



Brigadier (Retired) Gareth Paul Collett CBE CEng FIEExpE

**Understanding and mitigating the threat posed by
precursor chemicals used in the manufacture of
improvised explosive devices**

School of Defence Chemistry
PhD (Defence & Security)

Doctor of Philosophy
Academic Year: 2024

Supervisor: Professor Jacqueline Akhavan

Associate Supervisors: Dr Rachael Hazael
Dr Richard Critchley

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Academic integrity declaration

I declare that:

- the thesis submitted has been written by me alone.
- the thesis submitted has not been previously submitted to this university or any other.
- all content, including primary and/or secondary data, is true to the best of my knowledge.
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Abstract

Explosive chemical precursors (ECP) have been used to manufacture home-made explosive (HME) compositions for over a century. Ammonium nitrate (AN) fertiliser has dominated the landscape as the most used ECP in large improvised explosive devices (IEDs), whilst organic peroxides and the azides have been used as vital enablers to the explosive train within detonators and boosters.

Control measures are applied to many ECP through regulation, standardisation, or substitution, yet transnational criminal networks and terror groups continue to access and exploit the supply chain. When one ECP is controlled, the supply chain provides an alternative oxidiser or fuel, which does not appear (at first) to be of importance until it is discovered within an improvised explosive device (IED). First responders are most at risk when IEDs comprising HME are encountered, whether that discovery be within a viable device (a device that has been built correctly and is set to detonate), or as a partly synthesised product in solid or liquid form.

This thesis examines the current regulation applied to ECP globally and establishes a revised methodology to improve their identification and prioritisation at the strategic level, but also to assist governments in developing an understanding of the human factors associated with their diversion through Bayesian belief updating. Where HME is discovered, and not necessarily understood (whether this be under pre or post blast circumstances), the thesis provides thermochemical and explosive performance models to assist the first responder in risk reduction.

Keywords: Explosive Chemical Precursor (ECP); Bayesian Belief Updating; Network Analysis; Supply Chain; Home-Made Explosive (HME); Improvised Explosive Device (IED); Regulation.

Acknowledgements

Having served as the head of the bomb disposal profession in the United Kingdom and on His Majesty's deployed operations overseas, this PhD has been written for the victims of explosive violence and to remember friends and colleagues who never made it home. You are always in my thoughts.



***'Lest we forget'* – The EOD Memorial at the National Arboretum**

Events such as the Manchester arena bombing on 27th May 2017 demonstrate that acts of explosive violence remain close to home, they can happen at any time, and are not solely the curse of the failed and failing states dominating social media. Access to explosive chemical precursors (ECP) plays a pivotal role in that violence. Therefore, this PhD challenges a *'taboo'* subject – home-made explosives (HME) - exposing the wickedness of criminality behind illicit ECP diversion and how it can be better controlled. Given such a topic, I am hugely grateful to my supervisors for supporting what must have been an ethical nightmare for Cranfield University. There are so many people to thank, but the following deserve special mention.

Anicée van Engeland, thank you for starting this emotional journey through explosive violence with me, and for your presentation on International Security and Law to the Ministers and Attorney Generals of countries where Westerners rarely safely visit. This assisted the United Nations Development Programme (UNDP) in establishing a governance and rule of law programme under which community consultation to tackle the problem of ECP diversion was developed. Whilst many individuals such as Auke, Lucy, Stephen, Steve, Marie, Noora, Mohammed, Aleks, Abdullah, Nasser, Jes and Ghazi cannot be named in full, you turned a vision of risk reduction and victim assistance into reality. Please do not underestimate how your initial support facilitated access to the United Nations General Assembly (UNGA) for charities such as Action on Armed Violence (AOAV) and REVIVE, who continue your advocacy today.

Tracey Temple, thank you for securing 50% of the funding for this PhD and working extremely hard on the first paper surrounding strategic approaches to ECP regulation. You will be pleased to hear that this paper is now one of five mitigation procedures endorsed by the United Nations to counter-IEDs.

Jacqueline (Jackie) Akhavan, I thank you for that initial spark of academic interest in '*all things that go bang*'. You taught me explosive chemistry during my undergraduate degree at the Royal Military College of Science (RMCS) between 1989 and 1992, and then during my Masters in 2002. I know it has been painful for you - re-educating me on the finer aspects of thermochemistry – but this has facilitated the development of a simple HME calculator for first responders, which will preserve life. This was the hardest publication to pass peer review, but one that assists those at greatest risk.

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of the human factors associated with illicit diversion. This paper, published in the Security Journal, now forms part of future C-IED strategies, whether they be humanitarian or military. You may be called out of retirement to add the bells and whistles to any formal statistical approach – apologies in advance!

Rachael Hazael and Richard Critchley, you have both been fighting in the trenches from the outset. We have mulled over countless ethical possibilities and your advice and guidance on academic writing has been invaluable. I cannot remember how many drafts of each paper you commented on, but their format and content strengthened each time. Your principal focus centred on blast injury that may be incurred from the detonation of real-life IEDs recovered during security operations, not those based on small scale experimentation or modelling. Across several soil types, this work has provided a simple comparator between the crater size produced by theoretical spherical charges and those of a hexahedral nature commonly used by terrorists. I wish you both huge success in your academic careers as you gain further accolades in this discipline.

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List of Abbreviations

Abbreviation	Term
AGL	Artios Global Limited
ALARP	As Low as Reasonably Practicable
ALUMATOL	Ammonium Nitrate, TNT and aluminium powder
AMATOL	Ammonium Nitrate and TNT
AMMONAL	Ammonium Nitrate, Aluminium powder, charcoal and TNT
AN	Ammonium Nitrate
ANAI	Ammonium Nitrate and Aluminium
ANNM	Ammonium Nitrate and Nitromethane
AOAV	Action on Armed Violence
AQAP	Al Qa'ida in the Arabian Peninsula
AUS	Australia
AXO	Abandoned Explosive Ordnance
BARATOL	Barium Nitrate and TNT
BARONAL	Barium Nitrate, Aluminium and TNT
BCL	Brimstone Consultancy Limited
BDO	Bomb Disposal Operator
BRW	BURROWITE – see AMMONAL
BTI	Bertelsmann Stiftung Transformation Index
C-IED	Countering IEDs
CAN	Calcium Ammonium Nitrate

Abbreviation	Term
CCW	Convention on Certain Conventional Weapons
CFATS	Chemical Facilities Anti-Terrorism Standard
CHD	Cheddite
CHP	Hydrogen Peroxide (Concentrated)
CISA	Cybersecurity and Infrastructure Security Agency
CP	Chemical Precursor
CPI	Corruption Perception Index
CRIMP	Chemical Risk Identification and Mitigation Project
CTED	Counter Terrorism Executive Directorate
CWIED	Command Wire IED
DADP	Di-Acetone-Di-Peroxide
DAG	Directed Acyclic Graph
DDT	Deflagration to Detonation Transition
DNR	Donarit(e) – Ammonium Nitrate, TNT, Nitroglycerine and Starch
ECP	Explosive Chemical Precursor
EFP	Explosively Formed Penetrator
EOD	Explosive Ordnance Disposal
ERW	Explosive Remnant of War
ET	Explosive Train
EU	European Union
FBI	Federal Bureau of Investigation

Abbreviation	Term
FEFO	Bis (2-fluoro-2,2-dinitroethyl) formal
Fol	Figure of Insensitiveness
GICHD	Geneva International Centre for Humanitarian Demining
GNGT	(1-(5-tetrazolyl)-3-guanyl tetrazene hydrate (Tetracene/zene)
GPI	Global Peace Index
GTI	Global Terrorism Index
HME	Home-Made Explosive
HMTD	Hexamethylene Triperoxide Diamine
ICCT	International Centre for Counter Terrorism
IED	Improvised Explosive Device
IMSMA	Information Management System for Mine Action
INTERPOL	International Criminal Police Organisation
JIEDDO	Joint IED Defeat Organization
LA	Lead Azide
LS	Lead Styphnate
MA	Mine Action
MC	Main Charge
MEKP	Methyl Ethyl Ketone Peroxide
MF	Mercury Fulminate
MINOL	Mine-OL
NAS	National Academy of Sciences

Abbreviation	Term
NEQ	Net Explosive Quantity
OB or Ω	Oxygen Balance
OECD	Organization for Economic Co-operation and Development
OME	Ordnance, Munitions and Explosives
PBIED	Person Borne IED
PBX	Polymer Bonded Explosive
PC	Potassium Chlorate
PCFO	Potassium Chlorate & Fuel Oil
PETN	Penta-Erythritol-Tetra-Nitrate
PGS	Programme Global Shield
PIRA	Provisional Irish Republican Army
PSSM	Physical Security & Stockpile Management
RDX	1, 3, 5-triazacyclohexane
REVIVE	Reduce Explosive Violence, Increase Victim Empowerment
RSP	Render Safe Procedure
SII	Simple Initiating Impulse
TATB	2,4,6-triamino-1,3,5-trinitrobenzene
TATP	Tri-Acetone-Tri-Peroxide
TMD	Theoretical Maximum Density
TNT	2, 4, 6 Trinitrotoluene
TNTe	TNT Equivalence

Abbreviation	Term
UHP	Urea Hydrogen Peroxide
UK	United Kingdom
UNDP	United Nations Development Programme
UNGA	United Nations General Assembly
UNMAS	United Nations Mine Action Service
UNODA	United Nations Office of Disarmament Affairs
UNODC	United Nations Office of Drugs and Crime
UXO	Unexploded Ordnance
VBIED	Vehicle Borne IED
VOIED	Victim Activated/Operated IED
ZND	Zeldovich, Neumann and Doering

I Keep Six Honest Serving Men

"I keep six honest serving-men

(They taught me all I knew);

Their names are 'What' and 'Why' and 'When'

And 'How' and 'Where' and 'Who'.

I send them over land and sea,

I send them east and west;

But after they have worked for me,

I give them all a rest".

(Rudyard Kipling [1])

1 Introduction

1.1 Background

In 2020, The United Nations General Assembly (UNGA) published the following statement:

“The devastation caused by the increasing use of improvised explosive devices (IEDs) by illegal armed groups, terrorists and other unauthorized recipients ... has affected a large number of countries and has resulted in thousands of casualties, both civilian and military” [2].

How such armed groups, terrorists and unauthorised recipients acquire, manufacture, and use IEDs evolves at pace, including the synthesis of home-made explosives (HME) and the misuse of electronic components and chemicals considered dual-use in nature [3]. The definition of dual-use is provided by the Department for Business & Trade as:

“Goods, software, chemicals, information and technology that could be used for civil or military purposes [4]”.

As such, law enforcement must be more adaptable than the opponent to circumvent their decision-making in the dual-use arena, thereby ensuring longevity of countermeasures [5] against the IED. Never has there been a more pressing time to instigate such effective mitigation when the last decade (excluding recent events in Ukraine and Gaza) [6] has witnessed the following:

“Between 2011 and 2022, IEDs accounted for 49% of global reported civilian deaths and injuries, ground-launched weapons caused 23%, air-launched weapons caused 23%, and combined/unclear weapons caused 5%” [7].

“Between January 2010 and December 2022, 14,242 incidents involving IEDs were recorded in Western media, resulting in 147,482 civilian casualties (40,840 killed, 106,642 injured). In that time, IEDs accounted for 36% of all explosive weapon use recorded globally, and 49% of all civilian casualties from the use of explosive weapons” [8].

When such a vast array of components and substances may be used in an improvised system, the definition of *‘improvised’* sets remediation at odds with the intelligence cycle [9]. The word *‘improvised’* means to:

“Create, invent, or do something spontaneously or without preparation, esp. in response to circumstances, or as a result of necessity” [10].

Where should an appropriate intelligence focus be applied within a supply chain if *‘something’* (the IED) is being *‘created’* out of *‘necessity’* and in response to *‘circumstance’*?

Where do you start when the international community cannot agree [11] what constitutes an IED? Is it an IED, booby trap, artisanal mine, improvised mine, mine of an anti-personnel nature, or anti-personnel mine of an improvised nature [12]?

And what can be achieved to prevent use when the IED is classed as a weapon of necessity for the weak and cowardly compared to the strong and the brave [13]?

Therefore, this thesis decides to avoid argument on the definition of *‘improvised’* and *‘who’* the perpetrators are that use them, focusing on a specific research aim.

1.2 Research Aim

To narrow the opportunity for explosive violence by focusing on the regulation¹ that surrounds the explosive components of an improvised system. The research examines global supply chains available to criminals to identify whether the regulation applied to explosive chemical precursors (ECP) is sufficiently robust, and to advocate findings for improvement and change at the highest international level – the United Nations General Assembly (UNGA).

1.3 Research Objectives

The research objectives of this thesis are to:

¹ a rule or directive made and maintained by an authority realting to an ECP.

- Identify an appropriate methodology by which the threat posed by ECP can be better predicted and regulated (Chapters 2 and 3);
- Identify a methodology by which international approaches to countering the illicit diversion of ECP can be improved using artificial intelligence (Chapter 4); and
- Consider how the threat posed to first responders and the public can be better assessed and distributed at point of need, such as user-friendly App-based systems (Chapters 5 and 6).

This latter bullet can only be presented in the thesis as a visual excel format due to the classification that would likely be applied to any distributive system.

1.4 Literature Review

1.4.1 Context

The IED has fast become the definitive weapon of the new unconventional wars faced by the world today [14]. It is the weapon of the weak, not the cowardly [15], with HME being used in each part of an explosive train (the initiator, booster and main charge) to compensate for limited access to conventional energetic materials [16].

This research considers the IED within the context of HME and the ECP necessary for their synthesis [17]. This aspect is rarely considered, with the focus of law enforcement and technology applied to IED components that are not part of the explosive train (such as switches and circuit boards) [18].

Furthermore, the '*internet of things*' [19] can be seductive (humankind exists in a gadget collecting era), convincing law enforcement that the dastardliest of switches are being created for which there is no counter measure [20].

However, any competent bomb disposal operator (BDO) will debate that a switch is just a switch, it is a means of making, breaking, or changing the connections in an IED, and merely controls the stimulus to the initiating mechanism of the device [21].

Whilst components may be an important factor in countering IEDs (C-IED) [22], the IED becomes impotent if the combustion wave in an explosive train cannot progress to detonation [23]. Lee [24] defines the dependency upon progression as:

“Upon ignition of an explosive, a combustion wave propagates away from the ignition source. Combustion waves transform reactants into products, releasing the potential energy stored in the chemical bonds of the reactant molecules, which is then converted into internal (thermal) and kinetic energy of the combustion products. Large changes in the thermodynamic and gasdynamic states occur across the combustion wave as a result of the energy released. The gradient fields across the wave generate physical and chemical processes that result in the self-sustained propagation of the combustion wave”.

Given the confusing array of systems that could be used to promote heat transfer or shock wave in an explosive train, Proud [25] defines the components of an explosive train pertinent to this thesis as an initiator, a pyrotechnic delay (optional), a booster and a main charge (see Figure 1-1).

Whether the simple initiating impulse (SII) involves electrical energy, flame, spark or friction, if the progress of the shock wave in an energetic material cannot sustain detonation [26], then optimum mitigation has been achieved. Within this context, and considering the 5 components reported within literature most common to modern IEDs (the container, power source, switch, initiator and main charge (Figure 1-2) [27] [28]), the focus for research shifts naturally towards:

- cutting the link between explosive and non-explosive components; or
- degrading the ability of the explosive train to support a successful detonation.

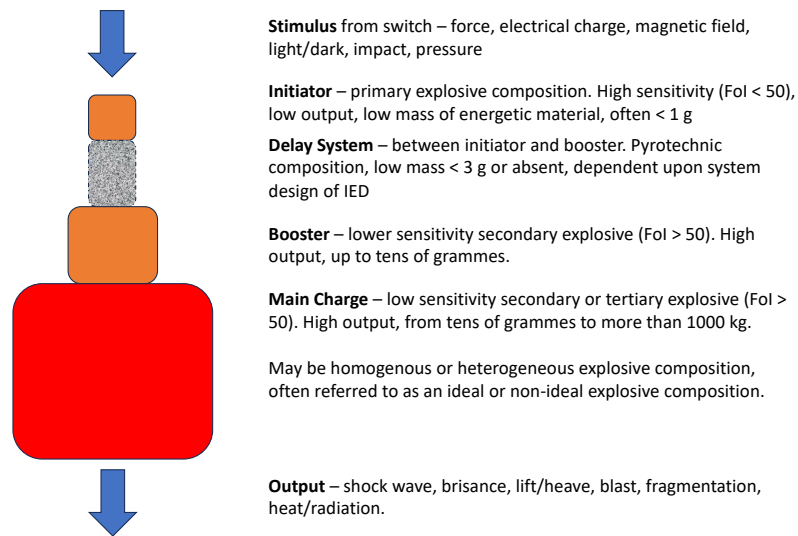


Figure 1-1: The explosive train (W.G. Proud)

Comment: In Figure 1-1 the terms Figure of Insensitiveness (Fol) and Brisance are described as follows:

- Figure of Insensitiveness is determined by the Rotter Impact Test, which characterizes explosives samples as the median drop height at which 50% initiation is achieved by a 5 kg drop-weight, compared to an RDX reference sample [29] [30].
- Brisance is the destructive crushing effect of an explosive on its immediate surroundings (within one charge diameter) [31], which can be seen in quarrying as the shattering of rock in direct contact with the explosive [32].

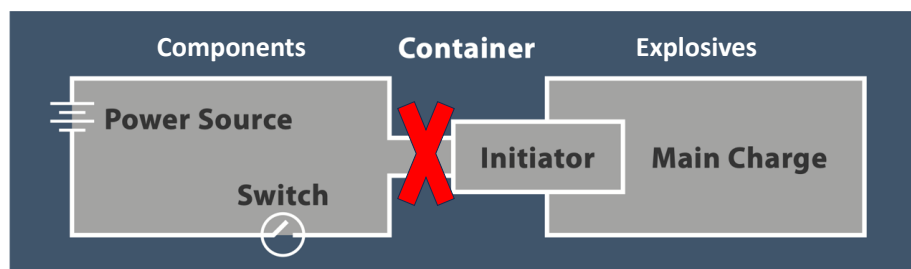


Figure 1-2: The common components of modern IEDs © BCL

1.4.2 HME within the Hierarchy of Energetic Materials

1.4.2.1 Definition

Within literature, a home-made explosive (or HME) is defined as:

“an energetic material produced from precursor chemicals, which are physically mixed or combined in a chemical reaction. Production often requires the use of other chemicals to synthesize the process, or to act as catalysts” [33].

This leads to two important sub-definitions:

1.4.2.1.1 Dependent

The precursor must rely on other chemicals for explosive synthesis. Examples of such dependent precursors would be:

- Glycerine, which is dependent upon nitric and sulfuric acid above certain concentrations to manufacture nitro glycerine (NG) [34].
- Hexamine, which is dependent upon concentrated hydrogen peroxide (CHP) and acidic catalysts [35] [36] to form Hexa-Methylene Triperoxide Diamine (HMTD).

1.4.2.1.2 Independent

The precursor chemical can be used independently for the chemical synthesis of an explosive and is not reliant on another ECP for that synthesis. Examples of independent precursors would be:

- Nitromethane, which is a detonable liquid in its own right [37].
- Barium Nitrate, which is a powerful inorganic oxidiser [38].

1.4.2.2 Basic Properties

Greater detail on the properties associated with HME can be found in Chapter 5. Explosives can be expressed as ideal (homogeneous) compounds such as PETN, RDX and TNT [39] (see Figure 1-3), or non-ideal (heterogeneous) mixtures such as ammonium nitrate and nitromethane (ANNM) [40]. HME is non-ideal in nature and comprises a fuel and oxidizer which are mixed together, but separated at the molecular level [41].

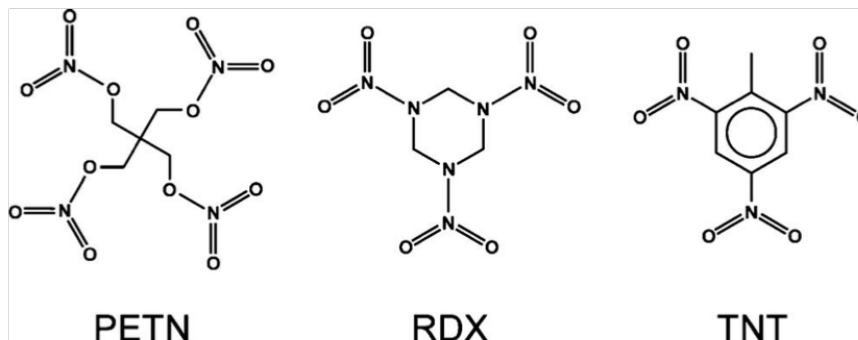


Figure 1-3: The molecular structure of PETN, RDX and TNT

When initiated by an SII, ideal and non-ideal explosives can deflagrate or detonate, dependent upon the '*effect*' that must be achieved on the surroundings. The type of effect could be:

- the production of blast in an underwater munition [42];
- the optimum spread of natural fragmentation from an artillery shell [43];
- attaining high detonation pressures to shatter material (brisance) [44];
- the production of gas in quarrying to produce a 'lift and heave' effect [45];
- or the driving of metal liners, such as shaped charges and explosively formed penetrators (EFP) [46], to achieve armour penetration.

Therefore, the properties of ideal and non-ideal explosives can vary considerably, dependent upon their role within a weapon system, a munition, or an item or ordnance.

1.4.2.3 Use

HME is often used when access to military and commercial explosives has been controlled by a State [47]. An example would be Somalia, where stringent controls have been applied to weapons and ammunition management [48], and the import of military and commercial explosives [49]. Given such constraints, Al-Shabaab commenced the manufacture of improvised dynamites from which to perpetrate atrocities in early 2017 [28], with the common constituents of some dynamites shown in Table 1-1.

Table 1-1: Common constituents of classic dynamites

Dynamite Classification	Composition [34] [50]			
	Nitroglycerine	Nitrate oxidiser	Fuel	Moisture
Guhr	75%		25% Kieselguhr	
Straight	60%	22% NaNO_3	17% woodmeal	1%
Straight	50%	35% NaNO_3	14% woodmeal	1%
Straight	40%	46% NaNO_3	13% woodmeal	1%
Straight	30%	52% KNO_3	18% charcoal	
Gelatin	66% gelatinised	25% KNO_3	9% charcoal	

HME has been developed within a myriad of military [51] [52] and commercial [53] explosive applications for centuries, with its first recorded use in a military compendium called the Wujing Zongyao, authored by Zeng Gongliang for Emperor Renzong of Song sometime between 1040 – 1044 CE:

“At night the thunderclap bombs were used, hitting the lines of the enemy well, and throwing them into great confusion. Many fled, screaming in fright.” [54]

“The thunderclap bomb contains a length of two or three internodes of dry bamboo with a diameter of 1.5 inches. Thirty pieces of thin broken porcelain are mixed with 3 or 4 pounds of gunpowder, and packed around the bamboo tube. The tube is wrapped within the ball, but with about an inch or so protruding

at each end. A gunpowder mixture is then applied all over the outer surface of the ball.” [55]

From there, gunpowder was used to craft other dastardly devices such as the ‘*heaven shaking thunder bomb*’ between 1211 – 1234 CE, which was an iron mine filled with black powder. Of the ‘*heaven shaking thunder bomb*’ it was written that:

“When the powder goes off, the bomb rips open, and the iron pieces fly in all directions. That is how it is able to kill people and horses from far away.” [54]

The last 70 years has seen HME develop within ideological IED propaganda [56] [57], based principally upon the triumvirate of opportunity [58] [59], availability [60] [61] [62] [63] and design [27] (see Figure 1-4).

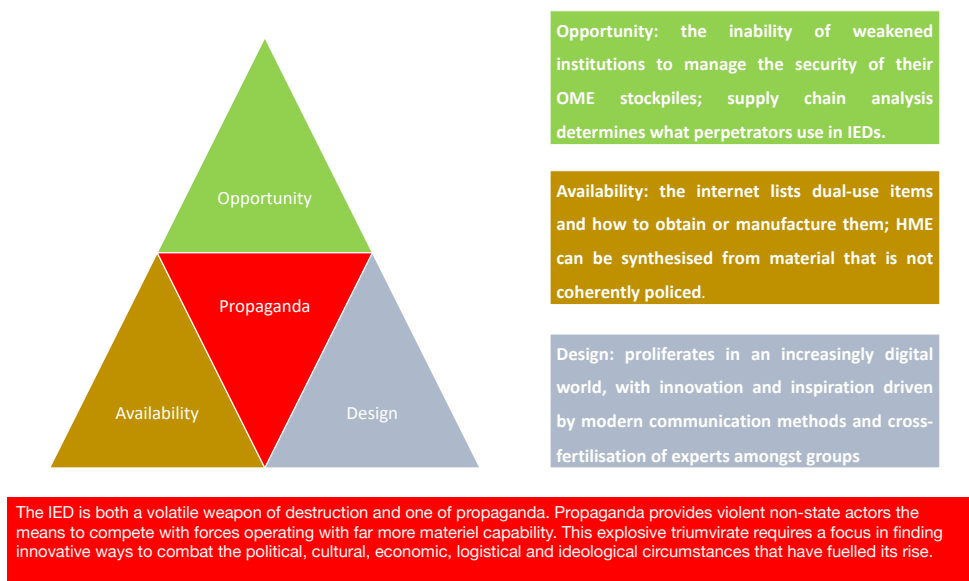


Figure 1-4: The triumvirate that drives HME use within ideological propaganda

In Figure 1-4, availability of precursors within the supply chain, opportunities presented to the belligerent by the state, and the propaganda of achieving success against a more powerful opponent, drive the IED design.

1.4.3 Explosive Chemical Precursors

An ECP is a chemical that may be used in the unlawful manufacture of explosives [33]. ECP appear as solids and liquids [64], which have a wide variety of legitimate applications. These applications are examined in Chapter 2, where regulation and control measures at the strategic level are reviewed. What is abundantly clear from literature review is that a blanket ban on all ECP is impractical and financially unviable as most chemicals have legitimate roles within society [63]. For example, nitric acid is a regulated precursor chemical, but it is pivotal in the nitration of compounds to produce fertilisers (for example ammonium nitrate and urea ammonium nitrate), as well as rocket propellants and explosives [65].

However, availability does facilitate the continued manufacture of compositions such as triacetone triperoxide (TATP) used for detonator compositions [66], or main charge compositions such as Al-Shabaab '*dynamite*' [67]. Both explosive compositions can appear as simple innocuous powders to the first responder, with photography in Figure 1-5 below provided from Brimstone Consultancy Limited (© BCL):

Explosive	Precursors	Appearance
TATP (Europe)	Acetone and Hydrogen Peroxide. Note: both precursors are independent (see paragraph 1.4.2.1.2)	

Al-Shabaab Dynamite and TATP detonator (East Africa)	Potassium nitrate, charcoal and locally manufactured nitroglycerine (NG). All precursors independent, less NG, which requires nitric acid, sulphuric acid and glycerol for synthesis	
--	--	--

Figure 1-5: An unremarkable appearance - TATP and improvised dynamite © BCL

1.4.4 First Responders

This research is not just about minimising the availability of ECP to manufacture initiators and main charges, but to understand their unique characteristics which progress a successful detonation [7]. This latter statement is necessary to improve and empower the knowledge of first responders [68] should regulatory process be circumvented, or supply chains yield suitable chemical alternatives. In an IED event, the first responder is there to formulate a threat assessment at the scene based on what they can determine, which leads to:

- saving lives;
- preventing damage to property;
- restoring a situation to normality as soon as possible;
- restoring freedom of movement in an affected area;
- assisting in the collection of items for forensic analysis; or
- facilitating the development of practical and technical IED countermeasures.

In this doctrinal capacity, the first responder will often ask themselves [69]:

- What HME has been encountered?
- What is the risk to self and the public in the worst-case scenario based upon the evidence?

- If it is a bomb factory, what (if anything) could be an ECP, and what are the likely synthesised products from those ECP?
- What is the safety distance criteria that should be applied to HME?
- What are the post-blast outcomes likely to be from a physiological, structural, and toxicological perspective?

All of the above questioning and analysis often needs to be conducted rapidly, with time being the worst enemy to the first responder. The following photograph demonstrates such a conundrum for an improvised main charge discovered by a first responder, and where the mechanical timer is not at all obvious (Figure 1-6). This photograph also provides very little evidence of the type of HME incorporated, other than the presence of an off-white prilled composition, with military grade detonators and detonating cord used as initiator and booster.

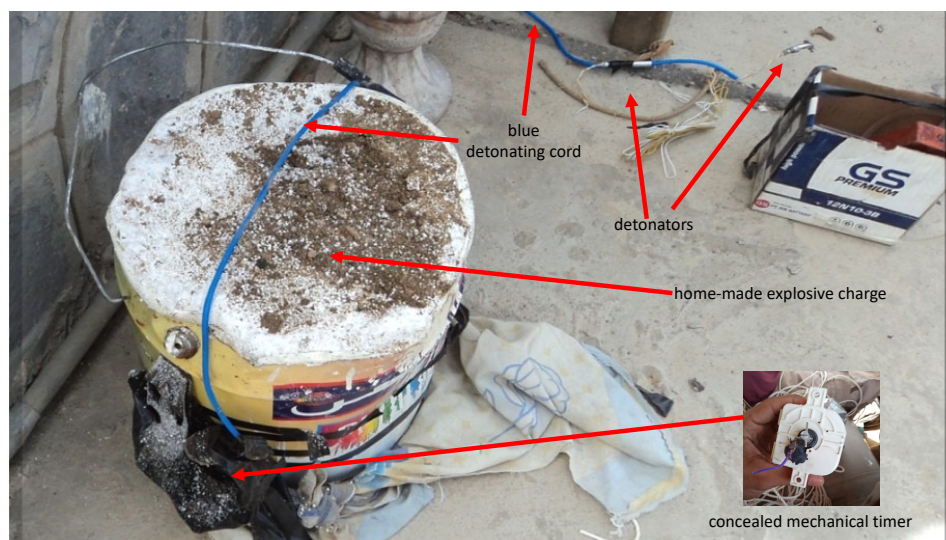


Figure 1-6: An improvised main charge in-situ © BCL

1.4.5 The Relationship between ECP and First Responder.

The initial BDO questions of “*what is it, where is it, who found it, when was it found, how was it found, why was it found*” etc, are international best practice [16]. They feature in the training manual of every first responder and at all levels of competency [70]. However, the environment engulfing explosive violence is now hugely complex and three-dimensional as Figure 1-7 demonstrates.



Key: the red circles represent UXO lying around and within the building; the red rectangles represent IEDs that have been placed on the ground floor and 2nd floor of the building; the trajectory of air-dropped munitions is shown in the earth below the building by red dotted lines

Figure 1-7: Complexity of the post-conflict urban environment © AGL

This 3-dimensional problem involves complete structures (damaged or otherwise), with Explosive Remnants of War (ERW), such as un-exploded ordnance (UXO), abandoned explosive ordnance (AXO) and IEDs, laid on top of buildings, within buildings, below buildings, or buried beneath rubble [33].

From the perspective of ECP, where the explosive is situated is not strictly relevant to the impact of this thesis – the location would apply equally to conventional explosives. The ‘*who*’, ‘*when*’ and ‘*where*’ is usually known to the first responder, with threat assessment strengthened by lessons identified in post-conflict reports relating to IED [71] and conventional weapon clearance [72] [73].

It is the ‘*how*’, ‘*why*’ and ‘*what*’ of Rudyard Kipling’s *Six Honest Men* [1] that establishes the link between the first responder and ECP. **How was the explosive made, why was it made, and what is the potential lethality should it detonate?**

This thesis therefore attempts to address these three ‘*honest men*’ as follows:

- the ‘*how*’ is investigated through supply chain analysis (Chapters 2 and 3);
- the ‘*why*’ is investigated through human factors and the application of Artificial Intelligence (AI) to inform C-IED initiatives (Chapter 4); and

- the ‘*what*’ is determined through performance analysis (Chapters 5 and 6).

