical reaction zone and radial expansion of the products [30], which would however considerably increase the complexity of the study.

Two experimental methods, at two different charge scales, have been investigated in an attempt to assess the P_{det} of UHP.

On the one hand, the ASV method allowed for determination of the detonation pressure on the constructed experimental Hugoniot of explosive detonation products, using 5 different inert acceptors. The first advantage of this method is the fact that one single shot leads to the determination of a point on the Hugoniot of the detonation gases, which is of particular interest with non-ideal explosives for which large quantities have to be used. Moreover the method is not limited to transparent materials as other optical techniques. The major issue with this method is the indirect determination of the parameters of interest. In fact, we calculate the particle velocity from the measured shock velocity in an inert acceptor and then use this value to further calculate the initial pressure at the interface, making the error on pressure proportional to the square of the measurement error on shock velocity.

On the other hand, for quick assessment purposes, we investigated the use of IWM using PDV for scaled-down UHP charges. Current observations are limited to a particle velocity at the UHP/PMMA interface

consistent with the calculated particle velocities in PMMA acceptors from the ASV method. However, the use of the IWM at small-scale on a coarse granular heavily confined low-density non-ideal explosive in small charge diameter has proven challenging, even if potential improvements have been identified. An alternative small-scale PDV-based method could be the Disc Acceleration eXperiment (DAX) [32], which has proven effective and reliable in providing a rapid evaluation of explosive performance, ie detonation velocity, pressure and expansion energy. Future work will investigate the application of the method to UHP, a non-ideal material with rather low detonation regime, using a scaled-up DAX charge geometry ensuring a steady detonation.

5 Conclusion

Within the scope of a performance assessment, the brisance of UHP was quantified through its predominant parameter, the detonation pressure (P_{det}). In this comparative study, we investigated P_{det} respectively at large and small scale using two distinct indirect methods. We determined an experimental 3.5 GPa detonation pressure for 5 kg unconfined UHP charges (0.87 g/cm^3 , 120 mm charge diameter) by measuring the shock wave velocity in adjacent inert materials using passive optical probes, which corresponds to an experimental 20% TNT equivalence for brisance. This experimental detonation pressure is also consistent with the thermochemical predictions from Explo5, taking into account the margin error due to the use of an ideal model for the calculations. Particle velocity measurements at the interface of a PMMA impedance window carried out with Photonic Doppler Velocimetry on scaled-down charges of 90 g UHP under heavy confinement (0.85 g/cm^3 , 30 mm charge diameter, 4 mm thick steel) are consistent with ASV results in the PMMA acceptors but further investigations are required to determine the detonation pressure, using a small-scale experimental set-up. The ASV method has proven reliable to assess the brisance of a non-ideal explosive for risk assessment purposes.

Symbols and Abbreviations

Al:	Aluminium
AN:	Ammonium Nitrate
ANFO:	Ammonium Nitrate Fuel Oil
ASV:	Attenuated Shock Velocity
CJ:	Chapman-Jouguet
D:	Diameter
DAX:	Disc Acceleration eXperiment
EoS:	Equation of State
GOF:	Glass Optical Fiber
ID:	Inner Diameter
IW(M):	Impedance Window (Method)
JWL:	Jones-Wilkins-Lee
L:	(charge) Length
M-BKW:	Modified Becker-Kistiakowski-Wilson
Mg:	Magnesium

OD:	Outer Diameter
P_{det} :	Detonation pressure
PDV:	Photonic Doppler Velocimetry
PMMA:	Polymethylmethacrylate
PTFE:	Polytetrafluoroethylene
PVC:	Polyvinyl chloride
PVDF:	Polyvinylidene fluoride
ROC:	Radius of Curvature
TMD:	Theoretical Maximum Density
TNT:	Trinitrotoluene
TPX:	Polymethylpentene
UHP:	Urea Hydrogen Peroxide
VN:	Von Neumann
VoD:	Velocity of Detonation

Γ :	Polytropic exponent
ρ :	Loading density

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