1.4.6 Impact of ECP on Communities

To determine the impact of the prohibited diversion of ECP, the damage inflicted on communities is published regularly by organisations such as AOAV and REVIVE [74], with careful delineation between the types of explosive weapons that cause injury. For example, the most recent report for global harm determines that IEDs make up for 49% of all civilian casualties [8] and that HME has been used in 13,500 mass casualty events since 1881 [75]. This may, at first, seem a low statistic given the passage of more than a century, until one considers the definition of a mass casualty event (see below), and where in one IED-related incident involving HME, the numbers killed and injured could be in excess of 500 [76] [77]:

“A mass casualty event is an overwhelming incident, which generates more patients at a time than locally available resources can manage using routine procedures. It requires exceptional emergency arrangements and additional or extraordinary assistance [78]”.

1.4.7 Impact of ECP on First Responders

Sadly, the first responder does not feature in regular casualty reporting [68] when, in reality, numbers can be significant dependent upon the adversary, training, equipment and resource shortfalls, and the political will to report with honesty [16] [71] [79]. In this latter point, the ‘*Six Honest Men*’ have been corrupted.

Griffith and Unger [80] have recently announced that 43% of first responder deaths have not been reported since 2005, and that of those reported, 35% were from IEDs containing improvised explosives (HME). It has also taken until 2020 for the UK and US to publish (in detail) data on the causality of IED deaths amongst military EOD personnel [71]. Such information is critical to inform threat assessment during operational interventions or during humanitarian mine action

(HMA) clearance, and to ensure that render safe procedures² (RSP) can be updated to the benefit of all [81].

As such, a methodology needs to be determined whereby a first responder can ascertain information regarding potential hazard quickly, particularly when mass casualty events are suspected. Chapters 5 and 6 consider what practical approaches can be provided to the first responder and how they can be transformed into user-friendly applications.

1.5 Exclusions to Research

Conventional military and commercial explosives are not considered in this thesis for 2 reasons outlined below.

1.5.1 International Efforts in Restriction of Military and Commercial Explosives

International efforts are in place to restrict access to military and commercial explosives as part of physical security and stockpile management (PSSM) [82] [83] and improved governance [47] [84]. Evidence of success is seen in the reduction of military and commercial grade explosives being encountered in IEDs across most regions [85], with HME becoming the favoured substitute in its own right [6], or used to bulk out dwindling supplies of military grade explosive [86].

This regulatory approach is a significant international achievement when one considers that a tertiary explosive such as ammonium nitrate and fuel oil (ANFO) is dependent upon a detonator and booster to achieve detonation [87]. Reliable military and commercial explosives were used considerably until their availability became more restricted. Additionally, 84 countries have sanctioned the Convention on the Marking of Plastic Explosives for the Purpose of Detection [88]. Within this convention, States agree to:

² An RSP is the application of explosive ordnance disposal methods to separate the components of an IED to prevent unintended detonation.

“destroy, mark, or render permanently ineffective all unmarked explosives not held by their authorities performing military or police functions within 3 years from the entry into force of the Convention in respect of their State”.

1.5.2 Reductions in Explosive Harvesting

The days of global contamination caused by conventional minefields are diminishing within the context of 21st century conflicts [82]. Maputo has been pivotal to this [89], with countries such as Mozambique and the Falkland Islands now declared free of mines [90]. This provides less opportunity for belligerents to access minefields and use the ordnance or the explosives within the ordnance for nefarious purposes. For example, the latest Landmine Monitor Report [91] highlights that of the 164 States signatories to the Mine Ban Treaty, 94 states have completed destruction of over 55 million mines, with the clearance of 219.31 km² in 2022 alone. However, Russian Federation expansionism is a conventional mine threat that shall require diligent monitoring at land and sea over the coming years [92].

1.6 PhD Academic Structure and Methodology

This thesis is structured around the regulation applied to ECP internationally and within conflict affected states. This is a multi-disciplinary research approach, looking at strategic and tactical issues within defence, security and humanitarian disciplines to determine the scope and scale of the problem faced by the international community, communities within states themselves, and the major causal factors. The thesis is presented in five peer-reviewed articles (Chapters 2 – 5) that focus not only on the regulation, standardisation³ and substitution⁴ of ECP, but also how risk and risk management could be applied to reduce illicit diversion.

Advocacy for regulatory change was applied at the highest international level (the Secretary General of the United Nations) in the form of briefings at the United

³ the process of making the concentration or reporting of an ECP conform to a standard.

⁴ replacing a problematic ECP with another chemical that performs the same function, but which is not synthesisable at all, or without considerable effort.

Nations Headquarters building in New York (with case studies and experimentation informing debate), and a ‘facts paper’ published by the author [93]. Access to the UNGA was facilitated by the United Nations Development Programme (UNDP), the Ambassador to the Conference for Disarmament, AOAV and REVIVE.

To address the risks faced by the first responder, dual-use chemical precursors found within open-source literature were reviewed to determine their viability to manufacture HME, and whether mathematical concepts could be applied to rapidly assess the performance of such non-ideal explosives at point of discovery. Scaled models were also applied to determine the likely mass of HME used during post-blast bomb scene management.

Throughout the academic journey, financial support has been provided by Brimstone Consultancy Limited (BCL), with the UNDP, who was the author’s principal employer until September 2022, providing access to staff, materiel and experimental locations as necessary. Artios Global Limited (AGL) were commissioned to produce graphics, with the Geneva International Centre for Humanitarian Demining (GICHD) providing photography as required. No supporting organisation felt it necessary to have their corporate logo shown on the thesis, but exacts copyright privileges on photography or data where annotated (© BCL, AGL, GICHD).

1.7 Ethical Considerations

Research involving the investigation of explosives and the perpetrators of explosions, requires due diligence. Each paper has received specific ethical approval from Cranfield University and supporting agencies (such as UNDP) as necessary. These approvals are included at Appendix A. There is only one paper that is not published in entirety (Chapter 3) due to those ethical considerations, but which highlights most specifically the availability of ECP to criminals and terror organisations when regulation, substitution or standardisation demonstrates weakness.

2 The use of a predictive threat analysis to propose revisions to existing risk assessments for precursor chemicals used in the manufacture of home-made explosives

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2.1 Abstract

Improvised explosive devices (IEDs) have generated over 137,000 civilian casualties in the past decade, more than any other explosive weapon system in the same period with a far-reaching impact on personal security freedoms across 50 affected countries. The aim of this paper is to consolidate existing risk management processes to control the availability of chemical precursors used in the manufacture of home-made explosives (HME) and to recommend global standards for market regulations in their composition, sale and use. This will be achieved by assessing the current regional regulations for three common chemical precursors (hydrogen peroxide, ammonium nitrate and potassium chlorate), and proposing a risk management process to identify key precursor chemicals that require greater control.

2.2 Introduction

Approximately USD \$5.7 trillion dollars-worth of chemicals are purchased on a yearly basis and transported through supply chains for personal, commercial or industrial use [94]. Dependent upon the restrictions imposed on supply, import/export, use and carriage, they circulate the globe by a variety of platforms where illicit diversion becomes possible. One of the issues facing states is the dual-use nature (where a chemical can be used both for beneficial and harmful purposes) of most chemical precursors that are considered by terrorists in the manufacture of Home-Made Explosives (HME). This makes regulation problematic given that some chemicals considered as explosive precursors (such

as potassium permanganate and sodium nitrite) appear on the World Health Organisation list of essential medicines [95], whilst others such as sulphuric acid are essential for industry. Therefore, many explosive precursors of interest can be found in retail stores, people's homes or in specialist applications.

Most of the global population pays little attention to explosive precursors; this is helpful to the terrorist as HME can exist as loose or compacted powder, as an emulsion, gel or plasticine, as a free-flowing liquid or a fine powder dispersed in the air. It can be prepared well in advance of planned activity or mixed prior to use.

The production of HME is nothing new in terms of explosive chemistry, but rather the types of fuel and oxidiser that are combined to deliver an explosive outcome are in constant flux according to their availability and traceability. When initiated by a suitable stimulus, these fuels and oxidizers deflagrate (burn rapidly) or detonate by the initiation of an explosive train (the passage of stimulus from detonator to main charge) [96] [97], dependent upon the 'effect' required (such as blast, fragmentation, heat, shatter, or the displacement of earth and rock by expanding gaseous products). Break the explosive train and an Improvised Explosive Device (IED) containing HME usually fails to function as intended. It is therefore the chemical components within an explosive train, not the physical components of an IED, that this paper considers of interest.

The explosive train may incorporate a mix of commercial, military and HME compositions, dependent upon supply chain availability and the sensitivity of the HME to detonation. For example, ammonium nitrate (AN)-based HME is insensitive to shock alone and requires a booster of more powerful commercial / military explosive to achieve detonation ([98] and [99]). This is recognised in Yemen's improvised sea mine where the ammonium nitrate and aluminium (ANAI) main charge requires a booster of more powerful explosive to achieve detonation [100, pp. 170, Table 41.1]. A large critical diameter (the minimum diameter of explosive required to progress detonation), which exceeds those of military explosives, is also required [101] [102], which is one of the primary reasons why AN-based explosions are often large in mass (in this paper, 25 kg

is considered the limit whereby an IED cannot be considered ergonomically man-portable). The fact that an IED comprises many '*standard*' components [27] facilitates exploitation. Exploitation informs risk assessment by promoting better understanding of the perpetrator's capability and intent and what opportunities may exist to obtain precursor chemicals. Through predictive threat analysis, these opportunities can be influenced. This is particularly important given that, for example, the current UK list of proscribed terrorist organisations encompasses 76 international organisations under the Terrorism Act 2000 and 14 organisations in Northern Ireland that were proscribed under previous legislation [103].

HME is most often used by non-state armed groups, terror organisations or criminal groups when access to the reliable performance of military and commercial explosives has been diminished through effective physical stockpile and security management [104] [105]. For example, Yemen has experienced many thousands of IED events this past three years, with over 90% of devices incorporating military ordnance, grenade fuzes and military or commercial detonators. There is little recourse for groups to manufacture HME at scale if access to other supplies continue.

Existing risk and risk management for precursors is based on standard techniques, which defines risk in terms of the hazard (the precursor) and the consequences of that hazard generating an explosive event. Consequence is based on probability and severity which, in the case of HME, drifts into the bracket of catastrophic on many well-publicised occasions. This approach is buried within complex regulation that influences risk reduction programmes at the national, regional and international level, dependent upon the consequences associated with that precursor. Action on Armed Violence (AOAV) suggests that whilst regulation should be one of our greatest weapons to counter the IED, it may be a significant weakness [106].

2.3 Research Methodology

This research is exploratory in nature, with the authors utilizing a mixed method approach regarding literature review, data analysis, and case study to establish initial perception of a risk assessment strategy that could be applied to the

regulation of explosive chemical precursors (ECP) used in the manufacture of HME. Through case studies certain precursor hazards that have been used in HME compositions and which are available to terrorists and criminals through knowledge exchange or literature. Trends analysis has been used to determine key step changes in historical ECP use when regulation has been amended to establish links to potential precursors of future interest, thereby facilitating pre-emptive mitigation. For example, if a chemical precursor were regulated, which other chemicals could perform a similar function within the supply chain and could that be anticipated?

Given the increased use of IEDs this past decade, and the variety of potential ECP available, the critical reasoning for the application of a Risk Assessment is demonstrated by three specific case studies. Each case study is taken through the proposed risk assessment strategy as an introductory proof of concept. New IED prevention and mitigation strategies are also introduced which, when combined with precursor regulation, can reduce the occurrence of incidents involving HME.

2.4 Literature Review

2.4.1 Regulation

In 2017 the United Nations Office of Disarmament Affairs (UNODA) reported that IEDs impacted upon lives and livelihoods within nearly 50 countries and territories globally, particularly Afghanistan, Iraq, Libya, the Syrian Arab Republic, Somalia and Pakistan [107]. As a weapons system they have also killed or injured more than 137,000 civilians this past decade, accounting for 48% of all casualties from incidents of explosive violence [58]. Wherever possible, regulation has been applied to restrict or regulate the availability of military and commercial explosives, or the ECP that are used in the manufacture of HME. Pivotal literature references by region are as follows: Australia [108]; Canada [109]; the European Union and Norway [110]; Singapore [111]; the United Kingdom [112]; and the United States (US) [113]. Minor screening interventions have also formed part of

academic study in South Korea [114] based on increasing threats to national security.

At the international level, Programme Global Shield (PGS) [115] attempts to enhance public safety through the security of global supply chains. Working with INTERPOL and the United Nations Office on Drugs and Crime (UNODC), PGS enhances awareness and information sharing on the global movement of the most common ECP used in IED manufacture to prevent their illicit diversion and trafficking.

In conjunction with PGS, INTERPOL runs a flagship programme called the Chemical Risk Identification and Mitigation Programme (CRIMP), which, over a period of 5 years, increases the capacity of member state agencies involved in counter-terrorism activities and infrastructure protection to identify chemicals at particular risk of diversion and misuse [116]. CRIMP's list of precursor chemicals follows PGS guidelines and several additional explosive chemicals that should raise concern within national governments agencies if found in quantity. Other initiatives complement the international approach further by gathering and sharing intelligence on devices with member countries to identify, locate and arrest suspected bomb makers.

The United Nations has raised awareness of ECP at the international level over the past five years, specifically with the adoption of General Assembly First Committee resolutions, which integrate the issues of IEDs into broader discussions on peace and security, enabling the arms control and disarmament community to consider their destabilising impact and to agree on steps to reduce their effect. Examples of awareness raising internationally are:

- resource mobilisation to the PGS initiative, recognising its important role in preventing the smuggling and illicit diversion of high-use explosive precursors [117];
- establishing an Office of Counter Terrorism to assist Member States in implementing the UN's global counter-terrorism strategy [118], specifically strengthening cooperation, needs assessment and gap analysis.

The approach to risk adopted by the European Union (EU) is also to categorise certain chemicals by restriction and reporting. Restricted explosives precursors are not generally available to members of the public above a certain limit value and their acquisition is subject to control and (possibly) licensing. For reportable explosives precursors, the emphasis is placed at online and offline retail, as well as online marketplaces, to report suspicious transactions. Specific detail lies within Regulation (EU) 2019/1148, which came into effect on 1st February 2021 [110]. The criteria for determining which measures should apply include:

- the level of threat associated with the explosive precursor;
- the volume of trade in the explosive precursor; and
- whether it is possible to establish a concentration level (threshold) below which the explosive precursor could still be used for the legitimate purpose it was intended but making it less likely to form a viable HME.

Regulation (EU) 2019/1148 does not permit the public to acquire, introduce, possess or use certain ECP at concentrations above certain limit values, expressed as a percentage of weight in weight (% w/w). However, members of the public are permitted to acquire, introduce, possess or use some explosive precursors at concentrations above those limit values for legitimate purposes, provided that they hold a licence to do so. This approach has been adopted by all EU Member States, as well as non-members (Norway and the UK), however certain aspects of the regulation will require transposition into national law through a new Statutory Instrument to come into effect. Table 2-1 summarises the EU legal concentration limits (thresholds) for precursors where access by the public is required.

Table 2-1: Precursor Chemicals - EU Concentration Limits (2019)

Precursor	Standard Limit Value (% w/w)	Upper Limit Value (% w/w)	Remarks
Hydrogen peroxide	12%	35%	
Nitromethane	16%	100%	Also explosive in own right
Sulphuric acid	15%	40%	
Nitric acid	3%	10%	
Ammonium Nitrate	16%	No licencing permitted	Maximum 16% by weight nitrogen content in relation to AN (which means 45.7% AN, discarding impurities)
Potassium chlorate	40%	No licencing permitted	
Potassium perchlorate	40%	No licencing permitted	
Sodium chlorate	40%	No licencing permitted	
Sodium perchlorate	40%	No licencing permitted	

Regulation (EU) 2019/1148 also requires that suspicious transactions and significant disappearances / thefts of the precursor chemicals shown in Table 2-2 be reported within 24 hours, although the definition of *suspicious* and *significant* is difficult to define.

Table 2-2: EU Reportable Precursor Chemicals (2019)

Precursors	Remarks
Acetone, calcium nitrate, calcium ammonium nitrate, hexamine, potassium nitrate, sodium nitrate, magnesium and aluminium powders, magnesium nitrate hexahydrate	For metal powders: with a particle size < 200µm; as a substance or in mixtures 70% w/w or more of Al or Mg

From the UK's perspective, Schedule 21 of the Poisons and Explosive Precursors Act [119] regulates the explosive precursors as per Table 2-1, but barium salts, mercury and phenol (above 60% w/w) are also listed. Reportable explosive precursors also mirror those in Table 2-2, with hydrochloric acid (10% w/w), hydroxides of potassium and sodium, and sodium nitrite being listed as reportable poisons.

Most recent developments at the national level have taken place in the US where the Department for Homeland Security (DHS) has worked with the National Academies of Sciences, Engineering, and Medicine (NASEM) in an attempt to augment / update Chemical Facility Anti-Terrorism Standards [120] and to establish a committee of cross-government experts to prioritize precursor chemicals and substances, analyse their movement through the national supply chain, examine national/international legislation and regulations pertaining to precursor chemicals, and identify potential control strategies. The committee's report [113] provides an excellent reference for potential mitigation strategies, which are adaptable in response to a variety of threats, specifically risk assessments pertaining to vehicle borne and person borne IEDs (VBIED and

PBIED), which have killed and injured more civilians than any other IED system. In the report, three specific criteria are examined as a risk assessment strategy:

1. the precursor's use in VBIED and PBIED;
2. the precursor's history of use in IED attacks (looking back over the past 50 years at large scale events);
3. the precursor's ability to be used in HME independent of the presence of another specific chemical.

On that basis, the report established three groups of precursor 'risk' as follows:

- Group A – chemical precursors that satisfy all 3 risk assessment criteria;
- Group B – chemical precursors that satisfy 2 of the 3 risk assessment criteria; and
- Group C – chemical precursors that satisfy one of the 3 risk assessment criteria.

Whilst Group A precursors are the ones where US national effort is principally focused, the precursors listed in Groups B and C provide a degree of predictive threat analysis whereby restrictions imposed on Group A would force perpetrators to change approaches over time.

As can be seen, there are several methods applied to minimise accessibility of precursors by their regulation and standardisation, but there is no single unified approach that sufficiently interrogates the associated hazards of such a fast-moving commodity in today's climate. Revised assessment methods underpinned by rigorous, yet simple practical steps are required so that they can be understood and replicated widely.

2.4.2 Precursor Chemicals: Fundamental Case Studies

Based on the wide selection of fuels and oxidisers that could be used to manufacture HME, three case study materials have been identified, each being widely available and having explosive properties reported in literature.

Ammonium nitrate (AN), a white crystalline salt of ammonia and nitric acid, is used widely in fertilizers, freezing mixtures (cool packs), anaesthetics

(manufacture of nitrous oxide) and is the most important raw material in the manufacture of commercial explosives and as a gasifiable oxygen carrier in rocket propellants [121].

Hydrogen peroxide is listed as one of the 100 most important chemical compounds [122] given its wide utility ranging from bleaching applications to rocket mono-propellants and oxidizers in the aerospace industry. In HME applications, hydrogen peroxide can be exploited to make detonators and main charges [123]. The most encountered peroxide-based explosives include triacetone triperoxide (TATP), hexamethylene triperoxide diamine (HMTD) and methyl ethyl ketone peroxide (MEKP).

Potassium chlorate (KClO_3) is a stable, white, crystalline solid with low toxicity to humans, commonly used as an oxidising agent, in the preparation of oxygen, and as a disinfectant. Since its discovery by Berthollet in 1787, it is the principal component of chlorate-based explosives (known as Cheddites), incendiaries, primer formulations, pyrotechnics and matchhead compositions [31]. Pure potassium chlorate cannot be detonated, but when mixed with a small percentage of fuel, an extremely sensitive explosive can be formed [124].

2.4.3 Applying an appropriate risk assessment

To apply an appropriate risk assessment to these types of chemicals the following topics need to be considered:

1. the intended end user of the chemical and their status on the Corruption Perceptions Index – this index denotes the ease of illicit diversion that may be possible within a national or regional supply chain [125];
2. the appropriateness of national or regional legislation. For example, if a particular threat does not transcend borders, is a national or regional regulation appropriate? If this is the case, then what monitoring is required to flag escalation?
3. the ease with which the precursor chemical can be substituted or standardised (the mitigation).

The solution calls for a simple iterative risk assessment which can be easily followed by any State that wishes to do so, and which allows precursors of significant interest to be referred to an appropriate higher authority (where necessary) for inclusion in a global regulation. Therefore, this paper proposes a risk management process to prioritise chemical precursors to ensure that the ones most readily available chemically and commercially are effectively managed by global standardisation.

The process is based on a series of assessments into key factors that influence the likelihood of a chemical precursor being used in HME. The more likely a precursor is to be used, the higher priority the chemical is given. The process begins when a new chemical precursor is identified in HME manufacture. If the chemical is already listed or known, but has not been assessed, it would be a priority 1 and move to the next decision point. If the chemical is dependent on other chemicals listed (i.e. HME cannot be synthesised without access to another chemical on the list), then it is designated priority 2 and can be considered after all priority 1 substances have been assessed and regulated.

The second step in the process is to determine the role of the chemical precursor in an explosive device. For example, if the chemical is used in detonator and main charge compositions it is designated a priority 1 and progresses to the next step. The reason for this is that the chemical can be used to generate the entire explosive train for a viable IED without recourse to any other chemicals. If the chemical is used in the main charge composition it is designated priority 2. If a detonator composition, it would be designated priority 3 (based on quantitative rate of use of improvised detonators in IEDs).

The way in which the chemical precursor has been used is the third step with priority being given to VBIED compositions (where loss of life and damage to property is significant) over man portable or person borne IED's. Analysis of historical use gives an indication of the intent and probability of encounter as well as the potential severity or lethality.

The fourth step is the commercial availability of the chemical in the global marketplace, which considers the quantity of the chemical manufactured annually

and its availability within the supply chain as well as the volume of annual trade. Chemicals are prioritised based on whether they are readily available (priority 1), moderately available (priority 2) or have very limited availability (priority 3) within a region. For the purposes of this paper, volumes for high production chemicals within OECD countries were considered, with priorities ranging from less than 1000 kg per year (priority 3) to more than 500,000 kg per year (priority 1). These reports do contain sensitive data but can be accessed for public research with permission.

The final assessment step for prioritisation is to consider the suitability of existing regulation (national, regional or international). Chemicals which have been designated a priority 1 through all other steps and that are not regulated should be prioritised for global regulation. Where regulation already exists but is not appropriate (based on precursor potential), these chemicals can be assigned priority 2 and held for action at a later date.

Future steps in this process may be to assess the specific hazard posed by these chemicals in accordance with the data acquired from steps 1-5. Involving an international expert panel, both the ease of standardisation and the ease of substitution can be accurately assessed and dynamically monitored to react quickly to any evolving precursors that are encountered by predictive threat analysis or forensics exploitation. Any significant risks can then be referred to the United Nations Counter-Terrorism Committee (CTC) for advocacy within a global regulation. Whilst these remarks seem relatively straightforward, substitutions may not be obvious, requiring funded research to progress them. Given the costs of research, development and implementation, there also need to be clear incentives from the market or elsewhere to initiate the process.

Figure 2-1 describes the possible process that the risk assessment could follow. It covers all elements of IED manufacture, not just the process by which the precursors are assembled to make HME.

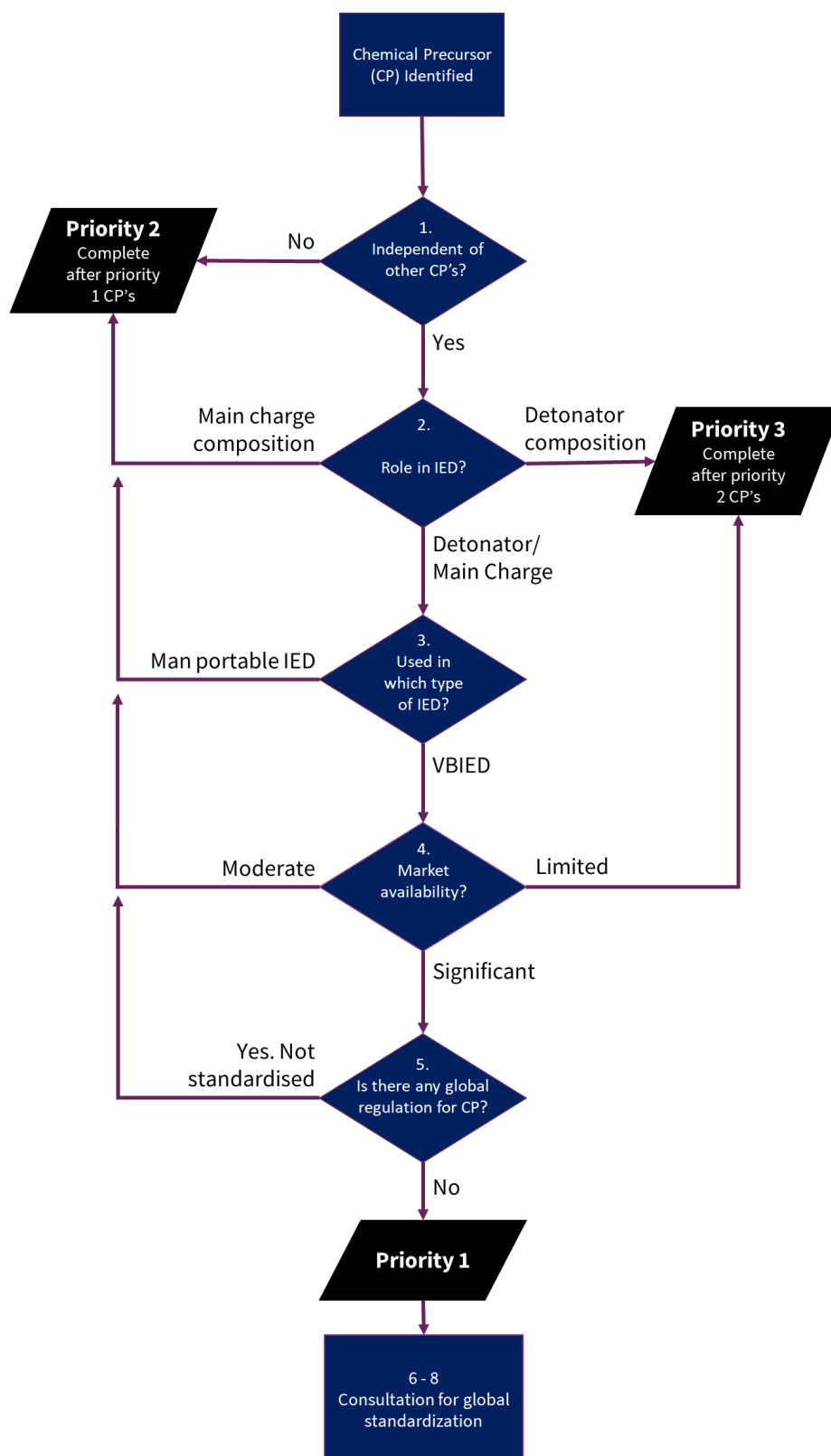


Figure 2-1: Criteria for hazard identification, risk assessment and risk control criteria process in relation to global regulation. (CP = Chemical Precursor)

2.5 Results and Discussion

2.5.1 Case Study 1 – Ammonium Nitrate

2.5.1.1 Historic examples of use

AN can be supplied at high density/low porosity at percentage concentrations greater than 90% w/w for Type A fertiliser applications or at low density/high porosity for use as an industrial grade explosive [101]. Where the percentage concentration is high, the product must be accompanied by a resistance to detonation certificate [126]. As such, the variation in limit ranges and legitimate use allows viable HME compositions to be pursued anywhere where AN is supplied, where security regulations are poorly observed, or where there is the potential for exploitation within global crypto markets (Martin, 2014).

Ammonium nitrate is not a new form of HME; it was identified as an explosive of choice during the historic bombing campaigns in Ireland/UK mainland circa 1970 - 72 [127]. Bomb disposal experts in Northern Ireland regularly identified the use of commercial blasting explosives such as AN and dynamite acquired from quarries [128]. In August 1971 alone, there were over 100 bomb explosions across Northern Ireland, the vast majority involving AN with a dynamite booster [129]. As such, access to commercial blasting explosives became a debate for governments of that time [130]. These devices regularly involved quantities exceeding 25 kg and there is detailed evidence from over 19000 IED attacks on UK territory, with 541 recorded incidents of main charge masses exceeding 25 kg between 1970 and 2007 [131]. Attacks such as this resulted in increased controls being applied to AN and dynamite with large quantities becoming impossible to obtain and with restrictions in nitrogen content of no more than 27.5% by weight (78% AN) a designated amount. This amount is not an arbitrary decision, and was based on experimentation of AN and diluents (such as ammonium sulphate, calcium carbonate and dolomite) going as far back as 1924 [132], throughout the 1950's [133] and more recently [134].

In 2016 an example of the catastrophic effect of the use of AN in HME and its strategic impact was the bombing of the Hadi shopping centre in Baghdad on 3rd July 2016 by Daesh, which killed 341 people and injured 246 others. The blast, fragmentation and enhanced heat of explosion destroyed the shopping centre causing damage estimated at USD \$4,300,000. The AN used in the attack comprised approximately 33% nitrogen by weight (94% AN), based on seizures of AN fertilizers from Islamic State forces in Anbar province earlier that year, which were suspected to have been diverted from national sales in Turkey [135].

2.5.1.2 Availability of ammonium nitrate on the global market

With so many agricultural economies relying on AN, the requirement for fertilizer has endured and the solution was thought to be the development of calcium ammonium nitrate (CAN). In 1967, research confirmed that the diluent, when added to AN, drastically reduced its detonability [136]. However, non-state actors soon developed a countermeasure to the ‘dumbing down’ and were able to separate the AN from the diluent and produce almost pure AN in the process. Detonations approaching TNT unity were achieved with certain fuels. As such, AN distilled from CAN continued to be used but its introduction made the manufacturing process time-consuming, thereby reducing the number of large-scale attacks and thus undoubtedly saving lives. The Provisional Irish Republican Army (PIRA) continued to experiment with CAN and in the early 1990’s orchestrated several successful attacks on the UK mainland by manipulation. This countermeasure may have existed as early as 1937, with Blinov articulating that desensitised AN could become detonable if manipulated [137].

Ammonium nitrate is also a common chemical found in cold packs (as are CAN and urea). Upon mixture with water, the reaction is extremely endothermic, producing ice almost instantly. The ammonium nitrate within a cold pack is readily exploitable and able to create energetic compositions. On 28th June 2012 the FBI issued a bulletin warning that cold packs containing AN had been used to manufacture IEDs [138], with several packs capable of yielding kilograms of almost pure product. Today, AN cold packs are still readily available within the global supply chain.

Annual production of AN sits in the region of 7 million tonnes, with Uzbekistan, Poland and the USA being the key manufacturers [139]. By 2026 the volume in AN manufacture is expected to have grown by 3.8% given the demands on food production for a growing global population [140]. AN therefore dominates the HME spectrum and has driven considerable legislative changes since 1969. These examples suggest either a determination by terrorists to seek out a notoriously insensitive precursor, or that it is relatively simple for non-state actors to access the supply chain.

2.5.1.3 Existing regulation on ammonium nitrate

One of the most prolific occasions of ammonium nitrate use in an IED is the Oklahoma bombing on 19th April 1995. There was a reported \$510M damage (US Dollar). Incidents such as this, and a succession of others using AN/CAN between 1995 and 2007 [63, pp. 24-25], led to Homeland Security Presidential Directive (HSPD) 19/2007 [141], which established a national policy, strategy and implementation plan on the prevention, detection of, protection against, and response to terrorist use of explosives in the United States. This directive established the Department of Homeland Security (DHS) as the lead agency for implementation. Soon thereafter, CFATS (Chemical Facility Anti-Terrorism Standards) were published, regulating over 300 chemicals that could be used domestically in a subversive fashion [120].

Table 2-3 below examines AN through the regulatory approaches adopted by NASEM, CFATS, the EU, Australia, Canada, PGS, Singapore, Norway and the UK. Subsequently, Table 2-4 demonstrates the global demand for varied compositions of AN [142].

Table 2-3: Comparison of percentage nitrogen content quoted in ammonium nitrate regulation

Precursor / Regulation	NAS	CFATS	EU	AUS	CAN	PGS	Singapore	UK/Norway
Ammonium Nitrate	Category A	≥23% N content w/w	≥16% N content w/w	Solid mixtures >45% w/w	≥28% N content w/w	14 Watch list	≥28% N content w/w	≥16% N content w/w
CAN	Category A	-	Regulated through suspicious transactions	-	-	14 Watch list	-	Regulated through suspicious transactions

Table 2-4: Ammonium nitrate classifications by weight concentration

Ammonium Nitrate Use	Chemical Composition	Hazard
Fertilizer Type A- UN/ADR Class 5.1. AN and AN-based high nitrogen fertilizers (high density & low porosity)	Mixtures of ammonium nitrate with added matter, ranging from 45% weight concentration to in excess of 90%	Oxidising; Non-combustible; May decompose; High resistance to detonation
Fertilizer Type B - UN/ADR Class 9	Non segregating mixtures between 45 and 70% weight concentration AN	Decompose when heated; self-sustaining decomposition
Fertilizer Type C – Unclassified. Self-sustained decomposition not possible	Mixtures of AN between 45 and 80% weight concentration with calcium carbonate/dolomite/ammonium sulphate	Decomposes when heated; decomposition stops when heat source removed
Industrial Grade Explosive - UN/ADR Class 1. Low density, high porosity prills combined with fuel oil (ANFO)	AN with more than 0.2% combustible material; sensitive AN fertilizer with 0.2% combustible materials; explosive preparations of AN	Deflagration to detonation following rapid decomposition; detonates with external shock

In summary, there is still a large likelihood that AN will continue to be used at a global scale. It is acknowledged that its use in HME is prolific and that regulation must be applied to restrict access to nitrogen content above 28% (80% AN by weight) for non-technical purposes to circumvent its use in HME. However, that regulation is not set at 28% across the board for public consumption and improved policing, security and education is required within the supply chain for all product types. Further mitigation will require advocacy, time and money. As such, AN should sit within a global regulation where all these conditions can be supported through effective resource mobilisation.

2.5.2 Case Study 2 – Hydrogen Peroxide

2.5.2.1 Historic/ examples of use

Peroxide based explosives have been used in 43% of Jihadist attacks involving explosives in the West between 2014 and 2018 [143]. In other regions of the world such as Indonesia, hydrogen peroxide use is seen as a new trajectory in terror-related attacks [144]. The primary solution to HME initiation problems evolved in the form of organic peroxide explosives (OPE), known since the 19th century ([145], [146] and [147]), and concentrated hydrogen peroxide (CHP) compositions, using hydrogen peroxide as the principal oxidizer with a variety of solid fuels. OPE and CHP are shock sensitive without the requirement of boosters [148] and unlike AN-based HME, could be manufactured in liquid or gel form, or even mixed at point of use, thereby improving versatility. Organisations such as al-Qa'ida soon began to provide knowledge exchange to other groups operating in the Middle East, Europe and the United States (raising the probability of encounter to high, and severity catastrophic [149]).

On 7 July 2005, 52 people were killed and over 700 were injured when four suicide bombers detonated 3 explosive devices on the London Underground and one on a London bus. Each bomb comprised mixtures of CHP. The Coroner's Inquest [150] identified that all the items necessary to manufacture the main charges and detonators used during 7/7 had been purchased within the local supply chain.

2.5.2.2 Availability of hydrogen peroxide

The global hydrogen peroxide market was valued at USD \$1.44 billion in 2020 and is expected to grow at a compound annual growth rate (CAGR) of 5.7% from 2020 to 2028 [151]. Rising demand for the product within the health industry because of COVID-19 is projected to remain a key factor fuelling market growth. The use of hydrogen peroxide is becoming more and more important in other fields of modern industry and may replace ammonium nitrate in a variety of emulsion and blended ANFO-emulsion commercial explosives given its 'green' nature (there are no toxic by-products such as nitrogen dioxide) [152].

2.5.2.3 Existing regulation relating to hydrogen peroxide

In response to the 7/7 incident, EU regulations were passed that limited the concentration by which the public could access hydrogen peroxide [153] and the way it could be marketed as an identified explosive precursor. Further updates have since been published (see Table 2-5). Therefore, examination of existing regulations (Table 2-6) identifies the following trend regarding hydrogen peroxide:

Table 2-5: Regulatory control of hydrogen peroxide

Precursor w/w/ Regulation	NAS	CFATS	EU	AUS	CAN	PGS	Singapore	UK/Norway
Hydrogen peroxide	Category A	≥35%	>12%	≥65%	≥30%	Watch list	≥20%	>12%

Table 2-6: Regulations pertaining to potassium chlorate

Precursor / Regulation	NAS	CFATS	EU	AUS	CAN	PGS	Singapore	UK/Norway
Potassium chlorate	Category A	Theft > 180 kg	>40%	≥65%(s) ≥ 10%(a)	Licence required	Watch list	Licence required	>40%

Except for Australia, the general thrust in regulation is to regulate public access to hydrogen peroxide where its concentration is below 35% w/w. This does deter use to a degree but does not remove the means by which enhancement increases the concentration to usable levels [154].

In summary, regulation has been amended to reflect OPE and CHP development (*mitigation*) but public-use concentration limits need to be considered at the global level (to reduce *probability*). Consideration should also be given to pre-empting how perborates and percarbonates could be exploited given their inherent source of readily available hydrogen peroxide within their chemistry (decreasing *probability*).

As such, hydrogen peroxide is another chemical precursor whereby there should be global harmonisation to restrict the specific w/w concentrations to levels that complicate the chemistry for determined individuals or groups, or by adding decomposition-promoting substances (such as enzymes) that frustrate attempts at concentration.

2.5.3 Case Study 3 – Potassium chlorate

2.5.3.1 Historic/ examples of use for potassium chlorate

One of the key factors of potassium chlorate that represents an area of concern to first responders is the presence of impurities that find their way into the composition during HME manufacture, whether they be chemical species such as acids, or low melting point solids. Each impurity lowers the melting point further and can lead to instability [155] [156, pp. 65-69]. Despite such sensitivity, potassium chlorate is a highly sought-after explosive precursor and one where predictive threat analysis provides some important observations. For example, potassium chlorate succeeded nitrate-based fertilizer as the HME of choice with the Taliban in 2013. It was used in 80% of all IEDs between March and May of that year, comprising a mixtures of potassium chlorate [157]. Inappropriate controls in the match and textile industry were cited as the primary reason for

potassium chlorate use following successful control of military stockpiles and the banning of AN (Case study 1) as a fertilizer in 2011 [158]. In this instance the research and development process for the Taliban took less than 2 years from the ban being put in place.

Potassium chlorate has been linked to several major vehicle-borne IED attacks in recent years, with its close cousin (sodium chlorate) traced to at least three al-Shabaab vehicle-borne IED attacks between 2016 and 2017 [159].

2.5.3.2 Availability of potassium chlorate

The potassium chlorate market is driven by the increasing demand for wood pulp bleaching to manufacture white paper and paperboard. This demand is set to increase by 5% between 2021 and 2026 according to global market key insights [160], with India's production in 2019 alone being in the region of 700 metric tons [161]. As such, potassium chlorate will remain a much sought-after commodity within the global supply chain.

In 2016, UN embargo monitors first flagged al-Shabaab's escalating use of commercial precursors in domestic IED production [162]. Al-Shabaab had infiltrated and gained covert access to the manifests of legitimate cargo vessels and was able to prosecute successful seizure operations of potassium chlorate. Based on this tactic, Somali security forces have recovered a broad variety of IED chemical precursors in the group's custody. In 2019, the UN Sanctions Committee added both potassium chlorate and sodium chlorate to a list of high-risk precursors requiring additional scrutiny due to their heightened risk of diversion into IED production [163]. The sanctions committee warned that Al-Shabaab's interest in the production of HME was escalating and that the effective seizure and use of commercial chemical precursors were an established part of their capability.

2.5.3.3 Existing regulation on potassium chlorate

Analysis of the regulation surrounding potassium chlorate can be found in Table 2-6. This table demonstrates that regulation continues to focus on variations in percentage w/w, or that illicit diversion of quantities greater than 180 kg should be reported to the authorities. This would seem to be rather an excessive quantity for such a potent precursor. And, whilst this regulation may be appropriate for

countries that enjoy effective security regimes within the supply chain, potassium chlorate remains exploitable in destinations where receipt and onward movement is questionable. Given that potassium chlorate is independent of other precursors and a natural (but less stable) second for AN, suggests it should also be another precursor considered within global regulation. Ultimately, the regulation of some precursors essentially begins a 'cause and effect' relationship where the use of potassium chlorate has become more prolific due to the regulations and therefore the difficulties in obtaining AN.

2.5.4 Application of Risk Assessment Criteria

Table 2-7 provides the projected priorities that should be afforded to AN, PC and hydrogen peroxide based on the assessment criteria proposed at Figure 2-1. Hexamine is also offered as a chemically dependent comparator for hydrogen peroxide since the production of HMTD, for example, is dependent upon it. Whilst hexamine requires no further action, AN, PC and hydrogen peroxide are not sufficiently regulated.

Table 2-7: Example of ammonium nitrate, potassium chlorate, hydrogen peroxide and hexamine being considered within a revised R.A. process

Chemical	Ammonium Nitrate	Potassium Chlorate	Hydrogen Peroxide	Hexamine
STEP 1	1 (independent)	1 (independent)	1 (independent)	2 (dependent upon hydrogen peroxide > 30% w/w to produce HMTD)
STEP 2	2 (main charge)	1 (main charge and detonator)	1 (main charge and detonator)	3 (detonators and boosters)
STEP 3	1 (VBIED - frequent)	1 (VBIED and PBIED)	1 (VBIED and PBIED)	2 (all types of IED - infrequent)
STEP 4	1 (Significant)	1 (Significant)	1 (Significant)	3 (many applications of limited scale)
STEP 5	2 (International but not standardised)	2 (International but not standardised)	2 (International but not standardised)	2 (national / regional appropriate)
STEP 6	Variance in nitrogen content (standardise) and control for specialist applications	Chemical is already standardised, so control, substitute or 'dumb down' for specialist applications	Variance in w/w % by region and country. Not possible to substitute or standardise dependent upon applications	Not possible to substitute or standardise in a number of applications. Regulation is essential.

Chemical	Ammonium Nitrate	Potassium Chlorate	Hydrogen Peroxide	Hexamine
STEP 7	Other oxidizers are available, what is the status on their regulation – refer these precursors to STEP 1	Other less potent oxidizers are available, what is the status of their regulation – refer these precursors to STEP 1	Standardize and substitute where possible. Consider use of decomposition promoting chemicals	Other detonators compositions exist, what is the status on their regulation – refer precursors to STEP 1
STEP 8	Refer to CTC	Refer to CTC	Refer to CTC	No further action

2.5.5 Future Steps

Having now considered PC, AN and hydrogen peroxide in this manner, a cursory comparison of international, regional and national risk mitigation strategies demonstrates that the importance given to an explosive precursor often varies.

With 193 Member States and 2 non-voting Members, the UN has by far the greatest reach and is therefore the most appropriate vehicle for advocacy in precursor risk reduction. The Counter Terrorist Committee (CTC) would, perhaps, be the most appropriate focal point since it is guided by resolutions 1373 [164] and 1624 [165] that attract funding to bolster the ability of Member States to prevent terrorist acts within their borders and across regions, and which can also direct technical assistance.

Most specifically, UNIDIR has completed research on C-IED threat mitigation and launched the C-IED Capability Assessment Maturity Model on 24th June 2020 [166]. This model allows Member States to conduct a risk assessment on their ability to counter the threat posed by IEDs. The use of precursors is specifically mentioned in '*Upstream Capacity Development Measure 6 [Control of IED Precursors]*', which assists a State recognise that certain materials may be misused in the manufacture of HME, how licencing and regulation might be applied, and that exploitation of recovered IED components can assist the protection of communities and improve information flow to entities such as border forces. Understanding of a State's precursor control is pivotal to any risk assessment being conducted at the national or regional level.

This paper supports the development of a systematic step approach to risk management whereby the hazard (severity / probability) associated with precursor chemicals are identified through rigorous analysis of their current and historic use, the importance of their role in the explosion process, and whether they are dependent or independent of other chemicals in application. The risk assessment must allocate priorities to those of most concern, weighted by their availability within the global marketplace and the appropriateness of the current

level in regulation applied. If the level of regulation is inappropriate at any level, then referral to the next step is required until the point is reached whereby a global intervention is required to direct the appropriate mitigation such as substitution or standardisation.

2.6 Conclusion

No precursor risk strategy can effectively prevent the ingenuity of non-state actors making HME. Nor is it possible to impose a blanket ban on certain chemicals due to their role in society. Real success in restricting the proliferation of explosive precursors can only be achieved through advocacy and cooperation between manufacturers, suppliers, retailers, and local/international law enforcement agencies, combined with the development and application of sound intelligence.

The common response has been to restrict their access by limiting supply of chemicals above certain concentrations and making reportable the supply of other precursor chemicals in large quantities, or to suspicious individuals. This type of risk assessment does make it much more difficult for individuals to develop HME, but the approach is inconsistent and loses sight of chemical precursors in countries where institutional oversight is lacking. Local security forces in countries where the rule of law is fragile become overwhelmed by extensive lists of chemicals, which limits effective control, suggesting that regulation must be applied more intelligently at point of manufacture for the repeated offenders.

The establishment of such global regulation on restriction, substitution or standardization must include those available at retail and online and requires advocacy. The United Nations is considered the most appropriate vehicle for advocacy given that the IED is now a matter of global security concern and resolutions pertaining to their use through terrorism are in force. Such a global risk reduction system would cost time and money to implement, would delay (not deny) access to a determined perpetrator, but knowing the direction of travel allows the international community the necessary space to implement focused and proactive strategies to preserve life and property.

Therefore, this paper offers an exploratory risk management process to prioritise chemical precursors to ensure that the ones most readily available chemically and commercially are effectively managed by global standardisation.

3 Urea Hydrogen Peroxide (UHP) as an improvised explosive: a threat assessment

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3.1 Statement on Classification

Throughout this research project, a clear distinction has been made between academic and restricted data. Citing Dr Maienschein (Lawrence Livermore National Laboratory) [167]:

“There is an inherent conflict between publishing scientific information and protecting it from adversaries, and this issue is very relevant to the field of improvised explosives. While scientific information should be published, information that will assist terrorists in development and application of improvised explosives must not be published in the open literature where they can gain access to it”.

This UHP paper has not been made publicly available due to its sensitive nature. Results were presented at a restricted security seminar in late 2022 [168], complementing a previous UHP-related Federal Bureau of Investigation (FBI) presentation in 2019 [169].

3.2 Abstract

Urea Hydrogen Peroxide (UHP) is an oxidising agent, widely used in the dental, cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide . UHP is a typical example of a dual-use industrial chemical, which exhibits the behaviour of a tertiary explosive. To properly assess whether UHP represents a threat to public safety as an explosive, we considered two critical criteria from a terrorist perspective, i.e. the availability of raw materials and the potential use as a main charge in Improvised Explosive Device (IED), building upon our previous academic work on UHP. As far as commercial availability is concerned, UHP is a viable Explosive Chemical Precursor (ECP) that has current and future

applications, its usage should therefore be monitored. As a tertiary explosive, UHP can sustain detonation at appropriate critical diameter and density, provided proper boosting material is available or manufactured. UHP could be used as a main charge in IEDs, most likely in blast-related applications, such as Vehicle Borne IED (VBIED) considering its detonation performance parameters.

3.3 Introduction and Method

Urea Hydrogen Peroxide (UHP), also referred to as Carbamide Peroxide is an oxidising agent, widely used in the dental, cosmetic and pharmaceutical industries as a solid source of hydrogen peroxide (HP) [170]. Like Ammonium Nitrate (AN), UHP is a typical example of a dual-use industrial chemical, which has proven detonable at large-scale [170], and exhibits the behaviour of a tertiary explosive [31]. Because of the market availability of this product, it has been assessed as a potential emerging threat. One might expect the design and the size of the ideal UHP-based Improvised Explosive Device (IED) to be in line with its inherent detonation properties. Our academic papers investigated the detonability at small-scale [171] and the detonation performance of UHP [172], deriving a 20% experimental TNT equivalence for brisance and 50% for explosive power compared to picric acid.

These equivalences are a useful source of information to assess the risks, predict the effects and potentially mitigate them. However, they do not provide all the answers within the scope of a threat assessment. The effect on target is not always the prior concern of terrorists and other key criteria come into play, such as the availability of raw materials, both for the improvised explosive itself and, particularly when considering a tertiary explosive, the explosive train required to detonate it.

A complementary approach to assess the threat of a potential misuse of UHP is hence to adopt the bomb makers' mindset (Figure 3-1), considering that UHP - related intelligence is rather immature to date, and no record of past terrorist use as a main charge in IEDs exists. The interest for UHP, though, no longer needs to be demonstrated. As a precursor, it has already been successfully used as a solid source of Hydrogen Peroxide for the manufacture of Tri-Acetone Tri-

Peroxide (TATP) in Uzbekistan in 2013 [169]. This falls outside the scope of our research, which studies UHP as an explosive in its commercial form.



Figure 3-1: Pictorial threat assessment of UHP

To assess whether UHP represents a threat to public safety and first responders as an explosive, the following critical aspects should be investigated:

- existing regulations or restrictions to acquire UHP or its chemical precursors;
- ease of manufacture;
- ease of initiation and performance concerning IED design; and
- required effect.

To further feed the threat assessment, we also compare the performance of UHP to Urea Nitrate (UNi), an improvised explosive with records of past terrorist use in IED attacks, notably the 1993 World Trade Centre bombing [173] [174] [175] [176]. This was not a random choice, with available supply chains playing a significant part [63]. UHP and UNi are also both adducts of urea. They combine oxidiser and fuel and exhibit explosive behaviour.

Hussein compared the relative explosive strength of UHP and UNi in one of the very few available academic papers on UHP energetic properties [177]. Both products are tertiary explosives, stable, rather insensitive and require a booster to ensure detonation. Unlike UHP, UNi is not sold commercially but can be

prepared by mixing urea and nitric acid [174]. Urea is therefore classed as an ECP dependent on other chemicals such as nitric acid to synthesise explosive compositions [178]. Throughout the research of UHP a clear distinction was made between commercially available carbamide peroxide and home-made UHP to determine if their use within IEDs was similar.

3.4 Results and Discussion

[The following text is approved for publication]. The flow chart for predictive threat analysis (Figure 2-1) has determined the level of consideration that should be placed on UHP as a chemical precursor to HME. This information has now been passed to UNODC and INTERPOL under Project CRIMP [116]

To properly understand the threat and assess the risk, two key criteria from a terrorist perspective are considered:

- the availability of raw materials; and
- the potential use as a main charge in IEDs.

To complete this threat assessment accurately, a difference must be established between commercial UHP and its homemade variant, with the following paragraphs summarised in Table 3-1.

3.4.1 Commercial UHP Classification

Commercial UHP (carbamide peroxide) is regulated, but surprisingly not within ECP regulation [110] [112]. Regulation is provided for consumer use as the adduct of urea and HP (which are both regulated ECPs [179]) and by concentration and availability through cosmetic regulation [180] [181]. HP content is restricted to no more than 12%, which follows ECP regulation, and UHP can only be procured by licenced practitioners. UHP's global annual trade quantity (May 2023) stands at 48,500 kg [182]. Commercial UHP is therefore an ECP with MODERATE availability (see Table 3-1). However, research has demonstrated [171] [172] that commercial UHP is an explosive, which can be used as a main charge composition INDEPENDENT of other chemicals. As a precursor to TATP

(significant relevance for detonator and small booster manufacture), commercial UHP is DEPENDENT on other regulated ECPs such as sulphuric acid.

3.4.2 Home-Made UHP Classification

Homemade UHP is DEPENDENT upon one regulated chemical for manufacture. Its synthesis is relatively simple for a terrorist to perform if they can access regulated concentrated HP and increase its specific gravity [183]. As such, the potential availability of homemade UHP is SIGNIFICANT, with main charge size dependent upon target and desired effect. Homemade UHP should therefore be classified as a DEPENDENT priority 2 ECP, using the same predictive threat analysis.

Table 3-1: Classification of UHP Based on Commercial or Home-Made Variant

UHP Variant	Precursors	Regulation	Use	Classification
Commercial	Urea, Hydrogen Peroxide	Manufactured under Cosmetic Regulation	VBIED main charge, PBIED main charge	INDEPENDENT PRIORITY 2
Commercial (detonators)	Carbamide Peroxide, Sulphuric Acid	Cosmetic Regulation, PGS List	TATP for detonator or booster compositions	DEPENDENT PRIORITY 2
Home-Made	Hydrogen Peroxide, AdBlue, Sulphuric Acid	PGS List PGS List	VBIED main charge, PBIED main charge	DEPENDENT PRIORITY 2

3.5 Conclusion

To properly understand the threat and assess the risk, two critical criteria from a terrorist perspective, i.e. the availability of raw materials and the potential use as a main charge in IED's, were investigated, building upon our previous academic work on UHP. As far as commercial availability is concerned, UHP is a viable and INDEPENDENT ECP that has current and future application in main charges

such as PBIED and VBIED. It can sustain detonation at appropriate critical diameter and density if proper boosting material is available or manufactured. This would classify commercial UHP as a tertiary explosive.

For detonator compositions, commercially available UHP can be used to synthesise TATP, thereby making it a precursor with utility across the entire explosive train. It should therefore be monitored as a real and present threat.

4 Introducing Bayesian Belief updating as a method to counter improvised explosive devices: a qualitative case study on identifying human behaviours associated with explosive chemical precursor diversion

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4.1 Abstract

Countering improvised explosive devices (C-IED) is a significant theme of the 21st century, particularly in regions with limited governance and a fragile rule of law. Many strands of activity are involved, with human interaction proving difficult to predict. However, Bayesian belief updating (used across several academic fields to provide insight into human behaviours) has never been considered.

Given the breadth of C-IED, this research focuses on a state affected by conflict, and where illicit diversion of explosive chemical precursors (ECP) for IED manufacture is supported by the population. It aims to represent (both visually and probabilistically) a methodology by which human relationships could be better understood, thereby promoting belief updating as new evidence becomes available. Such belief updating would refine focus and improve resource mobilisation.

4.2 Introduction

The international approach to countering improvised explosive devices [22] suggests that ‘*IED networks*’ are responsible for the diversion of commodities for use within improvised explosive devices. The IED network is defined within that approach as interconnected human and/or materiel nodes that may be identified, isolated or engaged. Commodities range from electronic components, such as relays and switches, to military and commercial explosives (such as plastic explosives, detonators, and detonating cord), and precursor chemicals used to manufacture home-made explosives (HME). By

attacking these networks, the intent of C-IED is to minimise component acquisition and IED use. However, such networks do not exist in isolation [184], they are a subset of broader criminality, with component acquisition promoted and inhibited by many different pressures and variables [185], such as supply chain availability and the relative advantage to be gained over the opponent by favouring one commodity over another. For example, global illicit trade involves the economic or ideological exchange of prohibited goods and services within interlinked '*dark*' networks, ranging from the trafficking of illegal narcotics and endangered wildlife to the exploitation of migrants, children, and sex workers [186]. These networks are well-established, lucrative businesses for transnational criminal organisations, and as such there is no need to establish one specifically related to IEDs. Given that they are estimated at U.S. \$2.2 trillion per annum, or 3 % of the world's global economy, these networks are protected, financed and extremely difficult to disrupt [187].

The scope for 'trafficking' IED components across '*dark*' networks is therefore extensive. As such, this paper focuses on the acquisition and use of explosive chemical precursors (ECP) used in the manufacture of HME since there has been a significant increase in their use over the past decade, despite improved regulation or other sensible measures such as substitution being applied. For example, hydrogen peroxide (a heavily regulated ECP) has been used in 43% of all Jihadist explosive devices in Europe over five years (Bergen & Sterman, 2018), whilst sodium nitrite (used as an oxidiser within certain HME), cannot be substituted by a less useful precursor since it appears on the World Health Organisation's list of essential medicines as an antidote to poisons [188]. The dual-use nature of most ECP considered useful in HME manufacturing therefore invokes a supply chain conundrum, which must be addressed at the global level [178].

Similar to wildlife crimes, drug smuggling, human trafficking and terrorism, the illicit diversion of ECP is accompanied by societal need [189] and behavioural prediction [190]. Criminal behaviour is based on the social learning theory [191], which considers how environmental and cognitive factors interact to influence human learning and behaviour. As such, the participating society is required to change, and for that to happen, human security must be strengthened, and visibly

so. If not, the problem endures, which has been one of the aspects of C-IED failure in Iraq due to the cyclical violence of the lived Iraqi experience at the individual and collective level, owing to repeated failures in reconciliation [192].

There is ample physical evidence of the illicit diversion of ECP and the widespread adverse effects of HME on economies [193], societies [194] and the environment [195], including broader security implications [196]. ECP use in HME manufacture is therefore likely where access is possible. This is because criminal supply chain activity does not conform to any regulation that can be policed effectively when national capacity is fragile [197]. Such criminality involves murder, intimidation, corruption, circumvention, concealment, avoidance, and pre-emption [198]. In many instances, this criminality embeds itself within the organisation providing the security function, whether by intelligence-gathering roles (such as reporting when consignments of importance are being delivered/transported), or simply turning a blind eye. Indeed, individuals' sole motivation may be the need to provide for the family [199] [200]. Causal factors such as this may therefore influence the human environment surrounding the illicit diversion of commodities and must be considered within any approach if identified.

NATO's C-IED strategy encompasses collective efforts to defeat an IED system by attacking networks, defeating devices, and preparing a force to operate effectively [22, pp. 1-5]. Within this doctrine, the IED system incorporates the personnel, resources and activities necessary to resource, plan, execute and exploit an IED event, with '*attack the network*' (AtN) identifying key nodes (such as a node of supply) for degradation. This degradation can be kinetic or non-kinetic, with such strategies sequenced or combined in some manner to achieve greater effect [201]. Degrading such a network aims to identify critical vulnerabilities against which appropriate countermeasures can be applied. Understanding and intelligence gathering therefore underpins the NATO C-IED approach for identifying critical vulnerabilities [202]. Such an approach helps to identify and assess the relationships or connections among people and organisations involved in crime, helping to understand and visualise the network.

Terminology such as '*critical node*' demonstrates that those of high importance or low redundancy levels can be selected to focus law enforcement efforts [203]. However, the approach is often initiated at the request of state or international governments, with few breakthroughs achieved [204]. It is shaped by the interests of leaders rather than being guided by a consultative process to assure the security needs of communities [205]. Such initiatives fuel corruption, repression, and violence, whilst neglecting social capital and social contracts that may govern any node, or a criminal organisation's ability to regain stability after a significant AtN setback [206].

Furthermore, human intelligence (HUMINT) is often overlooked in favour of technical intelligence by policymakers, leaving operations vulnerable to counter-intelligence [207]. An example of this is Afghanistan, where technical intelligence focused on developing equipment solutions to defeat the IED threat posed by the Taliban, as opposed to the Taliban's counter-intelligence cycle that outpaced most solutions delivered [208] [209]. Damage assessment is therefore difficult to verify in the NATO approach when people and their motives form the most vulnerable element of any network. Afghanistan and Iraq present recent historical examples where this long-term NATO strategy has failed through NATO's inability to neutralise transnational terrorist groups [210].

In terms of a humanitarian C-IED approach, the UNIDIR model considers sixteen upstream and downstream capacity development measures, which are either preventative or mitigative. These are described as all the activities a State may undertake to prevent and mitigate the use of IEDs [166, p. 11], with ECP mentioned explicitly in '*Upstream Capacity Development Measure 6*'. The upstream measure is entitled '*Control of IED Precursors*'. It attempts to assist states to recognise that some materials may be misused in the manufacture of HME and how restrictions may be applied to protect communities and improve information flow. Under the assessment criteria proposed within this model, the complexity of the human environment is not considered [205], and may also be compromised.

Therefore, common approaches to C-IED do not reveal the causal nature of the problem amongst the people. They lack a mathematical theory of evidence which Shafer [211] purported to be essential for serious research on problems relating to the rules of combination of evidence in complex systems. Current approaches systematically identify

points of failure (FMEA) within an '*IED System*' for interdiction, action or pressure, or where capacity development can be focused. This reductionist approach underplays the '*wickedness*' associated with criminal networks [212]. Using the illicit poaching of rhino horns as an ecological example [213], reductionism proves insufficient to resolve problems involving complexity and human beings. As such, military, humanitarian, and ecological approaches to C-IED provide limited resolution but, with the help of belief updating, based on community observations, may provide insights that facilitate effective countermeasures. It is within that modelling context where Bayesian belief updating is considered useful since it has been used across several academic fields to provide insights into human behaviours that influence decision-making [214].

4.3 Aim

The aim of this paper is to illustrate how community dialogue can be a useful tool to flesh out strategic options in dealing with an IED threat, and to introduce Bayesian belief updating as a method to improve focus, using the illicit diversion of ECP in a conflict-affected state as an example.

4.4 Methodological Approach

The methodology used in this research can be considered in seven steps: literature review; the identification of peer-reviewed mathematical modelling pertinent to C-IED; the consideration of ethics and approvals to underpin anonymity; minimising bias and controversy within data collection; identifying and understanding an appropriate ECP; determining the role of human beings in the diversionary process; and selecting the most appropriate modelling method from which to establish areas of focus and predict future success. The research does not distinguish between terrorism and organised crime since the act of illicit diversion of ECP is a criminal activity, whether used for terrorist purposes or otherwise [215].

4.4.1 Literature Review

Step 1 involved a literature review of the institutional approaches to C-IED adopted by states and armed forces concerning human security [216], including

a review of the international programmes undertaken to degrade criminal networks. This literature review is incorporated within the introduction.

4.4.2 Peer-reviewed mathematical modelling pertinent to C-IED

Step 2 comprised an examination of peer-reviewed mathematical modelling used to identify instability within regions, and particularly the region pertaining to the state considered within the research. It was found that academia applies mathematical modelling to regional instability through several published indices that analyse the impact of conflict, terrorism, and corruption within a state, and where the status of governance and the rule of law is placed in relation to stability. These indices provided meaningful statistical information to inform understanding of that state, and the most applicable to C-IED are summarised in Table 4-1, including their relevance to the research:

Table 4-1: Peer-reviewed indices relevant to C-IED

Index	Description	Relevance to Research
The Global Terrorism Index (GTI)	A comprehensive study analysing the impact of terrorism, covering 99.7 per cent of the world's population [217]	Examines human security, and the definition recognises that acts of terrorism have a psychological and physical impact on society for many years. This index positions a country as the most and least affected by terrorism. For this research, the authors are interested in the socio-economic conditions under which terrorism occurs within the state.
The Global Peace Index (GPI)	Comprises 23 indicators of the absence of violence or fear of violence within a state [218]. Positions the most and least peaceful countries within a regional context.	How the level of societal safety and security, the extent of ongoing domestic conflict and the attitudes of the local security forces towards the population affects the illicit diversion of ECP.

Corruption Perceptions Index (CPI)	The CPI aggregates data from several different sources that provide perceptions among business people and country experts of the level of corruption in the public sector [219]	The impact of corruption on the illicit diversion of ECP. Criminal threats and common distrust in society are linked to corruption [220] - the higher the level of corruption, the higher the distrust in society, which reduces interaction with law enforcement. This paper draws data from a country within the 'developing' bracket (limited ability to counter corruption).
The Bertelsmann Stiftung's Transformation Index (BTI). Governance and Rule of Law.	Considers transformation processes toward democracy and a market economy in international comparison and identifies successful strategies for steering towards peaceful change [221]	Whether or not communities have confidence in the rule of law and if any economic considerations motivate illicit diversion.

4.4.3 Ethics

Step 3 involved receiving ethical approval. There are obvious ethical considerations when researching sensitive material relating to C-IED and the human environment. The methodology of this paper was therefore guided by the normative ethical principle of '*do no harm*' [222]. Ethics approval was made and accepted by Cranfield University's Ethics Committee in early 2021, and subsequently the United Nations Development Programme (UNDP), which has been pivotal in completing this work. UNDP ethical approval insisted that any information be collected impartially by an implementing partner and safeguarded. It should be presented for this paper in a qualitative and '*stateless*' form; and that non-disclosure of implementing partners and experts be observed [223]. Confidentiality was assured through the establishment of community focus groups, not individuals or professions. Focus groups were not remunerated, and attendees at C-IED consultations were advised of their rights to participate, or to be present and simply observe rather than actively engaging in the discussion. Focus groups were aware that the overall intent was to identify areas from which to improve community safety. They were free to discuss various issues within consultation, such as drugs, gender, and sexual violence.

No comment, statement or answer by a focus group is identifiable. Several academics and historians expressed the desire to be cited directly, but the authors determined to withhold this for security and sensitivity.

Working within communities where non-state armed groups operate is also challenging, and few organisations manage to do it successfully. Ceasefires may stop the violence for a while, but they do not resolve conflict [224]. Therefore, this paper does not examine the capability and intent of any terrorist organisation mentioned, or seek to resolve conflict, but considers how ECP use could be diminished by better defining the causal factors on which to focus.

4.4.4 Minimising Controversy & Bias

Step 4 involved minimising controversy and bias.

The use of IEDs within, and by communities, has long been a point of controversy, with the IED narrative of the 20th and 21st centuries, linking them to terror organisations and brutal regimes [14]. Use driven by hate, support driven by fear or ideology. Stacey [225] initially advanced the importance of including sensitive and controversial areas, such as war crimes and ethnic violence, in their association with a group narrative. She argues that institutional behaviour is informed by presumptions of human behaviour, not the actual reasons for behaviour. It is from successes in such an approach that the sensitivity of gathering information on IED use was considered less '*taboo*' when debating issues concerning community safety. To ensure that such a controversial approach was acceptable, clearance was sought from the Prime Minister's Office, the Ministry of Interior, family protection directorates, victim support organisations, and the governors/community leaders of the locations where focus groups would convene. Access to affected communities was unanimously supported.

To ensure no bias from the authors, UNDP selected the implementing partner independently and through fair competition. The implementing partner needed to be of national descent given the mistrust towards international organisations yet divorced of the politics within the communities. Similarly, to prevent bias from the implementing partner, the organisation was provided direction from UNDP governance and rule of law representatives and international humanitarian law experts to introduce and discuss several thematic areas concerning human security and steer debate, not provide an opinion.

Locations for the research were identified from humanitarian organisations recording the impact of explosive violence within the country as part of the ongoing conflict. Those areas most heavily affected by IED attacks were chosen, but where safe access could be guaranteed. Focus groups were established only in areas separated by hundreds of miles and facing entirely different IED threats from non-state actors, criminals, and terror groups. Representation comprised

men and women from across society, including those working extensively within the supply chain and victims of explosive violence. Given all the above, risk of bias was reduced to as low as reasonably practical.

4.4.5 Choice of Precursor and Percentage use in IEDs

Following ethical considerations and approval from sponsors, Step 5 involved the identification of a suitable ECP within that state whose use could be determined. Ammonium nitrate was chosen given its significant volume of global trade [226], the overt involvement of international law enforcement towards its regulation [178], and increasing evidence of its use in that particular state through United Nations Security Council reporting.

For this research to determine the type and amount of ammonium nitrate used in HME, it was necessary to compare the volume of legitimate trade to that country and liaise with national demining organisations and local law enforcement to assess the volume used in IEDs. This would provide a percentage figure of use over several years where records were available.

4.4.6 Determination of Causal Factors in ECP Use

Step 6 involved the interpretation of information provided by the focus groups so that trends in ECP activity could be identified. The information provided by the implementing partner and focus groups was assessed by an expert panel to determine the most appropriate modelling method to represent and interpret data. Owing to the complexity of the information provided, a panel of defence, security and humanitarian experts was convened to interrogate the views of focus groups into root causality that could be used within an appropriate model. The expert panel was also provided access to the indices for the country in question (described at Step 2) and associated UN Security Council reporting. The expert panel adopted the following process to submit, review or reject the available evidence provided by ten (10) focus groups, based on its relevance to ECP diversion (see Table 4-2).

Table 4-2: Qualitative Acceptance Criteria

Focus Group	Implementing Partner		Panel of Experts		Authors
1	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
2	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
3	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
4	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
5	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
6	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
7	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
8	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
9	Validated	Submit	Validated	Submit	Accept

Focus Group	Implementing Partner		Panel of Experts		Authors
10	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject
	Validated	Submit	Validated	Submit	Accept
	Not validated	Review	Not validated	Review	Review
		Reject		Reject	Reject

4.4.7 Choice of Modelling Method

Following the collation of data and further literature review based on the data obtained (Steps 5 and 6), the authors identified Bayesian belief updating as the potential modelling method (Step 7). Firstly, the methodology supported reasoning under uncertainty [214], and has been successfully applied throughout human factors research across several disciplines such as engineering safety [227], failure mode analysis [228], security [229], poaching [213] and most recently genetics [230]. Secondly, Bayesian reasoning could conveniently update prior judgments when new evidence becomes available [231], making it ideal for changes in circumstance over time (as a state moves towards improved governance and rule of law for example). This would provide longevity to future research. Thirdly, further reading on the diversity and uncertainty of information in complex environments [232] led the authors to discount other theories such as FMEA, AHP and ANP. Bayes' theorem was therefore chosen as a viable method to assess ECP diversion since it provided '*weights of evidence*' to determine the level of risk priority that should be apportioned to effective decision-making, and which has proven successful in unpacking the complexity of poaching [213].

However, two fundamental problems have been addressed to build a Bayesian network around ECP. The first was to determine the structure of the network (the qualitative part, which is usually called a directed acyclic graph (DAG)), and the second was to determine the conditional probabilities associated with each node (quantitative). In this research, the experts sought to establish the DAG

associated with ECP diversion within the state, but stopped at anything further than establishing the most basic conditional probabilities. Based on those areas of potential focus identified, belief updating would need to be applied to determine successful outcomes, and which is funded throughout 2023 and 2024.

4.5 Results & Discussion

4.5.1 Ammonium Nitrate Use in HME

Senior law enforcement officials within the state identified that by far the largest explosive constituent of IEDs comprised military ordnance, owing to the limited security of ammunition stockpiles. However, discussion with the national demining authority and UNDP established that the use of ammonium nitrate (energised with aluminium) within improvised mines and IEDs over four years had been significant. Whilst the numbers in circulation are difficult to predict (they are only encountered during clearance operations), the use of AN between 2018 and 2021 could be determined from the Information Management System for Mine Action (IMSMA) as 92,000kg (see Table 4-3):

Table 4-3: Numbers of mines and IEDs recovered over four years containing HME
– source IMSMA [132]

Year	Improvised Mine	IED	Contain HME
2021	1204	1032	448
2020	923	512	287
2019	1536	786	465
2018	1691	918	522
TOTALS	5354	3248	1722

Port Authority data identified that 1,457,610 kg of AN had been delivered as part of legitimate trade over that same period, intimating that 6.3 per cent of total volume imported had potentially been used to manufacture IEDs and improvised

mines. This percentage is important since it establishes the start-point from which to determine whether usage would diminish over time by applying belief updating. For example, if the amount of usage is 6.3% in 2022 (based on data over 4 years) what would that percentage be in 2026, once the causal factors had been identified and belief updating implemented?

4.5.2 Vulnerabilities Identified Through Focus Groups

Of the ten focus groups established between November 2020 and December 2021, the authors can determine (alphabetically) eleven critical vulnerabilities specific to the illicit diversion of AN: awareness (lack of); bribery and corruption; coercion and intimidation; consultation (inappropriate international focus); domestic availability; employment (limited funded employment); idealism; inspection (limited checks); opportunity (relative advantage moving towards HME); security (lack of); and visibility (of overt criminality). These are described in more detail in Table 4-4:

Table 4-4: Vulnerabilities identified by focus groups

Vulnerability	Remarks
Awareness	Limited understanding within the supply chain regarding an ECP and its dual-use. As such, little attention was paid to the movement of agricultural or industrial products, less those with a corruptible value chain (food, fuel, water). Ammonium nitrate was seen solely as a fertiliser for agricultural use.
Bribery & Corruption	A heuristic and anecdotal view that access of criminal entities to some key contributors in the supply chain was known about, but not acted upon. The local security forces, immigration, port and customs authorities were cited as the most problematic, with significant irregularity in the payment of wages being the principal cause. The ' <i>shadow economy</i> ' available through terrorism and criminality was a method of obtaining income security.
Coercion & Intimidation	Punishments imposed by terrorist and criminal entities for non-compliance were an ominous undertone within some focus groups, but not all. Impotent justice systems were unable to react to reporting. The legal system was confession instead of evidence-based, leading to minimal prosecution and subsequent retribution for crimes reported. Little, if any, evidential process or the will of security forces to see an investigation to a conclusion.
Consultation	Lack of international investment on matters of priority within communities. The community need may not necessarily align with the international view of need, and the impact of IEDs has never been previously discussed. Explosive violence, sexual violence and drugs were cited as significant issues, leading to identifying many areas where governance and the rule of law levers could be better applied. Local security force response to IEDs was focused

Vulnerability	Remarks
	upon specific points of intervention (such as an individual) with no understanding of the long-term effect of that intervention. There had been no reduction in the number of events or civilian casualties due to such interventions. Indeed, IED use had increased by over 20% from the previous year.
Domestic Availability	Ammonium nitrate was reported to be commonly available for purchase at market, and in quantity. There is no understanding of regulation given that the need for nitrate fertilisers was widely shared across multiple households given food insecurity. IEDs comprising AN were considered easy to manufacture by those with a knowledge of explosives (no requirement for melt casting such as TNT).
Employment	The lack of jobs was seen as a critical driver amongst disaffected youth to support the illicit supply chain. The deteriorating security situation drove the necessity of cash incentives to feed the family. The government was not paying wages across several employment groups, including those with supply chain access. Coordination with endowment offices to intensify awareness was lacking. The shadow economy's attraction severely undermined any advancement toward achieving peace, justice, and strong institutions.
Idealism	There was little support for terrorism or criminal acts based on idealism. Of those consulted, very few recognised ideologies as a motive to stymie their communities.
Inspection	A lack of resources, or even funds to pay staff, prevented effective security regimes from being put in place.
Opportunity	The opportunity to use military and commercial explosives was diminishing due to improved physical stockpile and security management. The chance to use ECP existed, with access to the internet readily available. However, focus groups alluded that IED use was at an industrial scale, with users proficient in HME manufacture.

Vulnerability	Remarks
Security	Lack of investment in security architecture or facilities. Limited training. Multiple security entities with differing allegiance working within ports – some recognised within the peace process, others not. They have limited information technology and surveillance. Some institutions are more corruptible than others. ‘Insiders’ can flag and identify shipments of vital interest. Little evidence, if any, of criminal entities promoting opportunism but more organised planning. Trusted insiders manipulate access to ECP for use by organisations [233]. Tribal contracts override security contracts. Gathering accurate and meaningful metrics for illicit diversion had never been attempted, given limited national law enforcement [234].
Visibility	Mixed views on the visibility of criminal entities. Whilst a common principle in states with a robust rule of law would be to avoid law enforcement [235], observations were made that criminal elements did not necessarily hide their presence or involvement in some districts. It added to an individual’s ‘wasta’.

It must be pointed out that focus groups remained fully engaged throughout the research and were passionate about the impact of IEDs within their communities. They were keen to express views, which is paradoxical to the opinions and humanitarian imperatives of many international organisations [236]. Just as Stacey has surmised [225], it was a '*taboo*' topic that needed to be aired, so that improved international focus could be applied to the problem. Indeed, focus groups were so enthusiastic that they applied themselves to the materials provided (such as flip-chart, post-it, or picture), collating thoughts into areas of similarity.

4.5.3 The views of the expert panel, based on available data from focus groups, indices and reporting

The vulnerabilities identified by the focus groups were consolidated into 12 root causalities by the expert panel, as shown in Table 4-5. In terms of terrorism, corruption, human security freedoms and violence, there was a direct correlation to the peer-reviewed indices. For example, the GTI provided index scores relating to the modus operandi and intent of the world's four most deadly terror groups, including reference to their impact on the local population. Whilst the focus groups did not refer to these organisations by any western nomenclature, two of those four terror groups were described as hugely influential within the community, but not for all the reasons western definitions of terrorist organisations may reflect. It was, therefore, quite simple to pull several strands of observation under the heading of 'terrorism', to have confidence that the GTI rating was statistically accurate, to determine the main area of impact, which was almost exclusively security related, and to separate out those areas that were not solely attributed to security (such as idealism, intimidation, disaffection and so on).

Table 4-5: Definitions of root causality

Root Causality	Description
Idealism	The impact of idealism driving a society to be involved in illicit diversion
Terrorism (GTI)	The impact of terrorism on society to facilitate illicit diversion – assessed within the GTI scores for country
Corruption (CPI)	The impact of corruption on human rights as a driver to illicit diversion – assessed within the CPI scores for country
Human security freedoms (BTI)	The status of human security freedoms as a driver behind illicit diversion – assessed within the BTI scores for country.
Intimidation	The impact of intimidation, tribal or otherwise, on a society to be involved in illicit diversion
Disaffection	Societal disaffection, employment or otherwise, as a principal cause behind illicit diversion
Financial need	The basic need to provide for the family given insurmountable financial hardship
Regulation	The absence of, or poor understanding of, ECP regulation in the workplace
Accessibility	The accessibility of ECP within the supply chain at the point of delivery

Root Causality	Description
Opportunity	Opportunities being presented within society for illicit diversion to take place at the point of delivery and beyond
Volume of trade	The status in the volume of legitimate trade of an ECP to the state in question
Violence (GPI)	The status of negative peace as a driver for illicit diversion – assessed within the GPI for country

Furthermore, the expert panel noted that the country under research did not fall within the scope of international support concerning the policing of ECP due to the levels of violence and corruption present. Ports were integral to the economy, yet the influence of certain terror groups and their affiliations outside these ports was significant.

It was also evident from the focus groups that the illicit diversion of ECP had not been considered within the context of a change of attitudes and behaviours, but rather poorly informed FMEA [237]. For example, C-IED involves multiple functional areas and, therefore, relies upon an integrated and comprehensive approach that is joint, inter-agency and multinational. The focus groups responded that this was not the case, given limited capacity within the rule of law, and the absence of civil-military interaction. As such the main facilitator (effective cooperation) within the C-IED context was absent. This lack of coordination and cooperation filled law enforcement with the desire to obtain direct and immediate effects, acting on limited information to provide resolution. Such a kinetic approach led to greater discontent, thereby eroding the rule of law further. It did not reduce the IED threat to a manageable level that returned any tangible freedoms to the community. As such, there was limited knowledge and experience evident to support other C-IED pillars, or pursue any meaningful activity without the proactive involvement of the community.

4.5.4 System Modelling the Human Environment

4.5.4.1 The DAG

The DAG was constructed from the root nodes identified in Table 5, based on successful transition through the qualitative acceptance criteria (Table 2). Once this exercise had been completed, the expert panel agreed that the end state of the research was to determine the *probability that ammonium nitrate would be diverted for use within an IED*, and through belief updating, whether a focus on specific causalities would reduce that probability. Based on the root causalities identified, the expert panel began to consider how these root issues could be

depicted visually. It was important to identify common issues to some, to identify cross-over, and if any could be subsequently eliminated. For example, the GTI considered specific issues relating to terrorism, which mainly influenced security concerns within the focus groups, whilst idealism (commonly associated with terrorism) was a motivator of willingness to support illicit diversion because of social and tribal ties. As such, the DAG was consolidated into three generic non-root nodes based on focus group feedback, specifically SECURITY (S), WILLINGNESS (W) and AVAILABILITY (A). Whilst this may seem simplistic, the greatest difficulty was defining what was meant by each non-root node so that data could be manipulated correctly.

The expert panel defined: security risk as the *likelihood that current supply chain security protocols cannot inhibit illicit diversion*; willingness as *the likelihood that those with access to ECP will actively and knowingly support the process of illicit diversion*; and availability of supply risk as *the volume of annual trade in an ECP to a particular country based on legitimate need*.

The inter-relationships are shown in Figure 4-1 .

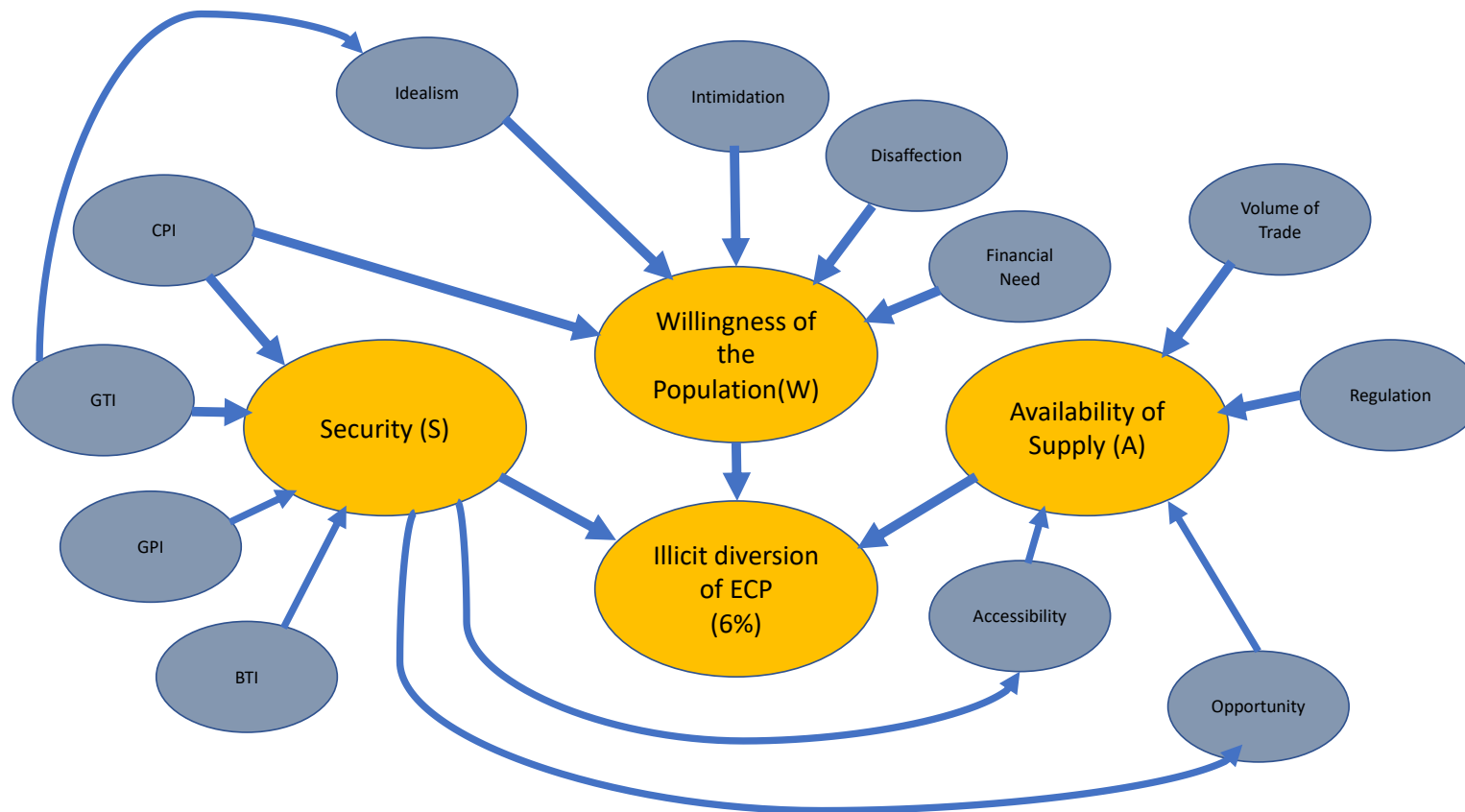


Figure 4-1: Suggested DAG for ECP diversion

It should be noted that the responses surrounding matters of security dove-tailed (for the most part) with the academic research conducted by the CPI, GTI, GPI and BTI. As such, the expert panel assessed that the statistical information provided within these indices for the state in question chimed with the views of the focus groups. Where there was a degree of cross-over, this was not ignored, with the expert panel linking nodes of common interest within the DAG. As can be seen, the willingness of the population was predominantly driven by human factors, with a degree of cross-over from the CPI and GTI. Again, the expert panel agreed that it was appropriate to capture the cross-over so that the basic model of probabilities could be refined as part of further work.

4.5.4.2 Establishing Root Probabilities

A DAG such as this requires the generation of conditional probabilities for several multi-parent nodes, whereby adjustment to S, W and A influences the degree of diversion. For this research, the initial degree of diversion was set as 6.3% for ammonium nitrate, based on use compared to volume of annual trade over 4 years. Given that this research is introductory, the expert panel set probabilities of diversion associated with the non-root nodes to High, Medium and Low, using the framework as shown in Table 4-6. For example, the GTI ranks Afghanistan and the United Kingdom as HIGH and LOW respectively, since the weighted average on the impact of terrorism in those countries returns scores of 0.91 and 0.477, respectively.

The input from focus groups relating to the root causalities in Table 4-5 was considered similarly. Based on this hypothesis, a reduction in the figure of 6.3 % ammonium nitrate used in IEDs would be expected over time if specific causalities were funded and acted upon. This approach mirrors the methodology associated with supply chain security risk assessment [238], suggesting that future research synergies may be possible.

Table 4-6: Probabilities associated with DAG

<i>Probability</i>	<i>BTI</i>	<i>CPI</i>	<i>GTI</i>	<i>GPI</i>
<i>High</i>	>0.7	>0.7	>0.7	>0.7

Medium	>0.5	>0.5	>0.5	>0.5
Low	<0.5	<0.5	<0.5	<0.5

4.5.4.3 Security Risk

The methodologies and results of the latest BTI, CPI, GTI and GPI indices all demonstrate that the case-study country should be set at HIGH for security risk. This is due to the levels of corruption within the security forces, significant economic instability, and the absence of effective governance and the rule of law (see Table 4-7).

Table 4-7: Diversion probabilities associated with indices relating to security

<i>Root Node</i>	<i>Impact</i>
<i>Bertelsmann Stiftung</i>	HIGH (>0.7)
<i>Corruption Perception Index</i>	HIGH (>0.7)
<i>Global Terrorism Index</i>	MEDIUM (>0.5)
<i>Global Peace Index</i>	MEDIUM (>0.7)

Given the considerable cost of security investment, the expert panel considered that supply chain security investment in conflict-affected states would do little to influence the illicit diversion of ECP. Therefore, it could be excluded from a DAG until such a time that BTI, GTI, CPI, and GPI index scores realised a return of < 0.7 in terms of 5-year weighted averages. For example, the United States has provided just under one billion dollars of security assistance in recent years [239], and the UN Security Council indicates two hundred million dollars in development assistance to ports and security infrastructure since 2017. There has been very little security improvement in that time, with the state remaining in a similar position on the indices year-on-year. As such, there has been little impact on improvements to governance, the rule of law or the economy. Therefore, is there any point in throwing more money at security relationships associated with ECP

when greater impact may be achieved in other areas? A trade-off is required, but evidence must be gathered to determine how that trade-off should be applied. It is hoped that belief updating will provide that evidence.

4.5.4.4 Willingness to Support

Initial conditional probability is determined from the consultations conducted relating to the root nodes of economics (the need to provide for the family), idealism, intimidation, corruption, and disaffection. Again, each root node is split into HIGH, MEDIUM and LOW based on the number of focus groups who responded. For example, if seven or more focus groups raised the issue of idealism as a problem in terms of illicit diversion, then the impact would be set as HIGH. If less than five focus groups raised the issue, then the impact would be set at LOW. During consultations, the following conditional probabilities were obtained (see Table 4-8):

Table 4-8: Probabilities associated with willingness

<i>Root Node</i>	<i>Impact</i>
<i>Economics (need)</i>	HIGH (>0.7)
<i>Idealism</i>	LOW (<0.5)
<i>Intimidation</i>	LOW (<0.5)
<i>Corruption</i>	MEDIUM (>0.5)
<i>Disaffection</i>	LOW (<0.5)

As can be seen above, it is the provision for family within this research that is by far the most significant contributor to ECP diversion, with >70% of focus groups citing this. For example, contributors to some focus groups had not received government salaries for over 12 months and had been required to turn to 'dark' network income streams to support the family. Coercion, intimidation, and targeted violence as incentives to carry out ECP diversion were not as dramatic as the research had anticipated, yet continue to drive the thought processes for international interventions within that state [240].

These findings would suggest that the international focus for C-IED in this state should be weighted towards salary incentivisation as opposed to security. Whilst efforts are made to do this, the majority are short-term and target specific community areas such as education [241], not those within the supply chain.

4.5.4.5 Availability of Supply

Again, community focus groups played a considerable part in determining the causal probabilities in this area, with the following attributes (Table 4-9):

Table 4-9: Probabilities associated with availability of supply

<i>Root Node</i>	<i>Impact</i>
<i>Volume of Supply (kg)</i>	HIGH (>500000)
<i>Regulation</i>	MEDIUM (>0.5)
<i>Accessibility</i>	LOW (<0.5)
<i>Opportunity</i>	HIGH (>0.7)

For supply volume, chemicals were only prioritised if they are on the PGS list [115]. Prioritisation is based on whether they are readily available (HIGH), moderately available (MEDIUM) or have minimal availability (LOW) within a country. For this paper, probabilities were based on the available annual volume of chemicals within OECD countries as follows: less than 1000 kg (LOW); more than 10,000 kg (MODERATE); and above 500,000 kg (HIGH)⁵.

Improvements to regulation are dependent upon its presence and an understanding of it. Six focus groups had never heard of a precursor chemical or its intended subversive use, let alone received any training in regulatory practice

⁵ The data within OECD reports can be accessed for public research with permission.

for those in supply chain employment. It was considered unlikely that many would recognise AN beyond a broad understanding of its agricultural use.

Focus group outcomes demonstrated that accessibility and opportunity are influenced by security. However, focus groups believed that opportunity (specifically insiders) instead of general accessibility drove diversion. Although fertilisers such as ammonium nitrate, urea, and potassium nitrate were openly sold in markets, they were not exposed in quantities sufficient to support such industrial-scale IED manufacture. This was being conducted 'somewhere' following a diversion within the national supply chain. Chemicals did enjoy a degree of security within ports (even if stored out in the open). However, the specific issue was a lack of training of security officials to know what was entering or leaving a facility, understanding who the end-user was, and how policing on route to the end-user, or once in the end-user's hands, could be managed.

4.5.5 Establishing the Final Bayesian Network

Based on the expert panel deliberations over security, and its short-term irrelevance given the limited return on investment, the final DAG was approved (see Figure 4-2), with the associated probabilities highlighted from focus group findings at Table 4-7, Table 4-8 and Table 4-9. Belief updating can now be conducted through Bayesian network analysis as more information becomes available to governance and rule of law programmes.

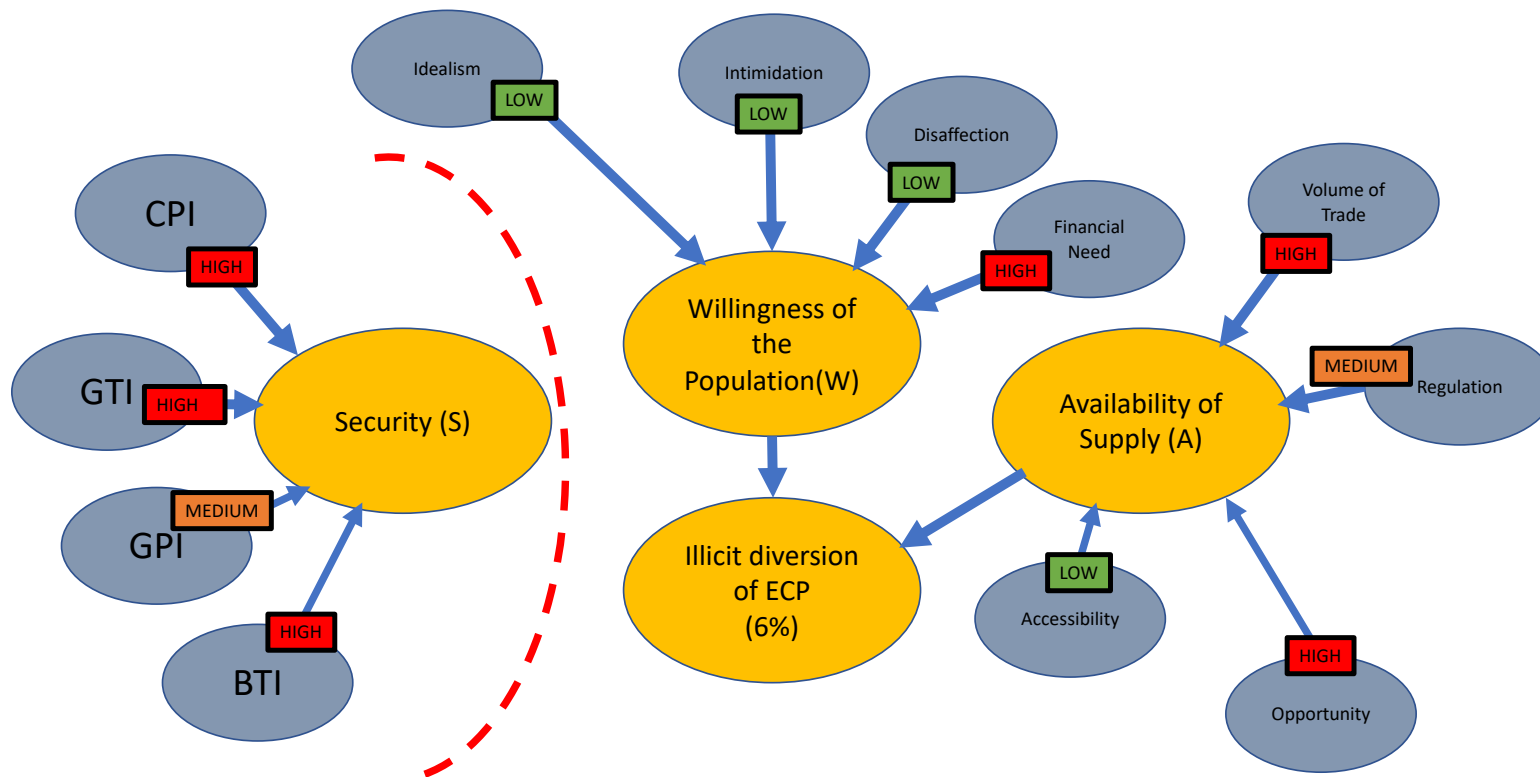


Figure 4-2: Revised DAG with associated probabilities

In this instance, the DAG and its associated probabilities highlight that the impetus for C-IED interventions concerning ECP should rest on reducing the willingness of the population to facilitate diversion through financial incentivisation, or reducing the volume of annual trade in ammonium nitrate. Addressing the financial need of a population is undoubtedly within the gift of donor governments as an economic recovery initiative, most likely centred on those professions with access to the supply chain initially. However, reducing the annual trade volume of fertilizer is difficult in a country experiencing significant food instability. Improvement can be achieved through substitution of ammonium nitrate with lesser potent fertilisers (such as urea), standardisation of nitrogen content from the supplier, increasing awareness of regulation, or reducing the opportunity for acquisition beyond the point of delivery if substitution and standardisation are not acceptable. If urea were a viable alternative for example, then effective risk and risk management would also require similar regulation for nitric acid [178], which is vital in the manufacture of urea nitrate explosives [50, p. B296].

4.6 Conclusion

In conflict-affected states, C-IED approaches are often initiated at the request of state or international governments. It is shaped by the interests of leaders rather than being guided by a consultative process to assure the security needs of communities. Damage assessment is, therefore, challenging to verify within any military and humanitarian C-IED response. This paper has used the concept of Bayesian networks to identify the causal factors behind the illicit diversion of a supply chain commodity (ECP), and offers a start point from which to progress belief updating. The methodology could be applied to any part of the C-IED process, military or humanitarian, thereby refining cost-benefit analysis and resource mobilisation.

Whilst a DAG has been established around ECP diversion within a state, it stops at anything further than establishing the most basic conditional probabilities that could inform more appropriate strategic interventions. The DAG proposes that

people and their motives form the most vulnerable element of the network, and that increased investment in security would do very little to improve the situation.

This is not obvious to international C-IED approaches within the state under study, and the application of belief updating in specific areas could return higher rewards.

In this research the willingness of the population to support the illicit diversion of commodities would seem to be the principal societal turning point, suggesting that resolution to the financial burden imposed on those areas of society with access to the supply chain should be pursued. International regulation on ECP exists within the context of availability but can be challenging to implement during conflict, or where food insecurity is a significant consideration. It suggests that the most appropriate place to apply mitigation is through consistent regulation and standardisation of ECP (or their substitution with less useful chemicals) at the point of manufacture, not at the point of delivery, since this is hugely costly to police when the rule of law is fragile. Such an approach would reduce the burden on overstretched resources attempting to apply mitigation within already compromised supply chains.

5 Calculating the Heat of Explosion (Q) for non-ideal explosives

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[Manuscript under publication – Propellants, Pyrotechnics and Explosives]

5.1 Abstract

Non-ideal explosives are typically highly porous, low-density heterogeneous materials. They differ from ideal explosives in that fuel and oxidiser are separated at the molecular level. As such, non-ideal explosives demonstrate lower detonation pressures and velocities than ideal explosives and more extended detonation reaction zones. These longer detonation reaction zones produce higher heat of explosion due to secondary and tertiary combustion reactions occurring behind the detonation front.

Since non-ideal explosives are increasingly used as homemade explosives (HME), it is often challenging to determine likely performance without detailed chemical analysis, or an understanding of loading density, critical diameter, and stoichiometry. Detailed analysis is not an option in security-related settings where preservation of life and property is often challenged by time.

Using Hess' Law of enthalpy, and empirical and quantitative thermochemical methods to determine the products of detonation, this paper introduces a simple method to determine the heat of explosion of any non-ideal explosive composition during three specific stages: anoxic detonation; anaerobic combustion; and aerobic combustion. The values calculated compare favourably to heats of explosion for non-ideal explosives published in open-source literature, suggesting that the approach can be developed into a user-friendly application for first responders.

5.2 Introduction

In the decade preceding COVID-19, non-ideal explosives were used in 43% of deliberate acts of explosive violence in Europe [143], with the United Kingdom, France and Spain having accounted for over 65% of such attacks [242].

Identification of explosive chemical precursors (ECP), which may be incorporated within an improvised explosive device (IED), can be hugely problematic for first responders and the public [243]. The choice of ECP available to criminals is broad, given the limited regulation applied to some energetic compounds [178]. As such, first responders across the international arena may be required to apply rapid judgement on the explosive performance of HME compositions. This is because of the overriding philosophy to preserve life, preserve property and return situations to normality within sensible timeframes [79] [16]. Judgement has been based on the knowledge of more conventional homogeneous explosives, not the heterogeneous nature of criminal compositions, with evacuation distance based on a bare charge mass equivalent of TNT [244] [245].

However, many non-ideal explosive compositions, particularly those based on nitrate esters, can be much more powerful than TNT [246] [247] and are relatively simple to synthesise [34] [248], suggesting that greater refinement of safety distance may be necessary [249]. The Geneva International Centre for Humanitarian Demining (GICHD) recently published an approximate comparison of non-ideal explosive performance based on functional groups to assist the humanitarian demining community – see Figure 5-1: TNTe of typical non-ideal explosive compositions (QV) © BCL Ltd [64]. This graphical representation clearly shows the dominance of nitrate esters. However, the publication does not identify the precise methodology by which TNT equivalence is measured. As this paper shall demonstrate, such an omission could under or over-estimate performance, leading to safety distance concerns for blast and fragmentation.

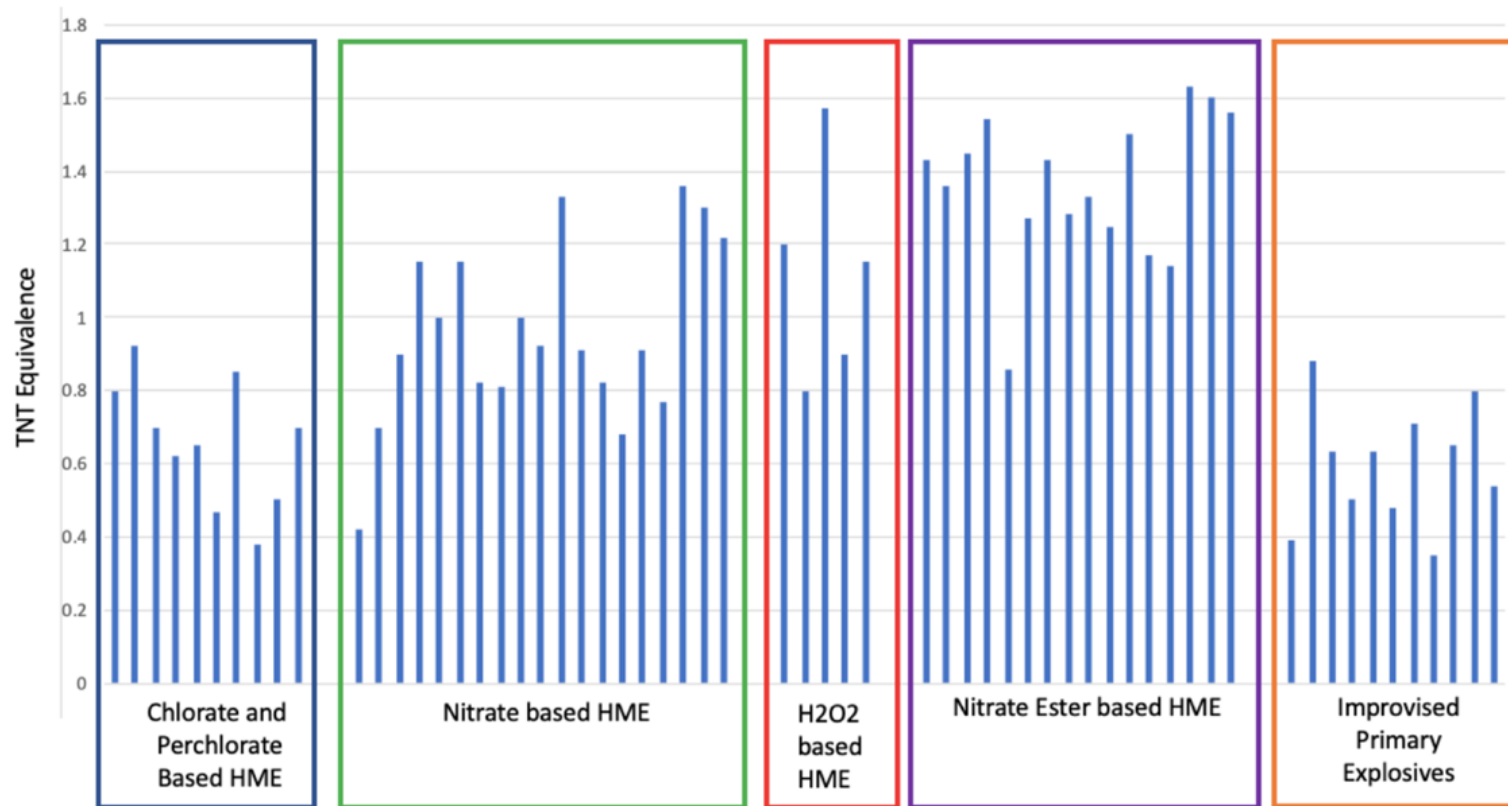


Figure 5-1: TNTe of typical non-ideal explosive compositions (QV) © BCL Ltd

Whilst media attention has often focused on typical non-ideal explosive compositions comprising ammonium nitrate, regulation has improved considerably for the most frequent HME encountered [112]. However, as supply chains become more heavily regulated, other fuels and oxidisers, or multiple mixtures of fuels and oxidisers, will be selected out of necessity and availability – the economics of supply and demand [250]. This has already been witnessed in Afghanistan, where regulation applied to ammonium nitrate led to the prolific use of potassium chlorate [157]. Therefore, such compositions must be assessed quickly and effectively at the point of discovery and based upon available information. This information could be based on intelligence provided to the first responder, on the chemical labels visible at the crime scene, on the physical appearance of partly synthesised or final product, the results of rapid chemical testing (if accessible), witness testimony, or affirmation from technical experts should they be available. The authors conclude that several 'ifs' face a first responder in what can only be described as a particularly challenging environment when timely decision-making is required.

Zeldovich [251], von Neumann [252], and Doering [253] (ZND) explicitly described a one-dimensional model of detonation for ideal explosives, comprising a leading shock front followed by a chemical reaction zone. For ideal explosives, all the potential energy contained within the explosive is released almost instantly in a short reaction zone [254] [255], with the typical ZND model describing the following:

- a vertical shock front (with associated ignition temperature (T_i), detonation pressure (D_p) and density (ρ_o)) within a *CHNO* explosive undergoing detonation;
- induction/reaction zones (where the dissociated molecules of the explosive form the principal products of detonation [24]); and
- a non-driving reaction zone where the products of detonation react with other species.

In this latter non-driving reaction zone, most additives to *CHNO* compositions compete with the gaseous detonation products to increase the heat of explosion

(Q_e) and alter the volume of gaseous products produced [256]. The heat of explosion is therefore driven by the enthalpies of formation of the explosive products ($CO_{(g)}$, $CO_{2(g)}$, $H_2O_{(g)}$, $NO_{2(g)}$ etc) dependent upon explosive composition, oxygen balance and stoichiometry. There is an order of precedence as to which products are formed first [257].

In current literature, the performance of ideal explosives comprising *CHNO* can be determined through the application of empirical and quantitative thermochemical methods published by Kamlet-Jacobs [258], Kistiakowsky-Wilson [257], Springall-Roberts [96] and Cooper [254]. Consideration has also been given to the performance of conventional explosives enhanced with highly reactive atoms such as chlorine, fluorine and aluminium [259], which are therefore non-ideal explosives by definition.

In contrast to the ZND model, non-ideal explosives can be considered to have multiple reaction zones behind the detonation shock front as shown in Figure 5-2, which influence performance. The line *AB* depicts the detonation shock front, with *CD* the point at which reactants are converted to products. The sonic locus depicts the region of the detonation driving zone where energy is released to sustain the shock front. Scott-Stewart and Kasimov [260] describe the sonic locus as an exact balance of heat release (Q) and flow divergence. The flow speed behind this region is sonic relative to the shock front and is therefore part of the non-driving reaction zone. As such, energy release is slower, detonation pressures lower, with a lack in oxygen balance being a contributory factor.

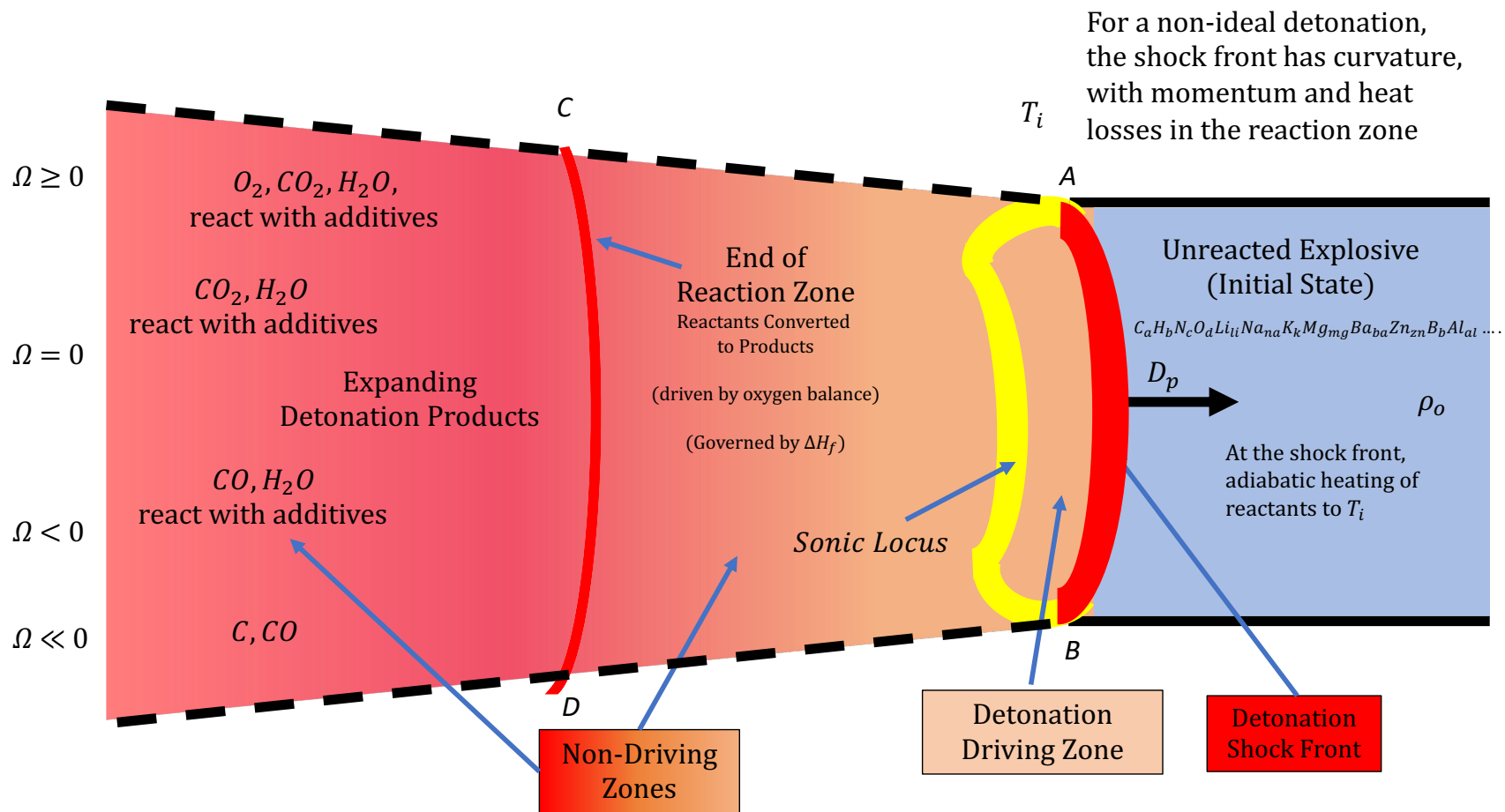


Figure 5-2: Schematic of detonation reaction zones in a non-ideal explosive

For example, in the case of a *CHNO* explosive such as *TNT* and *RDX*, the denotation velocity is typically proportional to the heat of explosion (*Q*), meaning that the higher the value of *Q*, the greater the denotation velocity [254] [24] [261]. However, this is not true for non-ideal explosives. Adding aluminium powder increases the heat of explosion [262], which is dominated by mass diffusion and conduction [263]. At the same time, the detonation velocity is decreased because of the endothermic effect of the aluminium powder during the primary reaction stage [264]. Whilst the aluminium does not react in the C-J plane (it is essentially an inert component), it generates high thermal loading [265] and produces an extended pressure pulse [266] when it reacts with the gaseous products of the detonation. The smaller the particle size (increasing surface area) and the nearer the approach to stoichiometry (the proportions where elements or compounds react fully with one another), the higher the heat of explosion [267]. However, if too much fuel is added, as can often be the case with HME, or the particle size of additive is too large, this detracts significantly from the detonation velocity to the extent that detonation may not occur at all [256] [268].

As such, one would expect non-ideal explosives comprising of finely powdered fuels or metal flakes, and oxidisers with excess oxygen, to have a lower detonation velocity than their homogeneous counterparts [260], but release significant energy upon detonation in a three-stage process outlined below (see Table 5-1).

Table 5-1: Energy release sequence in an explosive energised by aluminium

Stage	Event	Timescale	Reference
1	Anoxic Detonation – heat is produced from the '<i>detonation driving zone</i>' as the shock front dissociates explosive molecules. No apparent temperature rise from ignition temperature (T_i) is observed until the detonation products form. The heat of explosion (Q_e) can be calculated based on the molecular composition of the non-ideal explosive and Hess' law [269], regardless of the physical charge structure. The explosion products e.g. $CO_{(g)}$, $CO_{2(g)}$, and $H_2O_{(g)}$ are first produced from the active radical species, based on thermochemistry and oxygen balance. Additives do not participate in this highly exothermic reaction zone and act as an inert material, even absorbing and consuming part of the heat liberated, thereby reducing the total energy of the detonation wave. A drop in the detonation pressure (D_{cj}/D_p) denotes this.	The induction zone can take as little as 0.1 ns to dissociate the explosive into radical species. The reaction zone for ideal explosives such as HMX and TNT ranges from 20 – 80 ns.	[24] [257] [270] [271]

Stage	Event	Timescale	Reference
2	Anaerobic Combustion – the explosion products produced in Stage 1 then react with additives under the high temperature and pressure environment behind the C-J plane. Dependent upon the combustion products, the heat of explosion increases at the expense of gas volume. For metal explosives, the major products that liberate heat other than water, carbon monoxide and carbon dioxide can be metal carbonate, metal hydride, metal hydroxide, metal nitrate, metal nitride, and metal oxide.	10's to 100's of μ s.	[257] [268] [272]
3	Aerobic Combustion – if any additives remain within the non-ideal explosive after anaerobic combustion finishes, reactions then take place with oxygen in the atmosphere. It is assumed that full combustion takes place with atmospheric oxygen over a period of ms, and that this thermal energy release does not contribute to mechanical work, but rather the additional heat energy available to interact with the environment.	10's of ms	[268] [273] [274] [275] [276]

The energy release in Stages 1 and 2 represent the amount of energy available for the explosive to perform mechanical work on the surroundings, whilst Stage 3 contributes to additional thermal energy that the explosive could deliver over a period of ms (excess fuel and atmospheric oxygen dependent). Therefore, substance identification and an understanding of energy release are significant to the first responder, not least because of the mechanical work that the explosive can inflict on the surroundings (such as blast overpressure, impulse and fragmentation), but also potential thermobaric injuries caused during the aerobic combustion phase

5.3 Method

This paper reviews open-source approaches used to determine the oxygen balance and heat of explosion of ideal and non-ideal explosive compositions. It has sought clarification from organisations such as Fraunhofer Institute for Chemical Technology (ICT) to determine that existing modelling tools do not establish the detonation products for multiple HME formulations [277].

Based on the methods devised by Kistiakowsky-Wilson, Springall-Roberts, Kamlet-Jacobs, Keshavarz and Cooper [254] [258] [257] [96], this paper offers a generic chemical equation to predict the heat of explosion (Q_e) and TNT equivalence ($TNTe$) for any non-ideal explosive that may take the form of Equation 1:



This equation considers not only current HME formulations where regulation is applied [44] but also those formulations that may be devised as supply chains become constrained [64] [249] [278]. Typical compositions could therefore contain any number of the fuels and oxidisers listed in Table 5-2:

Table 5-2: A generic list of ECP that could be used in HME manufacture (© BCL Ltd)

Precursor Chemicals	Fuels		Oxidizers (including valence)
Acetic acid Acetone Ascorbic acid Citric acid Erythritol Ethylene glycol Glycerol/glycerine Hexamine Hydrazine Hydrochloric acid Hydrogen peroxide (dilute or concentrated) Methanol Methyl ethyl ketone Nitric acid Nitrobenzene Nitromethane Pentaerythritol Perchloric acid Phenol Sodium azide Sulphuric acid Urea	Organic: Artificial creamer Aviation fuel Black pepper Charcoal Cinnamon Cocoa Cotton Cumin Dextrin Diesel Flour Honey Icing sugar Kerosene Napthalene Paraffin wax Powdered milk Sawdust Shellac Sugar Tang Vaseline	Inorganic: Aluminium Antimony trisulphide Barium Iron oxide Lithium Magnesium powder Magnalium powder (Mg/Al) Phosphorous Potassium Sodium Sulphur Zinc powder	Chlorate salts (Na+, K+) Hypochlorite salts (Ca2+, Na+) Hydrogen peroxide (CHP) Metal peroxides (Ba2+, Na+) Nitrate salts (Ba2+, Ca2+, K+, NH4+, Na+) Ca2+NH4+ (CAN)) Perchlorate salts (Na+, NH4+, K+) Potassium permanganate Nitrites (Na+, K+)

TNTe has been chosen as the comparator, given its doctrinal use in energetic performance on land [279] and at sea [280] for over a century. However, it is acknowledged that *TNTe* for high and low explosives depends on the measurement method, and errors exceeding 30% are typical [281]. This is a significant margin for the first responder in terms of blast, fragmentation, safety distance, or indeed the thermal energy available to inflict quaternary physical injury [276]. For example, the values of *TNTe* for ideal and non-ideal explosives identified by the ballistic mortar test [282] are entirely different to that proposed by other methods such as peak overpressure/positive impulse [283] and the Trausl sand-crush test [284]. As such, it is essential to standardise the measurement by which any calculator operates, and base measurement upon theoretical and/or experimental literature findings. For this paper, the reference used is the heat of explosion under constant volume conditions (Q_v) where data for some non-ideal compositions in kJkg^{-1} can be found for Stage 1 and 2 reactions [247] [285] [286]. A comparison of Q_e (the heat of explosion calculated for those Stage 1 and 2 reactions) is then conducted against Q_v (the reference value) to determine accuracy. The potential thermal energy from any Stage 3 reaction is not calculated in this paper since it does not contribute to the mechanical work available to the explosion products [268].

TNTe for each explosive is then calculated as follows (see equation 5-2), with Q_{tnt} taken as 4091.6 kJkg^{-1} from literature [96, p. 99]:

$$TNT_e(\text{kJkg}^{-1}) = \left(\frac{Q_e}{Q_{tnt}} \right) \quad (5-2)$$

A 4-step process is then applied to the methodology, as can be seen in Table 5-3, with worked examples to underpin the theory at Appendices:

Table 5-3: Outline Method

STEP	Description
1. The establishment of a baseline programme in excel	As this is a proof of concept, an excel spreadsheet is constructed to determine oxygen balance (Ω) and heat of explosion for ideal compositions comprising empirical formula $CHNO$. The molar proportions of each atom in one gram of explosive are established to determine Q_e from Hess' Law. Kistiakowsky-Wilson and modified Kistiakowsky-Wilson rules are used as the primary vehicle to develop the likely products of detonation based upon the proportion(s) of fuel(s) and oxidiser(s) and detonation theory. The spreadsheet values are then interrogated against known literature values of Q_v for those ideal explosives to determine baseline accuracy of Q_e and Ω calculations. Comparison of Q_e/Q_v should be unity.
2. Derivation of formula for non-ideal explosives	A formula is then devised for the heat of explosion for non-ideal compositions, which could take any form from Equation (5-1). This formula is then tested against the molecular formulae for the ideal $CHNO$ explosive compositions examined in Step 1 to ensure that the values of Q_e and Ω obtained are identical. If this is not the case, then the formula in Step 2 is fundamentally flawed. Assumptions are clearly articulated to facilitate understanding and to influence refinement/automation of future models.
3. The introduction of powdered metals	Since so much literature is available on aluminium as an additive, aluminium is then introduced to the revised non-ideal explosive formula for TNT and ammonium nitrate (AN) compositions. This is to gain confidence in the thermochemical calculations. The oxygen balance and heat of explosion are then calculated and compared against

STEP	Description
	open-source literature values using the energy release sequence in Table 5-1. Results of Q_e are compared to Q_v values reported in literature. Values of TNT_e are then calculated using Equation (5-2).
4. The introduction of varied fuel and oxidiser mixtures	Non-ideal explosives of varied molecular composition are then interrogated with Q_e/Ω compared to open-source literature values. This step determines that the calculator can manipulate explosive compositions containing multiple fuels and oxidisers with confidence.

5.4 Assumptions

Given the complexity of thermochemical reactions during detonation and combustion, several assumptions underpin calculations. These assumptions are outlined in Table 5-4 to provide a simplistic baseline for the proof of concept.

Table 5-4: Assumptions

Assumption	Description
1.	Atoms want to achieve their highest oxidation state, which is also their lowest internal energy state. This means that the products of detonation of $C_aH_bN_cO_d$ explosives will strive to form $CO_{2(g)}$ and $H_2O_{(g)}$, dependent upon available oxygen (Kistiakowsky-Wilson and modified Kistiakowsky-Wilson rules apply).
2.	Additives do not react with $CO_{(g)}$, $CO_{2(g)}$ or $H_2O_{(g)}$ until those products of detonation have been formed from the active radicals.
3.	That there is sufficient hydrogen in the non-ideal explosive to bind <i>Cl</i> , <i>Br</i> , <i>I</i> and <i>F</i> to <i>HF</i> , <i>HCl</i> , <i>HI</i> , <i>HBr</i> etc
4.	The model assumes that more reactive elements of the non-ideal explosive compound form detonation products based on the hierarchy of the heats of reaction [257]. Additive oxidation will therefore commence with those detonation products with the highest enthalpies of formation. For example, $Al_{(s)}$ will compete with $CO_{2(g)}$ before it will progress to $H_2O_{(g)}$ and $CO_{(g)}$ to form $Al_2O_{3(s)}$. And, although $S_{(s)}$ and $Hg_{(l)}$ can have differing valence ($S=2,4$ and 6 , $Hg = 1, 2$) the most favourable energy states such as $SO_{2(g)}$ ($\Delta H_f -296.1 \text{ kJmol}^{-1}$) and $HgO_{(s)}$ ($\Delta H_f -90.7 \text{ kJmol}^{-1}$) would be considered by the calculator.

Enthalpies of formation used for calculation are listed in Table 5-5. Unless stated otherwise, all enthalpies are provided to one decimal place. These enthalpies provide a measure of the relative thermochemical stabilities of the molecules, intimately related to their structures [287]. For example, carbon dioxide displays

greater thermal stability than carbon monoxide, and aluminium oxide displays greater thermal stability than barium oxide. Values for Q_e and Q_v are presented as kJkg^{-1} and kJmol^{-1} .

Table 5-5: Enthalpies of formation used in calculations.

Species	Phase	Empirical Formula	Enthalpy of Formation ΔH_f (kJmol^{-1})	References
Aluminium	Solid	Al	0.0	Enthalpies of formation used for calculations in this paper are taken from literature [254], [96], [288], [289], [290], [291], [292] [293, p. 469] [294] [66]
Aluminium Oxide	Solid	Al_2O_3	-1669.8	
Ammonium Nitrate	Solid	NH_4NO_3	-365.3	
Barium	Solid	Ba	0.0	
Barium Nitrate	Solid	$\text{Ba}(\text{NO}_3)_2$	-988.0	
Barium Oxide	Solid	BaO	-558.1	
Baratol	Solid	$\text{C}_{0.028}\text{H}_{0.02}\text{N}_{0.013}\text{O}_{0.026}\text{Ba}_{0.00038}$	-295.0	
Carbon	Solid	C	0.0	
Carbon Dioxide	Gas	CO_2	-393.5	
Carbon Monoxide	Gas	CO	-110.5	
Diesel	Liquid	$\text{C}_{12}\text{H}_{23}$	-355.9	Equations refer to the phase of each compound (solid, liquid or gas). For example, where H_2O is quoted, this means $\text{H}_2\text{O}_{(g)}$, not $\text{H}_2\text{O}_{(s)}$ or $\text{H}_2\text{O}_{(l)}$.
Hydrogen	Gas	H_2	0.0	
Hydrogen Chloride	Gas	HCl	-92.3	
Hydrogen Flouride	Gas	HF	-268.6	
Hydrogen Peroxide	Liquid	H_2O_2	-187.6	
Lead Azide	Solid	$\text{Pb}(\text{N}_2)_3$	468.6	
Nitrogen	Gas	N_2	0.0	
Nitroglycerine	Liquid	$\text{C}_3\text{H}_5\text{N}_3\text{O}_9$	-370.7	
Paraffin Wax	Liquid	$\text{C}_{25}\text{H}_{52}$	-2460.5	

Species	Phase	Empirical Formula	Enthalpy of Formation ΔH_f (kJmol ⁻¹)	References
PETN	Solid	C ₅ H ₈ N ₄ O ₁₂	-530.5	
RDX	Solid	C ₃ H ₆ N ₆ O ₆	+70.3	
TATP	Solid	C ₉ H ₁₈ O ₆	-151.18	
TNT	Solid	C ₇ H ₅ N ₃ O ₆	-62.1	
3-NT	Liquid	C ₇ H ₇ NO ₂	-31.5	
Water	Gas	H ₂ O	-241.8	
Wood Meal	Solid	C ₅₀ H ₇₂ O ₃₃	-945.8	

5.5 Results and Discussion

5.5.1 Derivation of baseline programme in Excel to determine oxygen balance and heat of explosion– STEP 1:

The equation for a $C_aH_bN_cO_d$ explosive oxygen balance can be seen in Equation (5-3), which is widely published in literature [96]. The letters in subscript (a , b , c , and d) refer to the total number of atoms of carbon, hydrogen, nitrogen and oxygen in each molecule of explosive. The contribution of nitrogen (c) to the oxygen balance is zero, since nitrogen does not bind to the other elements, and is therefore absent from calculation:

$$\Omega = 15.999 \times \frac{(d - 2a - b/2)}{\text{molecular weight}} \times 100\% \quad (5-3)$$

Considering Equation 1, many fuels can be added to a $CHNO$ explosive, such as *Al, B, Ba, Ca, Cl, F, K, Li, Mg, Mn, Na, Pb, Hg, S* and *Zn*. Each will behave in its own unique fashion. To determine the oxygen balance for such non-ideal compositions, the following principles of chemistry are considered, based on the oxidation-reduction reactions described in Table 5-1 and the enthalpies of formation that accompany the reactions (ΔH_f in kJmol⁻¹):

1. Since *C* is oxidised to CO_2 , each *C* atom requires $2\text{O} = 2a$: ΔH_f -393.5
2. Since *H* is oxidised to H_2O , each *H* requires $\text{O}/2 = b/2$: ΔH_f -241.8
3. Since *N* goes to N_2 , there is no need of oxygen = $c \times 0 = 0$: $\Delta H_f = 0.0$
4. Since *Al* oxidises to Al_2O_3 , each *Al* requires $3\text{O}/2 = 3a/2$: $\Delta H_f = -1669.8$
5. Since *B* oxidises to B_2O_3 , the same argument for *Al* applies $3b/2$: $\Delta H_f = -1263.6$
6. Since *Ca* oxidises to CaO , each *Ca* requires one $\text{O} = \text{Ca}$ - $\Delta H_f = -635.5$
7. Since *Mg* oxidises to MgO , each *Mg* requires one $\text{O} = \text{Mg}$: $\Delta H_f = -601.8$
8. Since *Na* oxidises to Na_2O , each *Na* requires $0.5\text{O} = \text{Na}/2$: $\Delta H_f = -416.0$
9. Since *K* oxidises to K_2O , each *K* required $0.5\text{O} = \text{K}/2$: $\Delta H_f = -363.2$
10. Since *Zn* oxidises to ZnO , each *Zn* requires one $\text{O} = \text{Zn}$: $\Delta H_f = -348.0$
11. Since *S* oxidises to SO_2 , each *S* requires $2 \text{O} = 2\text{S}$: $\Delta H_f = -296.1$
12. Since the oxidation number for *H* and *F* are +1 respectively, each *F* requires one *H*, thereby reducing $\text{H}_2/\text{H}_2\text{O}$ by $0.5 = -\text{F}/2$: $\Delta H_f = -286.6$
13. Since the oxidation number for *H* and *Cl* are +1 respectively, each *Cl* requires one *H*, thereby reducing $\text{H}_2/\text{H}_2\text{O}$ by $0.5 = -\text{Cl}/2$: $\Delta H_f = -92.3$
14. Since the oxidation numbers of *H* and *Br* are +1 respectively, each *Br* requires one *H*, thereby reducing $\text{H}_2/\text{H}_2\text{O}$ by $0.5 = -\text{Br}/2$: $\Delta H_f = -36.2$
15. Since the oxidation numbers of *H* and *I* are +1 respectively, each *I* requires one *H*, thereby reducing $\text{H}_2/\text{H}_2\text{O}$ by $0.5 = -\text{I}/2$: $\Delta H_f = +26.5$

This approach is consistent with thermochemical code methodologies used to predict the detonation velocity of organic, inorganic and mixed explosives, whereby the more reactive elements of the explosive compound (those with the higher enthalpies) react first, and form detonation products based on the hierarchy of the heats of reaction [257].

The establishment of the baseline programme in excel from these principles was based on the manipulation of explosive compositions within Equation 3, using the appropriate Kistiakowsky-Wilson conditions. This step is not shown, as examples

of calculations using Equation (5-3) are widely published [96]. The next step is to derive the oxygen balance formula for non-ideal explosives.

5.5.2 Derivation of Non-Ideal Oxygen Balance Formula – STEP 2

From recent research at Cranfield University [178], only certain ECP are considered for HME manufacture and predictive analysis can determine future trends [113]. As such, Equation (5-1) constitutes the principal fuel and oxidiser compositions that could be readily encountered within geographical supply chains. The products of detonation and combustion depend very much on the oxygen balance of the explosive composition and the Kistiakowsky-Wilson and modified Kistiakowsky-Wilson conditions. It is therefore important to understand the role of constituent atoms within the explosive molecule during anoxic detonation and anaerobic combustion. The following examples demonstrate the effect of oxygen balance within an explosive as detonation occurs, using known explosive compositions to derive the formula.

5.5.3 Example 1. When the explosive is hugely oxygen deficient

When the amount of oxygen within the explosive molecule $C_aH_bN_cO_d$ is much less than carbon ($d \leq a$, or $O \leq C$), then $C_{(s)}$ will dominate the products of detonation, dependent upon the oxidation reactions between $CO_{(g)}$ and $H_{2(g)}$:

$$\therefore \text{explosion products} \rightarrow \frac{c}{2}N_2 + dCO + (a - d)C + \left(\frac{b}{2}\right)H_2 \quad (5-4)$$

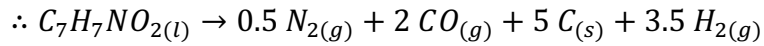
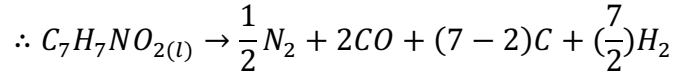
To determine if this is correct, consider the liquid explosive 3-nitro-toluene (3-NT), with molecular structure $C_7H_7NO_{2(l)}$. Using Equation (5-3), 3-NT has an oxygen balance of:

$$\Omega = 15.999 \times \frac{(d - 2a - b/2)}{\text{molecular weight}} \times 100\%$$

$$\therefore \Omega = 15.999 \times \frac{(2 - 14 - 3.5)}{137.14} \times 100\%$$

$$\therefore \Omega = -180.8\%$$

3-NT would require 8.75 additional $O_{2(g)}$ to form $CO_{2(g)}$ and $H_2O_{(g)}$, which means it is hugely oxygen deficient (-181%) [288]. Using the Kistiakowsky-Wilson rules [96], which state that carbon atoms would be oxidised to carbon monoxide first based on such a negative oxygen balance (>-40%), the products of detonation for an ideal explosive using Equation (5-4) would be as follows, which is consistent with literature [295]:



However, if those atoms in Group 7 of the Periodic Table with a valance of -1 were introduced to 3-NT (such as *F*, *Cl*, *Br*, and *I*) then, based on the assumptions in Table 5-4, these atoms would naturally compete with hydrogen in the detonation reaction zone [257] and the products would become:

$$\frac{c}{2}N_2 + fHF + clHCl + brHBr + iHI + dCO + (a-d)C + \left(\frac{b-f-cl-br-i}{2}\right)H_2 \quad (5-5)$$

Note 1: *a*, *b*, *c*, *d*, *f*, *cl*, *br* and *i* denote the number of atoms present within the molecular formula for explosive $C_aH_bN_cO_dF_fCl_{cl}Br_{br}I_i$. Note 2: All molecular weights from the periodic table are shown to two decimal places.

5.5.3.1 Example 2 - When the amount of oxygen exceeds that of carbon

When the amount of oxygen exceeds that of carbon, but the explosive remains oxygen deficient, then there will be insufficient oxygen to go beyond the formation of carbon monoxide and water. The following condition describes this relationship:

$$O > CO \text{ and } H_2O > O - CO \quad (5-6)$$

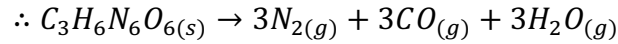
$$\therefore d > a \text{ and } \left(\frac{b-f-cl-br-i}{2}\right) > d-a \quad (5-7)$$

To determine if this is correct, consider *RDX*, with the molecular formula $C_3H_6N_6O_6(s)$. The detonation products favour a less negative oxygen balance than

3-NT (-21.6%). As such the products of detonation take the following form, which is consistent with literature and the Kistiakowsky-Wilson rules [96]:

$$\frac{c}{2}N_2 + aCO + (d - a)H_2O + \left(\frac{b}{2} - (d - a)\right)H_2 \quad (5-8)$$

$$\therefore \frac{6}{2}N_2 + 3CO + (6 - 3)H_2O + \left(\frac{6}{2} - (6 - 3)\right)H_2$$



If those atoms in Group 7 of the Periodic Table with a valance of -1 were to be added to *RDX* (such as *F*, *Cl*, *Br*, and *I*), thereby creating non-ideal conditions, then these atoms would naturally compete with hydrogen and the detonation products would become:

$$\frac{c}{2}N_2 + fHF + clHCl + brHBr + iHI + aCO + (d - a)H_2O + \left(\frac{b-f-cl-br-i}{2} - (d - a)\right)H_2 \quad (5-9)$$

5.5.3.2 Example 3 - When the explosive oxygen balance tends towards zero

In the situation where oxygen remains in excess of that required to compete in the formation of carbon monoxide and the products of hydrogen (such as H_2O and HF etc), but there is no excess of oxygen in the post-reaction phase, then carbon monoxide will oxidise to carbon dioxide. Such conditions are met when:

$$O \geq CO + H_2O \text{ but } O \leq CO_2 + H_2O \quad (5-10)$$

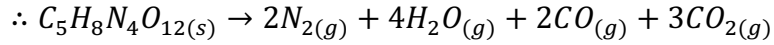
$$\therefore d \geq a + \left(\frac{b - f - cl - br - i}{2}\right) \text{ but } d \leq 2a + \left(\frac{b - f - cl - br - i}{2}\right) \quad (5-11)$$

The oxygen balance becomes even less negative and tends towards zero, where the Kistiakowsky-Wilson rules dictate an ever-increasing presence of $CO_{(g)}$, $H_2O_{(g)}$ and $CO_{2(g)}$.

To determine if this is correct, consider *PETN* with the molecular formula $C_5H_8N_4O_{12(s)}$ (oxygen balance -10%). The products of detonation can be determined as follows, which equates well with literature [96] [257]:

$$\frac{c}{2}N_2 + \left(\frac{b}{2}\right)H_2O + \left(a - \left(d - a - \frac{b}{2}\right)\right)CO + \left(d - a - \frac{b}{2}\right)CO_2 \quad (5-12)$$

$$\therefore \frac{4}{2}N_2 + \left(\frac{8}{2}\right)H_2O + \left(5 - \left(12 - 5 - \frac{8}{2}\right)\right)CO + \left(12 - 5 - \frac{8}{2}\right)CO_2$$



If those atoms in Group 7 of the Periodic Table with a valance of -1 were to be added to *PETN* (such as *F*, *Cl*, *Br*, and *I*), then these atoms would naturally compete with hydrogen and the detonation products would become:

$$\begin{aligned} \frac{c}{2}N_2 + fHF + clHCl + brHBr + iHI + \left(\frac{b-f-cl-br-i}{2}\right)H_2O \\ + \left(2a-d + \frac{b-f-cl-br-i}{2}\right)CO \\ + \left(d-a - \frac{b-f-cl-br-i}{2}\right)CO_2 \end{aligned} \quad (5-13)$$

5.5.4 Example 4 - When an oxygen surplus is evident within the explosive.

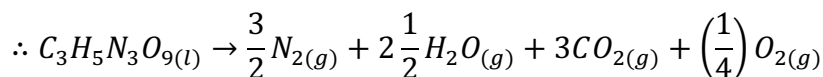
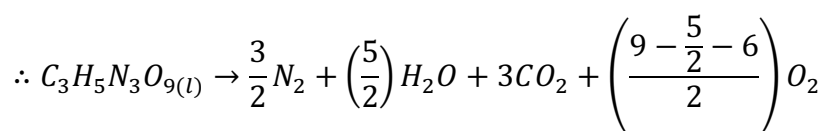
In a situation where there is an abundance of oxygen in the explosive such as nitroglycerine *NG* ($C_3H_5N_3O_9(l)$) then unused oxygen remains after the production of carbon dioxide and water. This is described by the condition:

$$O > CO_2 + H_2O \quad (5-14)$$

$$\therefore d > 2a + \left(\frac{b-f-cl-br-i}{2}\right) \quad (5-15)$$

The products of detonation would comprise $O_{2(g)}$, $H_2O_{(g)}$ and $CO_{2(g)}$ as follows [96]:

$$\frac{c}{2}N_2 + \left(\frac{b}{2}\right)H_2O + aCO_2 + \left(\frac{d - \frac{b}{2} - 2a}{2}\right)O_2 \quad (5-16)$$



If those atoms in Group 7 of the Periodic Table with a valance of -1 were to be added to *NG* (such as *F*, *Cl*, *Br*, and *I*), then these atoms would naturally compete with hydrogen and the detonation products would become:

$$\begin{aligned} \frac{c}{2}N_2 + fHF + clCl + brBr + il + \left(\frac{b - f - cl - br - i}{2}\right)H_2O + aCO_2 \quad (5-17) \\ + \left(\frac{2d - b + f + cl + br + i}{4} - a\right)O_2 \end{aligned}$$

Therefore, the valance of atoms in a non-ideal explosive containing some, or all the atoms annotated in Equation (5-1) can determine the overall products of detonation for a non-ideal explosive. The above process can be repeated for atoms within each Group of the Periodic Table, and mixtures containing atoms across multiple Groups.

5.5.5 Derivation of overall oxygen balance for a non-ideal explosive.

Examples 1 – 4 demonstrate the impact of Group 7 atoms on oxygen balance and products of detonation for ideal explosives. A similar situation applies to Groups 1 – 6, as shown in Table 5-6:

Table 5-6: Group and Valence Entry Points

Group Valence	Remarks
1 and 7 (Valence ± 1)	<i>K</i> , <i>Na</i> , <i>F</i> and <i>Cl</i> are highly reactive and possess valance +1/-1 respectively. This is therefore the entry point for atoms with valance +1/-1

Group Valence	Remarks
2 and 6 (Valence ± 2)	<i>Ca</i> , <i>Mg</i> and <i>O</i> are valances +2/-2 respectively. This is therefore the entry point for atoms with valance +2/-2
3 (Valence ± 3)	<i>Al</i> and <i>B</i> require 3/2 oxygen (valance 3). This is therefore the entry point for metals with valence +3/-3
4 (Valence ± 4)	<i>C</i> requires two oxygen atoms to achieve their preferred energy state (valence 4). This is therefore the entry point for HME compositions containing atoms with valance +4/-4

As such, the basic oxygen balance equation for an ideal explosive (Equation 3) can be refined according to the atomic composition of *O*, *C*, *H*, *N*, *Li*, *Na*, *K*, *F*, *Cl*, *Mg*, *Ba*, *Zn*, *Al*, *B*, *Pb*, *Sr*, *Br*, *I* as follows:

$$\therefore \Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} - \frac{Li}{2} - \frac{Na}{2} - \frac{K}{2} + \frac{F}{2} + \frac{Cl}{2} + \frac{Br}{2} + \frac{I}{2} - Mg - Ba - Zn - Sr - \frac{3Al}{2} - \frac{3B}{2} - 2Pb}{molecular\ weight} \right) \times 100 \quad (5-18)$$

This then provides the generic formula for oxygen balance for HME compositions as follows:

$$\therefore \Omega = \frac{15.999 \left(d - 2a - \frac{b}{2} + (2 \sum Valence(\pm 4) + \frac{3}{2} \sum Valence(\pm 3) + \sum Valence(\pm 2) + \frac{1}{2} \sum Valence(\pm 1) + \dots) \right)}{molecular\ weight} \times 100 \quad (5-19)$$

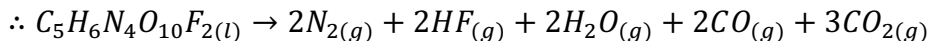
Note 3: *F*, *Cl*, *Br* and *I* atoms are positive values in the equation above since they compete with the hydrogen in water, thereby releasing oxygen from the water. Atoms such as *C*, *H*, *Mg*, *Li*, *Na* and *Al* attract a negative value in the equation because they compete for oxygen within the molecule.

5.5.6 Example 5 – Determining the detonation products of bisflourodinitroethyl formal (FEFO) and PBX 9407 (94/6 RDX/Exon 461).

In this example, *Cl* and *F* are introduced to the composition of a *CHNO* explosive. Detailed calculations can be found in Appendix A, with only the results highlighted in the main text.

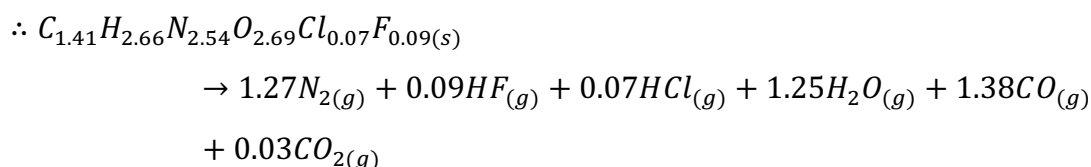
Consider *FEFO* with the molecular formula $C_5H_6N_4O_{10}F_{2(l)}$ and molecular weight 320.12 g. As the explosive is non-ideal, theory dictates that Equation (5-18), not Equation (5-3), should be considered to determine oxygen balance. This equation calculates the oxygen balance for *FEFO* to be -9.99%

The following products of detonation can then be determined from Example 3 (Equation (5-13)), where the conditions for a slightly negative oxygen balance are established:



The oxygen balance and products of detonation support reported literature values [289].

Consider *PBX 9407* with molecular formula $C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09(s)}$ and molecular weight 102.42 g [259]. Again, the explosive is non-ideal. One would therefore anticipate the oxygen balance and products of detonation to be based on Equations (5-12) and (5-18). Calculations at Appendix B realise an oxygen balance of -21.58%, with the following products of detonation determined:



5.5.7 Comparison of homogeneous and binary compositions, with Q calculated from Hess' Law – STEP 3

Using Equation (5-1) and Equation (5-19), Table 5-7 provides the calculated values of oxygen balance (Ω) and heat of explosion (Q_e) for ideal and binary non-ideal explosives compositions. These are compared with published literature values of heat of explosion at constant volume (Q_v).

AN/AI (88/12) is provided as the worked example at Appendix B.

Table 5-7: Literature and formula values for Q and oxygen balance for ideal and non-ideal explosives

Explosive	Literature Values			Formula Values		
	Q_v (kJmol^{-1})	Ω	Reference	Q_e (kJmol^{-1})	Ω	$\left(\frac{Q_e}{Q_v} \times 100\%\right)$
TNT	-929.34 (-4091.63) ⁶	-73.90	[96]	-929.30	-73.90	100.00
RDX	-1127.36 (-5075.50)	-21.60	[96]	-1118.90	-21.60	99.25
RDX/TNT (60/40)	-1057 (-4684)	-42.60	[96]	-1057	-42.60	100.00
NG	-1414.40 (-6228.46)	+3.50	[96]	-1414	+3.50	99.99
TNT/AI (80/20)	-756.36 (-5275)	-67.60	[247]	-786.60	-67.60	104.00
AN/AI (88/12)	-319.50 (-4934)	+6.92	[286]	-325.15	+6.90	101.80

⁶ Figures in (parenthesis) denote literature values for Q_v in kJkg^{-1} .

AN/Al (88/12) is a composition with a positive oxygen balance of +6.92% [286]. As such, it should follow the process described in example 3 where a CHNO explosive would tend towards the formation of $N_{2(g)}$, $O_{2(g)}$, $H_2O_{(g)}$ and $CO_{2(g)}$. However, in this example, there is no carbon present so the products of detonation would tend towards $N_{2(g)}$, $H_2O_{(g)}$ and $Al_2O_{3(s)}$. The empirical formula by molar quantities within 1g is therefore determined from calculation at Appendix B as:

$$H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447(s)} \quad (5-20)$$

Following the stages and assumptions described in Table 5-4, the aluminium competes with the detonation products formed, in this case $H_2O_{(g)}$ and any excess oxygen remaining after formation of the detonation products. The heat of explosion for this reaction is then determined from Hess' Law (5-21), with enthalpy values taken from Table 5-5:

$$\Delta H_{reaction}^{\theta} = \sum \Delta H_{f(products)}^{\theta} - \sum \Delta H_{f(reactants)}^{\theta} \quad (5-21)$$

The total heat of explosion produced during this process is shown in Table 5-8, along with the products of detonation at each stage:

Table 5-8: Reaction sequence for AN/Al (88/12)

Process	Products of Detonation	Q _e (kJkg ⁻¹)	Q _e (kJmol ⁻¹)
Stage 1	$H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447}$ $\rightarrow 0.010994 N_2 + 0.021988 H_2O + 0.005497 O_2$ $+ 0.004447 Al$	-1300	
Stage 2	$0.021988H_2O + 0.005497 O_2 + 0.004447 Al$ $\rightarrow 0.002224 Al_2O_3 + 0.022027 H_2O$ $+ 0.002160 O_2$	-3720	

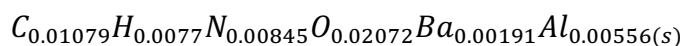
Totals	$H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447(s)}$ $\rightarrow 0.010994 N_{2(g)} + 0.022027 H_2O_{(g)}$ $+ 0.00216 O_{2(g)} + 0.002224 Al_2O_{3(s)}$	-5020	-325.15
$\left(\frac{Q_e}{Q_v}\right) \times 100\% = \frac{5020}{4934} \times 100\% = 101.8\%$			
$\left(\frac{Q_e}{Q_{tnt}}\right) \times 100\% = \frac{5020}{4091} \times 100\% = 122.7\%$			

From these results the calculator determines the accuracy for AN/Al (88/12) as 101.8% against the heat of explosion (Q_v) reported in literature.

5.5.8 Comparison of HME compositions comprising more complex mixtures, with Q calculated from Hess' Law – STEP 4

Following success of the valence formula with simple compositions, more complex interactions were interrogated against open-source literature values for Q_v . The example used in calculation is Baronal, a ternary mixture comprising barium nitrate, TNT, and Al (50/35/25).

Calculations at Appendix C identify the molecular formula for this non-ideal explosive to be:



As such, the oxygen balance for Baronal can be determined as -23.92% using Equation (5-19). There is therefore insufficient oxygen to produce $CO_{2(g)}$ and $H_2O_{(g)}$ during anoxic detonation (Stage 1). And, since barium and aluminium are inert '*passengers*' during that initial stage, they become major liberators of heat in the formation of their metal oxides during the anaerobic stage (Stage 2). Therefore, the products of detonation and heat of explosion can be determined from Equation (5-12) as (Table 5-9):

Table 5-9: Reaction sequence for Baronal

Process	Products of Detonation	Q _e (kJkg ⁻¹)	Q _e (kJmol ⁻¹)
Stage 1	$C_{0.01079}H_{0.0077}N_{0.00845}O_{0.02072}Ba_{0.00191}Al_{0.00556}$ $\rightarrow 0.004225 N_2 + 0.00385 H_2O + 0.00471 CO$ $+ 0.00608 CO_2 + 0.00191 Ba + 0.00556 Al$	-1837	
Stage 2	$0.0042 N_2 + 0.00385 H_2O + 0.00471 CO + 0.00608 CO_2$ $+ 0.00191 Ba + 0.00556 Al$ $\rightarrow 0.0042 N_2 + 0.00385 H_2O + 0.00471 CO$ $+ 0.000955 CO_2 + 0.005125 C + 0.00191 BaO$ $+ 0.00278 Al_2O_3$	-3675	
Totals	$C_{0.01079}H_{0.0077}N_{0.00845}O_{0.02072}Ba_{0.00191}Al_{0.00556(s)}$ $\rightarrow 0.004225 N_{2(g)} + 0.005125 C_{(s)}$ $+ 0.00385 H_2O_{(g)} + 0.00471 CO_{(g)}$ $+ 0.000955 CO_{2(g)} + 0.00191 BaO_{(s)}$ $+ 0.00278 Al_2O_{3(s)}$	-5512	-611.17
$\left(\frac{Q_e}{Q_v}\right)$	$\left(\frac{5512}{4767}\right) \times 100\%$	114%	
$\left(\frac{Q_e}{Q_{tnt}}\right)$	$\left(\frac{5512}{4091}\right) \times 100\%$	135%	

These values demonstrate an identical prediction of oxygen balance and Q_e within 14% of Q_v for baronal (-4767 kJkg⁻¹ [296] [285, p. 34]).

Table 5-10 shows the results obtained for seven further published non-ideal compositions and one lead-based composition (lead azide), which carries no oxygen within its molecular structure. A simple traffic light system depicts Q_e lying within 10% Q_v (GREEN), and those lying within 20% (AMBER). The common name for each explosive is annotated where known.

Table 5-10: Comparison of Non-Ideal Explosive Heats of Explosion to Literature

Explosive	Literature		Products of Detonation (to 5.S.F.)	Ω	Q_e (kJkg ⁻¹)	$\left(\frac{Q_e}{Q_v}\right)$
	(Q _v)	Ref.				
ANFO (96/4) (Diesel C ₁₂ H ₂₃)	-3950	[297]	$C_{0.00287}H_{0.05347}N_{0.02399}O_{0.03598}$ → 0.01199 N _{2(g)} + 0.02674 H ₂ O _(g) + 0.00287 CO _{2(g)} + 0.00175 O _{2(g)}	+5.61	-4438.5	1.12 (112%)
AN/Al (60/40)	-8866	[256]	$H_{0.02998}N_{0.01499}O_{0.02249}Al_{0.01483(s)}$ → 0.00750 N _{2(g)} + 0.00025 H ₂ O _(g) + 0.01474 H _{2(g)} + 0.00741 Al ₂ O _{3(s)}	-23.6	-9683.1	1.09 (109%)
ANFO/Al (92/5/3)	-4328	[298]	$C_{0.00359}H_{0.05285}N_{0.02299}O_{0.03448}Al_{0.00111(s)}$ → 0.01149 N _{2(g)} + 0.00039 C _(s) + 0.02642 H ₂ O _(g) + 0.00320 CO _{2(g)} + 0.00056 Al ₂ O _{3(s)}	-1.25	-4304.8	0.99 (99%)
Barium Nitrate/TNT (10/90) – Baratol	-4029	[299, p. B268]	$C_{0.02774}H_{0.01981}N_{0.01265}O_{0.02607}Ba_{0.00038(s)}$ → 0.00633 N _{2(g)} + 0.01636 C _(s) + 0.00991 H ₂ O _(g) + 0.00698 CO _(g) + 0.00440 CO _{2(g)} + 0.00038 BaO _(s)	-63.50	-4652.7	1.15 (115%)

Explosive	Literature		Products of Detonation (to 5.S.F.)	Ω	Q_e (kJkg ⁻¹)	$\left(\frac{Q_e}{Q_v}\right)$
	(Q _v)	Ref.				
AN/TNT/NG (70/25/5) Donarite	-3559	[293]	$C_{0.00555}H_{0.04438}N_{0.02263}O_{0.03573(s)}$ → 0.01132 $N_{2(g)}$ + 0.02219 $H_2O_{(g)}$ + 0.00555 $CO_{2(g)}$ + 0.00122 $O_{2(g)}$	+3.91	-3773.4	1.06 (106%)
AN/TNT/AL (40/40/20) – Minol 2	-6782	[296, p. 8]	$C_{0.01233}H_{0.02880}N_{0.01528}O_{0.02556}Al_{0.00741(s)}$ → 0.00764 $N_{2(g)}$ + 0.00117 $C_{(s)}$ + 0.00330 $H_2O_{(g)}$ + 0.01116 $CO_{(g)}$ + 0.00371 $Al_2O_{3(s)}$ + 0.01112 $H_{2(g)}$	-39.38	-6900.1	1.02 (102%)
KClO ₃ /Vaseline (90/10) - Cheddite	-4961	[299, p. C157]	$C_{0.00572}H_{0.01190}O_{0.02203}K_{0.00734}Cl_{0.00734(s)}$ → 0.00155 $KClO_{3(s)}$ + 0.00595 $H_2O_{(g)}$ + 0.00572 $CO_{2(g)}$ + 0.00580 $KCl_{(s)}$	+7.42	-5913.9	1.19 (119%)
Lead Azide (PbN ₆)	-1610	[96] [66]	$Pb_{0.00172}N_{0.0206(s)} \rightarrow 0.00172 Pb_{(s)} + 0.01030 N_{2(g)}$	-5.49	-1609.0	1.00 (100%)

Table 5-11 provides further calculation relating to 3 non-ideal compositions encountered by first responders [143] where literature reference on performance is not readily available. Whilst these results are merely speculative, they suggest that the calculator can provide rapid determination of HME performance in a security-related setting. The common names for compositions are annotated where known.

Table 5-11: Performance of non-ideal compositions without literature reference

Explosive	Products of Detonation (to 5.S.F.)	Ω	Q_e (kJkg ⁻¹)	$\left(\frac{Q_e}{Q_{TNT}}\right)$
H ₂ O ₂ /Sawdust (80/20) Concentrated Hydrogen Peroxide (CHP)	$C_{0.00833}H_{0.05903}O_{0.05253}$ $\rightarrow 0.02951 H_2O_{(g)}$ $+ 0.00833 CO_{2(g)}$ $+ 0.00318 O_{2(g)}$	+10.19	-5842.9	1.43
Sodium Chlorate/Nitrobenzene (72/28) (CO-OP Explosive)	$C_{0.01365}H_{0.01137}N_{0.00227}O_{0.02484}Na_{0.00676}Cl_{0.00676(s)}$ $\rightarrow 0.00114 N_{2(g)} + 0.00814 CO_{(s)}$ $+ 0.00569 H_2O_{(g)} + 0.00551 CO_{2(g)}$ $+ 0.00676 NaCl_{(s)}$	-13.01	-4904.1	1.12
AN/TATP/Al (85/5/10)	$C_{0.00203}H_{0.04653}N_{0.02124}O_{0.03321}Al_{0.00371(s)}$ $\rightarrow 0.01062 N_{2(g)}$ $+ 0.02326 H_2O_{(g)}$ $+ 0.00185 Al_2O_{3(s)}$ $+ 0.00203 CO_{2(g)}$	+0.54	-4057.0	1.00

The values of Q_e obtained from the valence formula in Table 5-10 present a ‘worst case’ situation for the first responder and differ (in some instances) from literature due to the enthalpies of formation chosen for the more complex hydrocarbons such as fuel oil, woodmeal, vaseline and paraffin wax. These values were scarcely found, yet are necessary for the critical evaluation of data. For example, if the formula for fuel oil is taken as $C_{18}H_{38(l)}$, then the enthalpy of formation for

this hydrocarbon (-378 kJmol^{-1} [300]) improves the accuracy of *ANFO/AI* calculations to 104%.

Additionally, barium is understood to continue energetic reactions well behind the shock front, where only a percentage of its oxygens react with carbon [301]. As such, it is reasonable to determine that experimental literature values for Baronal and Baratol may always be lower than those calculated in these examples since the equation of state considers optimum conditions.

Loading density, critical diameter, porosity, particle size, confinement and homogeneity of oxidiser/fuel mixing, are also of huge importance in any effective calculation of explosive performance, since each aspect plays a role in the deflagration to detonation (DDT) transition [260]. For example, if density and critical diameter are below certain values for any explosive then DDT cannot progress [302]. However, some explosive compositions can behave in a unique fashion. For example, compositions comprising TNT may experience decreasing critical diameters with increasing density (and increasing detonation velocity with loading density), whilst others such as ammonium nitrate may exhibit the opposite effects [303]. Therefore, a focus on the thermochemistry within this model does mitigate significant ‘unknowns’ associated with HME manufacture, thereby calculating the worst-case conditions for the first responder. It removes the complexity of Chapman-Jouget detonation velocities and simplifies the thermochemistry behind driving and non-driving detonation reaction zones. Indeed, if the complexity of detonation velocity (D) were required, then perhaps it could be predicted from the Q_e values obtained in Stages 1 and 2 of the detonation process, and using the equation of state for D and Q proposed by Kamlet-Jacobs [258] and Cooper [254].

Finally, the standard enthalpy of formation is pivotal in thermochemistry. The accuracy of calculations could be improved using a rotating bomb calorimeter for the types of fuels used in non-ideal explosive compositions. Examples of this would be ground coffee (used in the 7/7 bombings in London [304]), or the type of diesel commonly found in fuel stations. However, combustion calorimetry is hugely difficult to conduct since the precision in experimentation needs to be $\pm$

0.01-0.02% to have an uncertainty in an enthalpy of formation of $\pm 1 \text{ kJ mol}^{-1}$ [287]. Additionally, non-ideal compositions containing sulphur or halogens would require specific testing conditions given the highly erosive nature of the gaseous products. Therefore, it may be prudent to simply consider those fuels with the lower enthalpy values if the precise detail of the hydrocarbon (for example) cannot be determined.

5.6 Conclusion

The heat of explosion of non-ideal explosives has been historically difficult to model due to the significant departure of highly non-ideal detonations from idealised one-dimensional wave propagation. A simple method has been introduced for predicting the heat of explosion for both $C_aH_bN_cO_d$ explosives, and explosives comprising mixtures of organic, inorganic and organometallic compounds. This method is useful to the first responder since an in-depth knowledge of the chemical or thermochemical properties of explosives is not required. Compared to TNT equivalence criteria published in literature, this procedure combines accuracy and simplicity to predict the performance of a wide range of energetic materials based on the valence of the atoms that exist within any composition, and at what stage reactions take place. The model also allows the thermal energy release sequence to be predicted under ideal conditions should there be excess fuel in the composition and sufficient atmospheric oxygen to contribute to quaternary blast injuries.

Variance from reported literature does exist, but at a scale much reduced from other methods of TNT equivalence (no more than $\pm 15\%$ in examples as opposed to $\pm 30\%$). This variance is a consequence of the unpredictable chemistry accompanying non-ideal detonations within the detonation and non-detonation reaction zones (for example the role of barium nitrate in Baratol and Baronal), or the enthalpies of formation that are chosen for complex hydrocarbons or polymers such as vaseline, diesel and sawdust. This paper demonstrates that the variance tends towards over-compensation, which from a risk and risk management perspective would be considered as low as reasonably practical.

As such, the valence equation can be used to determine the risk posed by HME as part of predictive performance analysis, therefore allowing evacuation distance for blast and fragmentation to be accurately determined. A general equation for approximate HME performance for a first responder can therefore be developed as a hand-held Application, providing timely levels of assurance whilst more complex interventions follow behind.

6 Understanding the explosion risk presented by ammonium nitrate and aluminium home-made explosives detonated as surface charges in hexahedral main charge containers

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[Manuscript undergoing publication in Journal of Shock Waves]

6.1 Abstract

Ammonium nitrate and aluminium (AN-Al) has been used as a typical homemade explosive (HME) by non-state actors since the turn of the century. Despite the regulation applied to ammonium nitrate above 16 % nitrogen content and an aluminium particle size below 200 μm , their use has been widespread in Afghanistan, Columbia, Iraq, Syria and Yemen. Containers used to utilise AN-Al as a man-portable improvised explosive device (IED) are typically hexahedral in shape, not the spherical or hemispherical geometries used to theorise risk mitigation. This is particularly important in post-blast investigation where explosives of a non-ideal nature are often used in non-spherical containers.

Given the breadth of HME available to criminals, the explosion performance of forty (40) hexahedral containers filled with AN-Al of unknown manufacture is examined. Performance of the AN-Al is determined through the surface detonation of these containers on alluvial soil, with apparent crater volume compared to theoretical calculations for spherical charges of TNT detonated in that same medium. A conversion factor for hexahedral main charges to spherical charges is then established to achieve more accurate predictions of the explosion risk using Kingery-Bulmash and Bowen curves. The paper provides worked examples for practical application and a methodology by which predictions of charge mass in other mediums such as asphalt can be determined.

6.2 Introduction

The prolific use of ammonium nitrate (AN) within man-portable improvised explosive devices (IEDs) has recently undergone literature review [178] [113],

with aluminium (Al) as a metallic fuel rising in ascendance since the turn of the century in conflict-affected states such as Afghanistan, Columbia, Iraq, Syria and Yemen [305] [60] [158]. The addition of Al to AN is of significance, given its ability to make AN more sensitive to detonation than other types of AN-based HME, such as AN and fuel oil (ANFO) [306]. For example, the addition of Al to AN at a certain percentage and particle size is reported to reduce critical diameters from 60 mm to 20 mm, with detonation velocities above 3850 ms^{-1} achieved [307].

Whilst regulation does apply to both AN (above 16% nitrogen content) and Al (below a particle size of $200 \mu\text{m}$) [110], the United Nations General Assembly (UNGA) is now focusing on the regulation of ECP used to manufacture HME [308], since supply chains continue to facilitate their amalgamation into viable IEDs [113]. As such, HME performance poses a significant challenge to the scientific community given their non-ideal nature [309], relative ease of manufacture [14], and simplicity of placement [16]. Therefore, it is of great importance to understand the explosive power of such compositions to increase knowledge of their effects on people and structures and to represent that knowledge within recognised blast terminology such as Friedlander Blast Waves [310], Scaled Distance [311] [312], Pressure-Time curves [313] [314] [315] and TNT equivalence (TNT_e) [316].

Most historical data for blast in air examines the criteria surrounding a surface (or near surface) detonation of spherical or hemispherical charges [315], and does not consider containment. However, most IEDs comprising AN-Al utilise everyday hexahedral explosive charge containers, such as HDPE jerrycans, palm oil and water carriers (see **Figure 6-1**). Their use as a man-portable explosive device is purely ergonomic – they must be easy to carry, easy to conceal, and simple to place. Less exposure during emplacement means less chance of being caught [317]. As such, IEDs are often found lying horizontally on the surface (if command-activated) or buried just beneath the surface (if victim-activated) [318]. Open-source military counter-IED literature also refers to HME containers of hexahedral form as the most widely used in recent conflicts of Western interest [319].



Figure 6-1: Examples of Containers Used in Trial © BCL & Artios Global

Limited instrumentation within conflict-affected states makes scientific measurement of explosive performance and determining the composition of HME difficult. Therefore, a significant amount of information is lost to risk managers when practical measurement, such as crater size and volume from controlled detonations of confiscated items, would be an appropriate methodology to calculate TNTe of actual compositions, not those made for small-scale trials. As such, crater formation is a suitable tool to study blast phenomena, the explosive properties of different HME, and their impact upon soil and geological strata under such stress [320] when technology is the limiting factor.

However, the physics of crater formation is complicated and relates to the dynamic physical properties of soil, the medium in contact with the soil (such as air or water), the soil-medium interface, and the position of the explosive charge relevant to the soil-medium interface [321]. For even the most carefully performed cratering experiments, there can be deviations in dimension measurements in the region of 10%, up to as much as 40% [322]. As such, large sample sizes are

necessary to reduce margins of error and improve coefficients of determination (R^2). It is also desirable to perform trials where similarities in soil type to previous academic work exists; this provides consistency. This paper therefore considers 40 surface firings of AN-AI main charge compositions confiscated during security operations in alluvial soil (a soil medium commonly reported in cratering literature).

6.3 Literature Review

The most recent papers relating to surface explosions of spherical charges have been published by Ambrosini [323], P Cooper [324], Nagy [325] and Adushkin [326]. These trials were built on the considerable work conducted by H Cooper in alluvial soil during the Cold War [327]. However, the only publication that addresses non-spherical surface charges is that of Bjelovuk [328], who conducted numerous trials using hexahedral charges on asphalt. No literature on other soil types using hexahedral charges, or where a comparison to spherical charges has been attempted, can be identified by the authors of this paper.

Those historic crater trials derive a specific formula for crater dimension based on charge geometry and proximity to the soil surface (buried, surface or near-surface). For example, Westine [329], Rickman et al [330], Payne et al [331] and Luccioni [321] [332] have focused upon deriving formulae to determine crater size for buried charges, whilst the works of Cooper [327] and Kinney & Graham [315] focus on the surface or near surface.

To facilitate a useful trial of this nature, there must be commonality in reference data. As such, the formation of a crater from a surface explosion (and its measurement) must be described to obtain consistent and usable data. The crater dimensions defined by Kinney & Graham [315] and Cooper [324] are therefore used in this paper (see Figure 6-2), where D [m] represents the apparent crater diameter (that which can be seen in the post-blast phase), D_r [m] the actual crater diameter (that which cannot be seen), and H_2 [m] the apparent depth of the crater (another visible measurement).

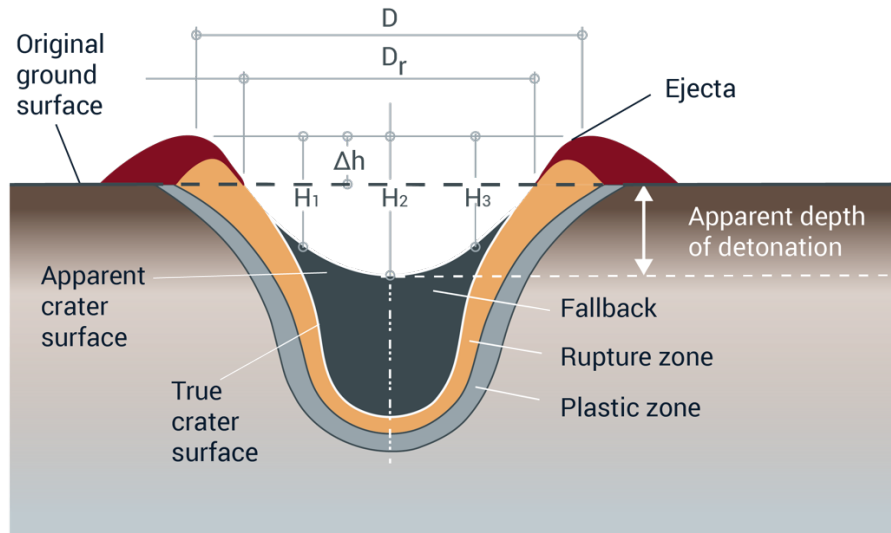


Figure 6-2: Crater Dimensions Considered During Trial © Cranfield University

The formulae of interest to this paper are described in Table 6-1 and have been derived over 50 years from the crater methodology described at Figure 6-2. Sometimes expressed as W in equations, M refers to the explosive mass of *TNT* in [kg], V_a is the apparent crater volume [m^3], D is the apparent diameter [m], D_r the actual diameter [m], E_{CR} the cratering efficiency for the soil type [324], and P_k the area of hexahedron (length x height [$L \times H$]) of the charge in direct contact with the soil surface [m^2] [328]:

Table 6-1: Empirical Formulae Available for Crater Calculations

<i>Author</i>	<i>Soil Type</i>	<i>Charge Shape</i>	<i>Charge Position</i>	<i>Empirical Formula</i>	<i>Equation Number</i>
<i>Ambrosini [323]</i>	<i>Various</i>	<i>Spherical</i>	<i>Surface</i>	$D = 0.51M^{1/3}$	(6-1)
<i>Bjelovuk [328]</i>	<i>Asphalt</i>	<i>Hexahedral (L:H 1 – 1.5)</i>	<i>Surface</i>	$M = 617.952V_b^{0.794}P_k^{0.309}$	(6-2)
<i>Cooper H [327]</i>	<i>Alluvial Soil</i>	<i>Spherical</i>	<i>Surface</i>	$H_2 = 0.5V_c^{1/3}$	(6-3)
				$R_a = 1.2V_c^{1/3}$	(6-4)
<i>Cooper P [324]</i>	<i>Alluvial Soil</i>	<i>Spherical</i>	<i>Surface</i>	$D = 2K_{alluvium}(2E_{CR}M)^{1/3}$	(6-5)
<i>Kinney & Graham [315]</i>	<i>Various</i>	<i>Spherical</i>	<i>Surface</i>	$D_r = 0.8M^{1/3}$	(6-6)
<i>Adushkin & Khristoforov [326]</i>	<i>Various</i>	<i>Spherical</i>	<i>Surface</i>	$D = 0.606M^{0.34}$	(6-7)
				$V_a = 0.0143M^{1.038}$	(6-8)
				$H_2 = 0.152M^{0.331}$	(6-9)
<i>Nagy [325]</i>	<i>Clay</i>	<i>Spherical</i>	<i>Surface</i>	$D_r = 0.55679M^{1/3}$	(6-10)

These empirical equations achieve relatively consistent results for ideal explosives such as TNT, PETN and TATB. However, limited data exists on non-ideal explosives such as AN-Al under similar circumstances, whose properties can vary dependent upon the nature of the AN and Al used (such as fertiliser grade or technical grade AN, powder or flake aluminium), the booster explosive [333], the stoichiometry of the composition, the loading density applied, the type of confinement [334], moisture ingress and ageing [302] [303].

For example, ANFO is a non-ideal explosive [335] and does not possess the shattering or brisance effect that one would experience from TNT when in direct contact with rock. It possesses a velocity of detonation (v) of 3140 ms^{-1} and explosion energy of 3940 Jg^{-1} [335] as opposed to 6850 ms^{-1} and 4091 Jg^{-1} for TNT [96]). ANFO has a longer detonation reaction zone than TNT, thereby giving up its explosive energy over microseconds as opposed to sub-microseconds [336]. This slower energy release results in much lower detonation pressures (P_c) and therefore less brisance than TNT, which promotes the cracking as opposed to shattering of rock. ANFO also generates a greater gas volume than TNT (980 ml g^{-1} [337] as opposed to 739 ml g^{-1} [96]) thereby creating a 'heave' effect within the medium as the gaseous products of detonation seep into the cracks formed in the soil [310].

The realistic physical properties of unknown HME recovered from security operations, and their ageing, is evident in Figure 6-1. These are the IEDs that terrorists actually build, not benign laboratory grade samples. Recent work by Collett et al [338] also improves understanding of non-ideal explosive behaviours, allowing predictions of TNT_e within 10% for heat of explosion (Q_e). Performance is determined from the following equation relating to oxygen balance and respective heats of formation from Hess' Law:

$$\Omega = \frac{15.999 \left(d - 2a - \frac{b}{2} + (2 \sum \text{Valence}(\pm 4) + \frac{3}{2} \sum \text{Valence}(\pm 3) + \sum \text{Valence}(\pm 2) + \frac{1}{2} \sum \text{Valence}(\pm 1)) \right)}{\text{molecular weight}} \times 100 \quad (6-11)$$

$$\therefore \Omega \Delta H_{reaction}^{\theta} = \sum \Delta H_{f(products)}^{\theta} - \sum \Delta H_{f(reactants)}^{\theta} \quad (6-12)$$

As such, there exists a gap in academic knowledge concerning:

- 1) formulae to predict the size of an explosive charge used based on non-spherical containers;
- 2) how such formulae can be applied to charge position (buried, surface or near surface) and soil medium; and
- 3) risk to life posed by non-ideal explosives confined within non-spherical containers.

This paper aims to address these criteria for surface-laid IED charges recovered and disposed of by humanitarian agencies in a conflict affected state.

6.4 Methodology

Working closely with the United Nations Development Programme (UNDP), 40 hexahedral containers comprising AN-AI of unknown explosive performance recovered from security-led operations, were detonated on an undisclosed demolition area between 18 December 2019 and 21 March 2021. The sample size of containers can be seen in Table 6-2, with the dimensions of each container, and the mass of the explosive filling, shown in Table 6-3.

Table 6-2: Quantity of containers available for trial

<i>Container</i>	<i>Quantity</i>	<i>Comment</i>
5L	10	Intelligence reporting identified AN-AI HME manufactured in bulk, but the precise AN-AI stoichiometry was unknown. 20L containers were by far the most available within the supply chain.
10L	10	
20L	15	
40L	5	

Table 6-3: Container dimensions used for trial

<i>Container</i>	<i>L [m]</i>	<i>W [m]</i>	<i>H [m]</i>	<i>Area [m²] P_k</i>	<i>Volume (m³)</i>	<i>Mass of AN-Al [kg]</i>	<i>H:L ratio</i>
<i>5 L</i>	230	100	270	0.0621	0.00621	7.1	1.17
<i>10 L</i>	226	194	324	0.0732	0.01421	16.3	1.43
<i>20 L</i>	290	240	400	0.1160	0.02784	32.6	1.38
<i>40 L</i>	400	240	580	0.2320	0.05568	65.2	1.45

Where:

- *L*, *W* and *H* [m] represent the length, width and height dimensions of the container;
- *P_k* [m²] represents the area of the container (L x H) laid on the surface of the soil;
- Volume [m³] represents the L x W x H of each container; and
- H:L represents the ratio of H divided by L for each container.

Each container was laid in a configuration typical of their original placement (Figure 6-3) with detonation achieved using a 100 g plastic explosive donor charge (85% RDX, 15% wax) and an Electric Instant detonator (450 mg PETN) at the centre face. Given the limited explosive mass of initiator and donor charge (100.45 g) compared to main charge mass, they are not included in overall NEQ calculations.

The donor charge was placed in the location of the '20' in the figure shown below. This is the intersection of the opposing corner diagonals (the centre of the container face). For safety reasons, no attempt was made to remove the yellow or blue detonating cord within the container cap of any IED, or to use the detonating cord as the means of initiation.

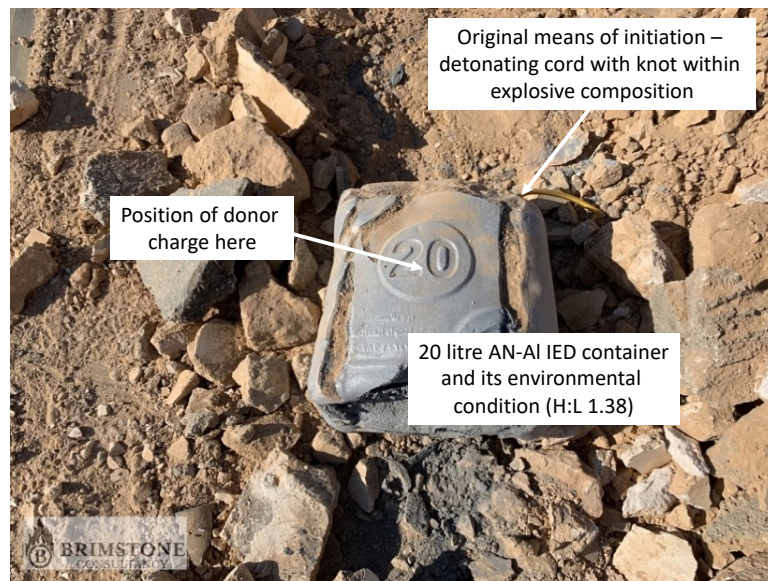


Figure 6-3: Position of Containers on Surface - Representative of a 20L container and its Condition © BCL

The soil type in the experimental area was determined from geological tables as dry compacted alluvial soil. For ethical reasons the precise location is not disclosed. However, the properties of that soil type are shown in Table 6-4, which are similar to those used by Cooper [324] [327], Kinney & Graham [315] and Ambrosini [323] to determine diameter (D), (D_r) radius (R , or $D/2$), and apparent crater depth (H_2) for many hundreds of surface detonations, thereby facilitating an appropriate trial data set.

Table 6-4: Properties of alluvial soil used in trial

<i>Soil Property</i>	<i>Value</i>
<i>Specific Gravity [Gs]</i>	2.6
<i>Minimum Void Ratio</i>	0.48
<i>Maximum Void Ratio</i>	0.91
<i>Maximum Dry Unit Weight [kNm^{-3}]</i>	19.66
<i>Moisture Content [%]</i>	10.66
<i>Liquid Limit [LL%]</i>	Non-Plastic

Plastic Limit [PL%]

Non-Plastic

Cratering Efficiency E_{CR}

0.5

However, it was noted that each hexahedral container produced an elliptical crater, not a hemisphere (see Figure 6-4), which was similar to the findings of Bjelovuk [328] for asphalt. As such, it was necessary to determine the apparent crater diameter (D) and apparent crater volume (V_a) using the following equations, where a and b are the major and minor axes of a semi-ellipse:

$$D = 2 \sqrt{\left(\frac{a}{2} \cdot \frac{b}{2}\right)} \quad (6-13)$$

$$V_a = \frac{1}{2} \cdot \frac{4}{3} \pi \left(\frac{a}{2} \cdot \frac{b}{2}\right) H_2 \quad (6-14)$$

$$\therefore V_a = \frac{\pi ab H_2}{6} \quad (6-15)$$

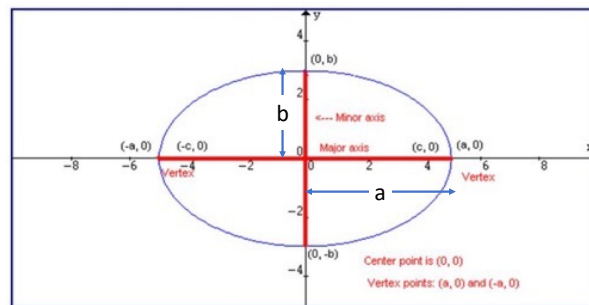


Figure 6-4: Representative Crater Shape from Trials

Post detonation, a , b and H_2 measurements were calculated [m] using a laser measure. Each dimension was recorded to 2 significant figures. No material was removed from the crater to determine the actual crater depth. The reasons for this were three-fold:

- Safety - the area used for the controlled demolition was a historical range of many decades;
- Environment - heat and humidity precluded spending long periods out in the open; and
- Security – minimising time out in the open due to ongoing conflict.

The apparent crater volume was determined using equation (6-15).

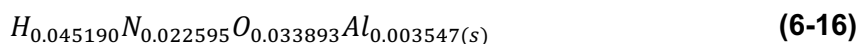
Apparent crater volumes were then compared to the calculations offered by Cooper [324] [327] for the same soil type in Table 6-1 (equations (6-3) (6-4) and (6-5)). Given that their results for Adushkin, Ambrosini, and Nagy were obtained for clay-type soils and asphalt, their data was discounted. However, given the similarities in crater shape between these trials and the results of Bjelovuk, a correlation between surface detonations on asphalt and alluvial soil was attempted for hexahedral explosive charges using equation (6-2) [328]. The aspiration was to achieve a methodology by which hexahedral detonations in alluvial soil could be used to determine crater sizes from hexahedral charges in asphalt.

Once trials were completed, 10 x 100 g samples of AN-Al were removed from surplus environmentally damaged containers awaiting bulk disposal to determine the composition of the HME and its likely TNT_e based on the predicted heat of explosion (Q). Sampling was carried out by UNDP explosive experts, with a Scanning Electron Microscope (SEM) utilised at the University of Wales Trinity Saint David (UWTSD) to determine whether the Al was a fine powder, flake, or a mixture of both.

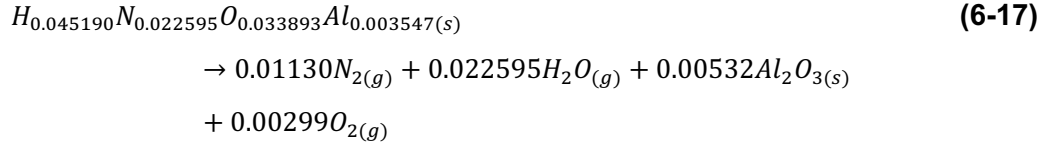
6.5 Results and Discussion

6.5.1 TNT equivalence

From the 1000 g sample collected, the mean stoichiometric composition of the AN-Al was determined from the dissolution of AN to be 90.43/9.57 AN-Al. Using this composition and methodology offered by Collett et al [338], the molecular formula of the AN-Al was determined as:



From this molecular formula, the products of detonation were calculated as follows, using the modified oxygen balance equation (see equation (6-17)) for non-ideal explosives [338]:



From this molecular formula and using the enthalpies of formation identified by the authors [338], Hess' Law (equation 8) determined the heat of explosion (Q) of the AN-Al to be -4272.93 kJ kg⁻¹, with an associated oxygen balance of +9.56%. This equates to a TNT_e of 1.04 (see equation (6-18), where the Q value for TNT is taken as -4091.63 kJkg⁻¹ from literature [96]:

$$TNT_e = \frac{Q_{ANAL}}{Q_{TNT}} = \frac{-4272.93}{-4091.63} = 1.04
 \tag{6-18}$$

Results of SEM analysis (see Figure 6-5) identified that no specific particle size criteria was applied to the selection of aluminium for this HME, but rather the availability of that aluminium within the supply chain. The aluminium used was a crude product, likely obtained from the sluff of engineering applications, with a particle size ranging between 10 – 100 µm and a mean particle size distribution of 63 µm. However, the particle size was within the scope of regulatory prohibition (< 200 µm), suggesting that waste Al from engineering applications should, perhaps, be graded before disposal [178].

The SEM also identified that the aluminium flakes had a coating of $Al_2O_{3(s)}$, suggesting that the AN-Al had been mixed with the AN and exposed to the environment for some time. This was also evident from the degradation of some containers where the HDPE had split longitudinally due to loss of ductility [339] and the explosive filling expanding [318]. It was impossible to determine the precise length of environmental exposure, other than to confirm with the authorities that containers had been recovered in August 2018, with disposals commencing in December 2019, and the trials concluding in March 2021. As such, the IEDs had been exposed to diurnal cycling in a largely arid sub-tropical country for about 18 months before disposal. This would allow for the HDPE

containers to degrade, for moisture uptake, for oxidation of the aluminium, and ‘caking’ of the explosive filling. ‘Caking’ causes AN-based explosives to lose their durability and explosive properties over time through loss of porosity [340] [341], thereby reducing detonation velocity up to 50% [342].

All of these findings support explosion theory predictions that the performance of the AN-Al would be less than that of HME compositions comprising fine Al powder [267] made for trials, but still capable of achieving theoretical detonation velocities in the order of $3160 - 3850 \text{ ms}^{-1}$, and detonation pressures (P_{cj}) between 2.1 and 3.5 GPa [307].

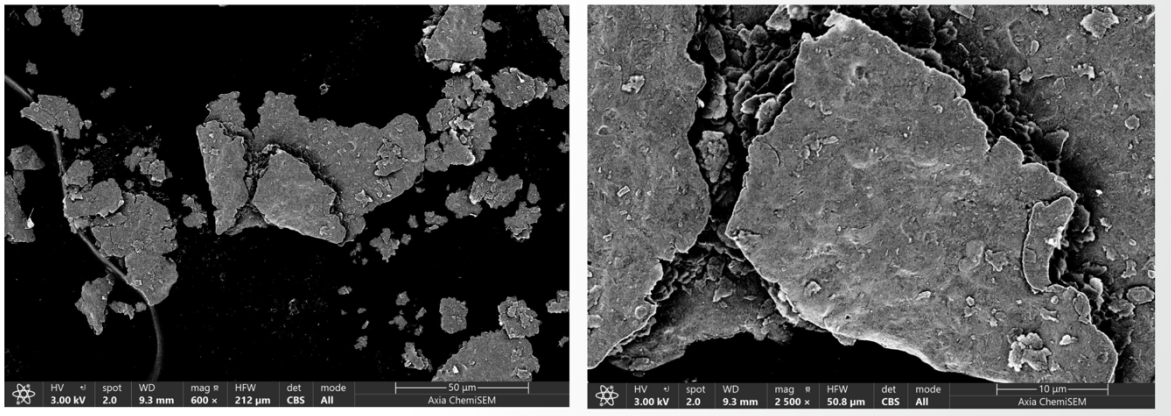


Figure 6-5: SEM results for Aluminium Composition (the grey flakes) within AN-Al at magnification 600 (left) and 2500 (right).

6.5.2 Cratering performance and explosive characteristics

The results of each firing are presented at Appendix E, with their mean values highlighted in Table 6-5 below. The columns from left to right determine:

- the mean mass of AN-Al within each container size [kg];
- the mean density of AN-Al from each container size [g cm^{-3}];
- the mean TNT equivalence for each container size [kg];
- the mean scaled charge mass $M_{tnt}^{1/3}$ [$\text{kg}^{1/3}$];
- the mean experimental widths (D_{Exp}) and depths (H_{2Exp}) of craters for each container size [m] compared to Cooper’s theoretical values for a spherical surface detonation (D_{Cooper} and $H_{2Cooper}$) [m];
- the mean apparent crater volumes (V_e) for each container size compared to theoretical values for Cooper (V_c) [m^3]; and
- the ratio of mean experimental crater depth (H_{2Exp}/H_{2C}) and crater volume for hexahedral charges compared to Cooper (V_e/V_c).

The comparison with Cooper [327] [324] is calculated using equations (6-3), (6-4), (6-13), and (6-15).

Table 6-5: Mean results of each container detonation

<i>Explosive</i>	<i>Mass [kg]</i>	ρ [gcm ⁻³]	TNTe [kg]	$M_{int}^{1/3}$ [kg ^{1/3}]	D_{Exp} [m]	D_{Cooper} [m]	H_{2Exp} [m]	$H_{2Cooper}$ [m]	H_{2Exp}/H_{2C}	V_e [m ³]	V_c [m ³]	V_e/V_c
AN-Al	5.68	0.914	5.91	1.81	0.498	0.759	0.219	0.158	138%	0.028	0.032	88%
	13.04	0.917	13.56	2.38	0.617	1.002	0.340	0.209	162%	0.067	0.073	92%
	26.08	0.936	26.08	3.00	0.741	1.262	0.440	0.263	168%	0.127	0.145	88%
	52.16	0.936	52.16	3.79	1.010	1.590	0.490	0.331	147%	0.261	0.291	90%
		0.926										
	Mean Value over all 40 firings								156%			89%

These results identify a hexahedral to a spherical relationship of apparent crater volume (V_e/V_c) in the alluvial soil of 89%, where the ratio of container in contact with the surface (H:L) lies between 1 and 1.5 (see above). Similarly, apparent crater depth provided a relationship of 156% (H_{2Exp}/H_{2C}). As such, it is possible to predict, based on $M^{1/3}$ and the properties of alluvial soil, that hexahedral HME charges display a relationship to spherical charges of:

$$V_e = 0.89V_c \quad (6-19)$$

Graphically (see Figure 6-6) the equations for V_e , V_c and M can be represented as:

$$V_e^{1/3} = 0.1687M^{1/3} \quad (6-20)$$

$$V_c^{1/3} = 0.175M^{1/3} - 5 \times 10^{-11} \cong 0.175M^{1/3} \quad (6-21)$$

Note that R^2 for the trials achieves unity.

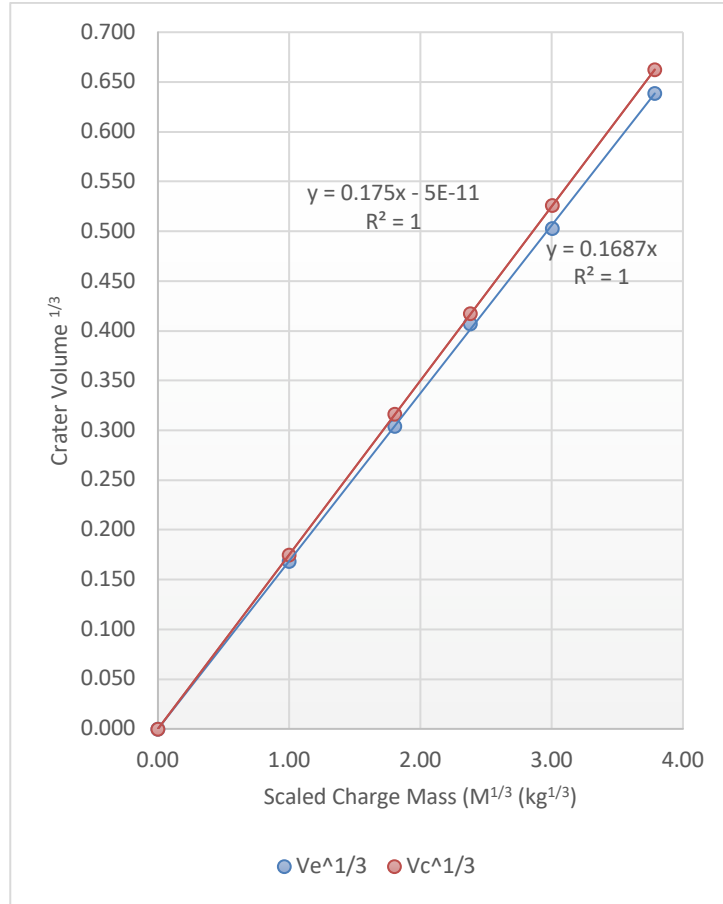


Figure 6-6: Graphical Representation of Experimental Crater Volumes for Rectangular Charge Containers Compared to Theoretical Volumes obtained from Spherical Charges

With the cratering comparison complete, Appendix 1 also determined the average density of the AN-Al explosive to be 0.926 g cm^{-3} . This was calculated by taking the mean value of density in Table 6-5. Given that the mixture comprises approximately 90/10 AN/Al from dissolution, the velocity of detonation (v_{mix}) can be established from the characteristic velocities (D_i) of both AN [343] and Al [324], and their theoretical maximum densities (ρ_{TMD}) of 1700 and 2700 g cm^{-3} respectively [324] [344]. The velocity of detonation v_d [ms^{-1}] and detonation pressure (P_{cj}) [GPa] of this composition are therefore predicted from the actual and theoretical maximum density (TMD) as follows:

$$v_{mix} = \sum D_{iAN} D_{iAl} = (0.9 \times 5050) + (0.1 \times 6850) = 5230 \text{ ms}^{-1} \quad (6-22)$$

$$\rho_{TMD} = \sum \rho_{iAN} \rho_{iAl} = (0.9 \times 1700) + (0.1 \times 2700) = 1.8 gcm^{-3} \quad (6-23)$$

$$\therefore v_d = v_{mix} \left(\frac{\rho}{\rho_{TMD}} \right) + 1.5 \left(1 - \frac{\rho}{\rho_{TMD}} \right) = 5.230 \left(\frac{0.926}{1.8} \right) + 1.5 \left(1 - \frac{0.926}{1.8} \right) \quad (6-24)$$

$$\therefore v_d = 3419 ms^{-1} [307] [324] \quad (6-25)$$

And detonation pressure P_{cj} [307] [324]:

$$P_{cj} = \rho \frac{v_d^2}{4} = 0.926 \left(\frac{3.419^2}{4} \right) = 2.84 GPa [307] [324] \quad (6-26)$$

Both values lie within the ranges of detonation velocity, and detonation pressure reported for AN-Al compositions of 90% AN and 10% Al [306] [345] [346].

6.5.3 Comparisons with other soil mediums

Bjelovuk reports [328] that the mass of explosive M [kg] (in terms of TNTe) is proportional to the apparent crater volume V_b [m³] and the surface area of the charge in contact with the ground P_k [m²] for container L:H ratios of 1:1.5 on asphalt.

Asphalt was chosen by Bjelovuk given that most IEDs within Europe present as surface or above surface detonations within this medium [113] [347] - it is difficult to dig into asphalt by hand. As such, a man-portable IED container is likely to be placed on the ground or worn as a person-borne IED (PBIED), whilst an IED within a vehicle may be above the ground by some distance 'x' (determined by the height of the load-carrying area) [113]. Such a statement can be further supported by international community concerns over the increased presence of IEDs within urban settings [348].

The correlation of apparent crater volume between alluvial soil and asphalt for hexahedral containers can be seen in Appendix E, which is summarised below (Table 6-6), where the columns from left to right represent:

- the mean mass of AN-Al within each container size [kg];
- the TNT equivalence of that mass of AN-Al [kg];
- the mean scaled charge mass for each container $M_{tnt}^{1/3}$ [kg^{1/3}];
- the mean apparent experimental crater volumes (V_e) for each container size in alluvial soil;
- the theoretical values for Bjelovuk in asphalt (V_b) [m³]; and
- the ratio of mean experimental crater volumes in alluvial compared to Bjelovuk (V_e/V_b) and Cooper (V_e/V_c) in asphalt.

Table 6-6: Comparison of experimental crater volumes in Alluvial Soil and Asphalt

<i>Exp</i>	<i>Mass</i> [kg]	TNTe [kg]	$M_{tnt}^{1/3}$ [kg ^{1/3}]	V_e [m ³]	V_b [m ³]	V_e/V_b	V_e/V_b
<i>AN-Al</i>	5.68	5.91	1.81	0.02	0.008436	334%	375%
				8			
	13.04	13.56	2.38	0.06	0.022536	299%	323%
				7			
	26.08	27.12	3.00	0.12	0.045107	282%	322%
				7			
	52.16	54.25	3.79	0.26	0.082456	316%	353%
				1			
	Mean Value over 40 firings					304%	339%

Table 6-6 demonstrates that (based on the *TNTe* for AN-Al used in the trials) the crater volumes produced by hexahedral surface charges on alluvial soil are roughly 300% larger than those calculated for asphalt (the ratio of V_e/V_b). Calculations further suggest that the volume relationship between spherical and hexahedral charges in alluvial soil is 339% than that in asphalt for the same mass *M* [kg] of explosive.

The results demonstrate that cratering in asphalt and alluvial soil for rectangular surface charges can be expressed as follows, with worked examples being provided at Appendix E:

$$M_{asphalt} = 617.952 V_b^{0.794} P_k^{0.309} \quad (6-27)$$

$$V_b = 0.339 V_c \quad (6-28)$$

$$V_a = 0.89 V_c \quad (6-29)$$

$$V_a \approx 3 V_b \quad (6-30)$$

Where:

- $M_{asphalt}$ = the mass of explosive [TNT_e in kg];
- V_b = the apparent crater volume [m³] created by the detonation of a hexahedral surface charge in asphalt
- P_k = the area of the container in contact with the surface [m²];
- V_c = the theoretical apparent crater volume from Cooper in alluvial soil [m³];
- V_a = the apparent crater volume from the surface detonation of a hexahedral container in alluvial soil [m³]
- the ratio of mean experimental crater depth (H_{2Exp}/H_{2C}) and crater volume compared to Cooper (V_e/V_c).
- the H:L ratio of the hexahedral charge lies between 1.0 and 1.5.

Given that the cratering efficiency (E_{CR}) for a vast number of soil types has been calculated over the years and is available at these literature references [324] [349], further work may be able to utilise the following equation of Cooper to deliver approximations for other media given that the crater radius (R_a), P_{cj} and $M^{1/3}$ can be determined by simple calculation (see equations 1 – 6 and 18):

$$R_a = (0.46 + 0.027 P_{cj})(2 E_{CR} M)^{1/3} \quad (6-31)$$

6.5.4 The impact on people and structures

Now that the performance of HME in spherical or hexahedral containers can be determined from crater size in alluvial soil and asphalt, these parameters can now be applied to the impact of such explosions on people and structures, or the safe cordon and evacuation distances required that should a device be discovered.

Whilst explosions have varied effects on engineering structures [350] [351] [352], the physiological response of civilians to blast, who are often the unintended victims of IEDs, can be much harder to determine. The most vulnerable organs in the body to blast are our lungs and ears, which through many decades of testing on animal species has led to an empirical scaling for humans [324]. Designed by Bowen in 1968 [353], empirical scaling predicts the lethality from a Friedlander blast wave for persons in front of a reflecting surface, or in the free field (see Figure 6-7).

In Figure 6-7 the adult male at (a) is set against a reflecting surface in the standing and prone position. The Friedlander blast wave approaches left to right and top down respectively. At position (b) the adult male is standing or prone in the free-field. The Friedlander blast wave approaches from the left. Curves can also be demonstrated for babies (the most vulnerable class), small children, and women.

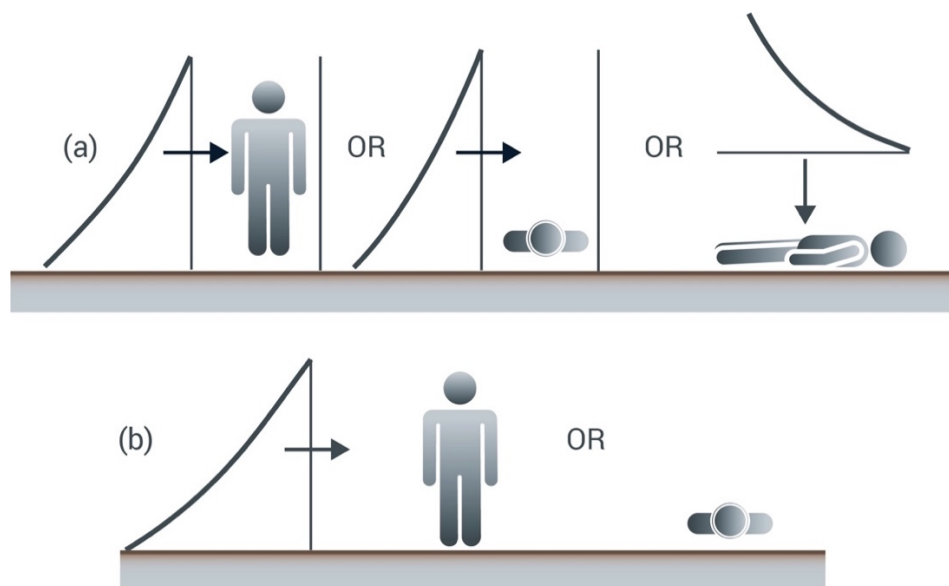


Figure 6-7: Orientations of Human to Friedlander Blast Waves [50] [13]

In recent years, Bowen's predictions have been updated by Bass [354] and Panzer [355] to determine that:

"For blast waves with short positive phase durations ($T < 2$ ms), the load on a person standing in the free field is comparable to that on a person in front of a

reflecting surface. For long positive durations ($T > 20$ ms), the load on a person standing in the free field is lower than for a person in front of a reflecting wall”.

Whilst these differences are minimal, the updated experimentation allows varying degrees of lethality (1, 50 and 99%, for example) to be displayed graphically as one image, (see Figure 6-8) which is useful for comparison to calculated data:

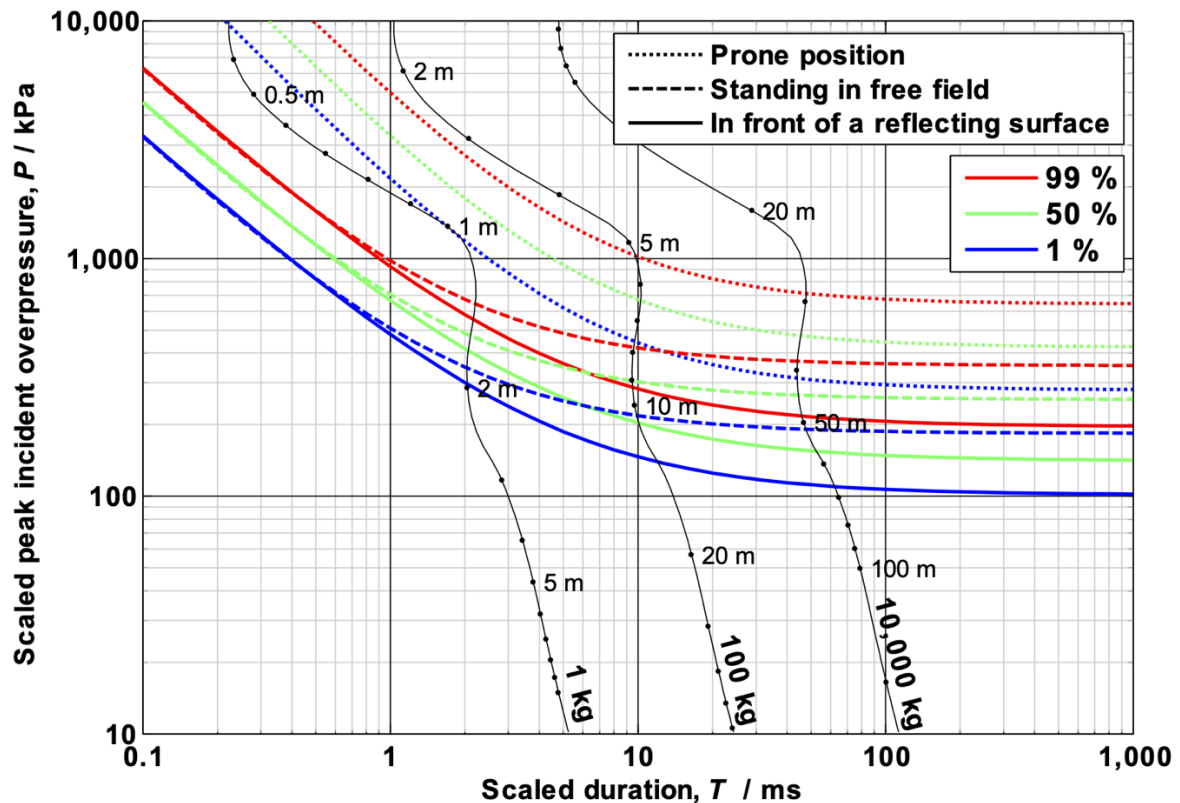


Figure 6-8: A graphical representation of scaled incident peak overpressure versus scaled duration for degrees of lethality on adult male orientations in the reflected and free field © Cranfield.

To demonstrate the utility of such information to the first responder, suppose that forensic analysis determined that an explosive was indeed AN-Al, and that crater analysis determined the charge mass to be approximately 28 kg. In this case, Table 6-7 uses detonation equations from Kingery & Bulmash [279], Bulson [356] and Vasilis et al [357] to calculate the scaled incident peak overpressure (P_s) and scaled duration curves (T) for TNTe 24.36 kg at distances of 1, 5, 10 and 20 m.

These calculations are shown for completeness as an excel sheet at Appendix F, using the distance of 10 m as the calculation example.

Table 6-7: Blast consequences for Worked Example 2

<i>Range (R) [m]</i>	<i>1</i>	<i>5</i>	<i>10</i>	<i>20</i>
<i>NEQ (kg)</i>	28	28	28	28
<i>TNTe (kg)</i>	24.36	24.36	24.36	24.36
<i>Peak Incident Pressure (Ps) [kPa]</i>	7293.10	271.54	61.71	18.72
<i>Incident Impulse (Is) [kPa.ms]</i>	408.73	305.88	164.81	87.17
<i>Peak Reflected Pressure (Pr) [kPa]</i>	64912.97	994.37	153.60	40.14
<i>Reflected impulse (Ir) [kPa.ms]</i>	7366.60	816.39	364.08	170.66
<i>Shock Front Velocity (U) [ms⁻¹]</i>	2609.78	617.21	419.63	370.59
<i>Arrival Time (Ta) [ms]</i>	0.245	4.28	14.60	41.03
<i>Positive Phase Duration (T+) [ms]</i>	0.575	4.93	8.34	10.81
<i>Decibel Level</i>	189.79	161.82	149.79	137.75

From these new 'Bowen' curves, the impact of HME compositions of unknown composition can be determined from the size of the crater they leave behind within a soil medium, which informs coroner inquests and cordon and evacuation distance for blast accordingly. For example, the calculated peak incident overpressures (P_s) from Table 6-7 would inflict the likelihood of death on an individual standing in the free field as follows (see Table 6-8):

Table 6-8: Incident overpressure inflicted upon male at distance

<i>Distance R [m]</i>	<i>1</i>	<i>5</i>	<i>10</i>	<i>20</i>
<i>Ps [kPa]</i>	7293.10	271.54	61.71	18.72
<i>T+ [ms]</i>	0.575	4.93	8.34	10.81

<i>Lethality</i>	$\geq 99\%$	$\geq 50\%$	$< 1\%$	$< 1\%$
<i>Lung Damage</i>	Yes	Yes	Yes	Yes

If these calculated values are then transposed to Bass' scaled graphical representation (Figure 6-8), then additional information can be gleaned by the first responder as Table 6-9 demonstrates.

Table 6-9: The actual impact on a human male - 70 kg

<i>Distance R [m]</i>	<i>1</i>	<i>5</i>	<i>10</i>	<i>20</i>
<i>Ps [kPa] Bulson</i>	7293.10	271.54	61.71	18.72
<i>T+ [ms]</i>	0.575	4.93	8.34	10.81
<i>Lethality</i>	$\geq 99\%$ even in prone position $\geq 50\%$ in front of a reflecting surface or $\geq 1\%$ standing in the free field $< 1\%$ in all cases $< 1\%$ in all cases			

Therefore, the original Bowen curves depict lethality based on lung damage, but the revised plot allows first responders to determine the effects of orientation at distance too. It may not, for example, be possible in open spaces (such as busy markets) for people to find hard cover, so what is the minimum distance required whereby a person would survive blast injury in the prone position?

6.6 Conclusion

The size and shape of a crater caused by ideal and/or non-ideal explosives are a practical method to determine the mass of explosives used in an explosion event.

Sadly, significant amounts of data are often lost due to the inability of nations to facilitate scientific collection, or through a lack of understanding by first responders of the complex theories involved.

Calculation is often based on spheres and hemispheres, not the actual geometry of the IED main charge container, or the warhead used. However, comparing cratering efficiency is possible between classical spherical charge predictions and hexahedral charges. In most cases, all that is required is a knowledge of the soil type, the apparent crater volume (V_a) [m^3] or the area of the container (P_k) [m^2] in contact with the surface to progress meaningful calculations.

This paper focuses solely on alluvial soil and asphalt, but existing equations in literature circulation can be adapted to provide efficiencies for other soil types. In each case, the crater size can determine the potential impact on people and structures using well-established methodologies such as Bowen and Bass curves.

7 Discussion

7.1 Introduction

The previous chapters detail the implications of ECP within the supply chain and address specific areas of weakness, which are regulatory and anthropological in nature. The papers are current (statistics and case studies represent research conducted between 2021 and 2024), with literature review addressing historical (11th to 20th century) and future trends (21st century).

Models have been developed using predictive threat analysis (risk and risk management), Bayesian belief updating, thermochemistry and quantitative trials data to analyse areas of weakness and offer degrees of resolution. The findings justify a need for the following, which were reported to the UNGA in 2022 [358]:

- advocacy to improve ECP regulation at the strategic level;
- improved understanding regarding human factors associated with the illicit diversion of ECP;
- app-based programmes to assist the first responder in the pre and post-detonation phase where HME and their precursors are encountered; and
- further research in crater and charge geometry to better reflect the impact of HME formulations on humans and structures.

The thesis will now consider the relevance of the research findings and their academic underpinning. For research relevance, it shall demonstrate where the knowledge has been applied throughout this journey, and where it is likely to be used in the future. Academic underpinning intends to demonstrate the efficacy of the data gathering and experimental design, which generated the equations and models that can be used by first responders.

7.2 Research Relevance

7.2.1 The Global Supply Chain

Chapter 2 identifies that the regulation surrounding ECP varies regionally and internationally. Even those ECP with the most stringent of regulation, and which appear on the PGS international watch lists [115], can still be accessed within the supply chain because there is no overarching process to underpin governance. Whilst AN, PC and CHP have been used as global case studies, their independent nature has been abused in a significant number of terror related incidents since 1970 [63], and within countries that would be considered of 1st World standing [359].

In the case of the Manchester Arena bombing [360], intelligence reporting identified that Salman and Hashem Abedi ordered significant quantities of sulphuric acid and hydrogen peroxide, of which only a portion was used to synthesise the TATP used in the bomb. At the time of the incident sulphuric acid was a reportable (not regulated) ECP under EU regulation 98/2013 [361], and the hydrogen peroxide obtained fell below a concentration where suspicious activity would be reported (see Table 2-5). The acetone recovered was a universal solvent and common ingredient of over-the-counter nail polish remover [362].

As such, these two individuals were able to construct a viable PBIED explosive train (detonator and main charge) in the region of 30 kg in weight [61], comprising organic peroxides, which could kill people up to 20 m away. Using the flow chart process offered in Chapter 2 (Figure 2-1), each precursor was classed as INDEPENDENT of other ECP, yet available in HIGH volume. However, with regulation and standardisation already applied to CHP in Europe, the manufacture of a PBIED this size was not considered likely by the security services given the effort that would be required to raise the concentration of hydrogen peroxide from 12% to above 35% [154].

However, Manchester indicated that a determined perpetrator will exploit the supply chain and use whatever chemical synthesis techniques are available to turn the most heavily regulated ECP into viable explosive compositions given

such disparity in the international governance. Whilst it is not known at open source what websites the Abedi's visited, or where the chemicals were ordered, the methodology on how to safely synthesise TATP can be found easily within a few keystrokes [363]. Perhaps more worrying, the synthesis of TATP (including other explosive peroxides such as HMTD) from unrecognised ECP such as the percarbonates and perborates [364] is also readily available.

Given the relevance of the research to an increasing global problem, and the advocacy required, the findings of Chapter 2 were taken to UNGA 77 in September 2022 [358], where advocacy for improved regulation was presented by the author and Ambassador to the Conference of Disarmament. Pre-papers were also submitted by the author in late 2021 [93], demonstrating the lead time that is required to implement life-saving regulatory changes at the international level. The letter demonstrating the impact of the research is shown below (see Figure 7-1), with the following strategic recommendations specific to IED harm issued to all Member States. The impact of Chapter 2 within the advocacy is highlighted **RED**):

- Improve international collaboration: sharing threat-intelligence and IED data (**understand**);
- Enhance national Explosive Ordnance Disposal (EOD) capabilities to match the threat (**mitigate**);
- **Increase international regulation to reduce access to** dual-purpose components and **precursors**;
- Increase international funding to support 3rd party IEDD operations in affected areas (**mitigate**).

“Your recent paper published in the Heliyon journal, and your support to Action on Armed Violence’s series of papers on IED harm.....shall inform future policy going forwards. The recommendation from your area of study was to increase international regulation to reduce access to dual-purpose components and precursors” [Ambassador to the Conference for Disarmament].

Following UNGA 77, the United Nations subsequently issued technical guidance on ECP regulation from the Counter-Terrorism Executive Directorate (CTED)

[365], with the 2023 Counter-Terrorism strategy adding ECP to the list of Member State mandates as follows [366]:

*“.....IEDs, including **explosive precursors**, continue to be **used extensively** in terrorist activities.....and **urges further attention** to the issue.....and requests the Secretariat to **strengthen precursor threat mitigation**.....underlining the importance of.....cooperation on crime”.*

INTERPOL has also recently completed a review on the analysis and detection of explosives and explosive residues [367], citing this work as follows:

*“Gareth Collett has published a **fantastic report** focused primarily on **precursors for Homemade Explosives (HME)** including **recommendations for preventative actions that could limit access to the materials. It should be required reading for any analyst in the field**”.*

As for the UK, the PhD has contributed to the review of extant regulation surrounding ECP, poisons and cosmetics. Following UNGA 77 the Secretary of State laid before parliament Statutory Instrument 2023 No. 63 on 23rd January 2023. This came into force on 1st October 2023 as ‘**The Control of Explosives Precursors and Poisons Regulation 2023**’, [368], which (following Manchester) mandates additional requirements relating to:

“the supply of a regulated ECP, the provision of information to workers within the industry, precautions to be taken by online market places, and the improved reporting of suspicious transactions”.

Using predictive threat analysis, the Secretary of State is to publish a report on success by 1st October 2028. Most specific to this research, and in relation to the ECP’s of concern highlighted by the author to the UNGA (see extract of publication at Appendix D [93]), Table 7-1 identifies the ECP that have been afforded regulated status in the UK by priority, and where concentrations have been better defined.

Predictive threat analysis has also paid dividends in academic research, with Chapter 3 of **the thesis identifying commercial UHP as an ECP absent from**

all regulatory lists, other than those relating to cosmetics. This has now been rectified, with commercial UHP classified as INDEPENDENT and home-made UHP classed as DEPENDENT on other regulated ECP. This has been, however, too late for the Control of Explosives Precursors and Poisons Regulation, but UHP shall feature in the 2028 report along with perborates and percarbonates.

Note: Appendix D [64] was submitted to the UNGA and listed those ECP named within international regulation and where there was a discrepancy between the EU, UK, USA, AUS, Canada, Singapore, the CFATS system, and PGS list protocols. Appendix D used Figure 2-1 to assign a DEPENDENCY to each ECP and to describe how substitution or standardisation can be applied. Areas highlighted RED demonstrate where regulation does not exist in some regions.

Table 7-1: Amendment to Schedule 1A to the 1972 Act

Precursor	Standard Limit Value (% w/w)	Upper Limit Value (% w/w)	Remarks
Ammonium Nitrate	16%	No licencing permitted	Moved to top of list.
Hexamine	N/A	N/A	NEW ADDITION in relation to HMTD and RDX manufacture
Hydrochloric Acid	10%	N/A	NEW ADDITION
Hydrogen peroxide	12%	35%	No change
Nitromethane	16%	100%	No change
Sulphuric acid	15%	40%	NEW ADDITION (now regulated, not reportable)
Nitric acid	3%	10%	No change
Phosphoric Acid	30%	N/A	NEW ADDITION
Potassium chlorate	40%	No licencing permitted	No change
Potassium perchlorate	40%	No licencing permitted	No change
Sodium chlorate	40%	No licencing permitted	No change
Sodium perchlorate	40%	No licencing permitted	No change
Sulphur	-	-	Added to the list of reportable items.

Figure 7-1: UNGA 77 Side Event Response



Geneva, 12/12/2022

FROM:

Colonel Philippe LEJEUNE
Military Advisor of the Ambassador to the Conference of Disarmament

Dear Mr Collett,

I am writing to thank you for your continued efforts in the C-IED arena, but more specifically, your recent publications on regulatory practices surrounding explosive chemical precursors. Your recent paper published in the Heliyon Journal, and your support to Action on Armed Violence's series of papers on IED harm, funded by France, featured at UNGA 77 as a tabled side event. From that side event, four specific high-level recommendations have been taken forwards by the UN secretariat, and shall inform policy going forwards. The recommendation from your area of study was to increase international regulation to reduce access to dual-purpose components and precursors. I cannot thank you enough for your support and effort in this arena and I trust that this justifies the long hours applied to your PhD.

Le commissaire en chef de 1^{ère} classe Philippe Lejeune
Conseiller militaire
de la Représentation permanente de la France
auprès de la Conférence du désarmement

TO:

General (Retired) Gareth Collett CBE
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7.2.2 The Efficacy of Current C-IED Approaches

Chapter 4 described the role that human factors play in the illicit diversion of ECP and demonstrated that current C-IED initiatives, whether they be military [22] or humanitarian [166], do not appropriately address the motivations behind the willingness of people to support such activity.

The research supports theories that communities (not governments or institutions) are pivotal to the success of any governance and rule of law programme, and that **taboo subjects such as IEDs can be discussed** without consequence if appropriate ethical and cultural sensitivities are considered [225]. Not all the people that support illicit diversion can be classed as ‘*wicked*’ criminals [212] if we are to consider what we would do to feed and protect our own families under the direst of circumstances. This was summed up by Lieutenant General Thomas F. Metz, the head of the Joint Improvised Explosive Device Defeat Organization (JIEDDO), who said of Iraq as far back as 2008 [369]:

“...the young person who goes and places the IED may just...get paid \$100 a night to put in the IED and they do it to feed their family”.

Not even the UK’s PREVENT duty guidance covers this aspect of necessity, focusing solely on three specific strands:

“tackling the ideological causes of terrorism, intervening early to support people susceptible to radicalisation, and enabling people who have engaged in terrorism to disengage and rehabilitate [370]”

The relevance behind this research is linked specifically to the fact that no IED network exists independently, despite military doctrine stating that they do [22], and that by mandating such a reductionist and myopic approach, C-IED initiatives become sub-optimal [212]. However, the intelligent application of Bayesian belief updating [231] to determine the societal turning points that facilitate degradation of an IED system can improve resource mobilisation by identifying principal areas for focus and monitoring tangible progress over time. Essentially, the international community assists those inappropriately classed as the ‘*wicked*’ when evidence

underpins such support **and** identifies the type of support that should be offered – in this case simple *‘pay for work schemes’*.

As such, ECP provide a useful focus at community level since the use of AN in the country of study had been significant. What better focus than an ECP of global interest with over 50 years of regulatory discipline applied to it. This Bayesian focus complements Chapter 2 as regulation at the strategic (States) level did not appear to prevent illicit diversion of ECP at the tactical (community) level since reasons for support to criminality (willingly or otherwise) were misunderstood by both C-IED practitioners and Ministries.

There is **therefore an interconnectedness between Chapters 2, 3 and 4, which demands a ‘Systems Thinking’ approach to ECP** [371] [372]. Such an approach to complex problem solving was first pointed out by Richmond who recognised the importance of involving the state, its institutions, and people under such circumstances [373]. This is not John Lennon’s *‘Power to the People’* [374], since Richmond states that:

“We must have a common language and framework for sharing our [institutional] specialized knowledge, expertise and experience with local experts [the community]...or complex solutions to problems become less viable”. (Richmond 1991)

This suggests that the thorny knot of ECP regulation requires **strategic policy and communities capable of comprehending systems and complexity** given the increased use of IEDs [375]. Bayesian belief updating can provide that intuitive simplification. As Wade states, *“it can conceptually model individual parts of a system and view them a-typically”* [376], whilst research by Arnold and Wade shows that *“perceptual wholes can reduce the conscious accessibility of their parts”* [377].

This approach allows ECP complexity to be unravelled within supply chains and at point of use as decision makers require less detail from which to act. It is a methodology by which complexity is reduced by stripping out excess information that is largely irrelevant. The solution to ECP threat mitigation therefore lies within

the advocacy of the United Nations to Member States (the strategic) and informed analysis of the causal factors through community dialogue in IED affected States. Chapters 2, 3 and 4 have achieved that - IED numbers are falling in the country of interest since community focus groups were established within the governance and rule of law programme.

However, there is a cost to all of this. Most certainly, the community requires tangible and visible proof of the benefits to be gained through being involved. If there is no proof, then there is no reason not to continue being '*wicked*'. Bayesian belief updating will need to be monitored over time to draw any sound conclusions, however it has been extremely successful in countering poaching of rhino horn in Africa since 2017 [213]. In a world of budgetary constraints, funding for UNDP is limited to 31st December 2025 [378], but it is hoped that such methodologies can be made available to C-IED facilitators within NATO and other defence and security institutions.

Cranfield University's Counter Improvised Explosive Device Capability course is a principal starting point, with access now available to staff employed within the multitude of global streams and disciplines involved in C-IED [379]. One of the key objectives of this course is to perform basic analysis of an IED System and identify ways in which it may be countered at various levels and the means available to do so.

7.2.2.1 The Performance of ECP

Chapter 5 identifies that the performance on non-ideal explosives is difficult to determine given their heterogeneity and composition [309]. This is further obfuscated by TNT equivalence, which is wholly dependent upon the testing criteria [281], and the fact that most 'real-life' IED compositions are left exposed to the environment and suffer a degree of degradation [340] [341].

As such, there is very little literature on a likely performance standard for HME, which is of concern to the first responder. Chapter 5 therefore provides a singular performance standard based on heat of explosion equivalence (Q_e), thereby

providing consistency in reporting and to within an accuracy of $\pm 10\%$ of known literature values (see Table 5-5).

For the humanitarian community, this allows them to update publications, which provide open-source detail on HME, and which have, to date, cherry-picked the TNT equivalence presented [64].

A screenshot of the excel model created to underpin Chapter 5 is provided below (see Figure 7-2), with the calculations shown for a four-part composition of HME that comprises AN, TNT, NG and starch (80/14/4/2). The Q_e value of this composition is identified as -3406 kJ kg^{-1} (TNTe 0.83), with an oxygen balance of $+5.78\%$ calculated using equation (5-18) from the empirical formula below:

$$C_{0.004843}H_{0.043941}N_{0.022367}O_{0.035267} \quad (7-1)$$

Historically, this composition was known as Donarite (or Donarit) [380], demonstrating that perpetrators can use ageing open-source data to identify viable explosive compositions of interest.

The Q_v value for Donarite published in literature is -3497 kJ kg^{-1} (TNTe 0.85), with an oxygen balance of $+5.7\%$ [293], which suggests a Q_e accuracy of 98% for this non-ideal composition (see equation (7-2)).

$$Accuracy = \left(\frac{Q_e}{Q_v} \right) \times 100\% = \frac{0.83}{0.85} \times 100 = 98\% \quad (7-2)$$

Screenshots of the data sheet for donarite and the calculator explainer are also shown at Figure 7-3 and Figure 7-4.

Whilst the calculations in excel are complex, they are ripe for automation in an app-based system. To provide the first responder with confidence, the outcome of calculator use for five other HME compositions compiled from the PGS list and used by criminals [243] are shown at Table 7-2:

Table 7-2: Calculator determinations for HME comprising PGS precursors

Composition	ECP Involved in HME manufacture from PGS list (Chapter 2)	Q_e (kJ kg ⁻¹) (Based on calculator from Chapter 5)	Remarks
TATP	Acetone (PGS) Concentrated Hydrogen Peroxide (PGS) Sulphuric Acid (PGS)	0.89	Literature value for Q_{tnt} vary between 0.71 [147] – 1.16 [381]. As such, the value of 3765 kJ kg ⁻¹ is taken from most recent literature [382], suggesting a Q_{tnt} of 0.92.
'Al-Shabaab' Dynamite	Potassium Nitrate (0.45) (PGS) Charcoal (0.15) Nitroglycerine (0.40) (Nitric Acid (PGS), Sulphuric Acid PGS), Glycerol))	1.26	There is no current literature value provided for Shabaab Dynamite. However, the heat of explosion in dynamites is driven by the nitroglycerine content [383], with

Composition	ECP Involved in HME manufacture from PGS list (Chapter 2)	Q_e (kJ kg ⁻¹) (Based on calculator from Chapter 5)	Remarks
			this particular composition first published by Phokion [34] in 1928.
Cheddite	Potassium Chlorate (0.9) (PGS) Wax (0.1)	1.19	Literature value for Q_{tnt} 1.21 [147]
HMTD	Hexamine Concentrated Hydrogen Peroxide Citric Acid	1.22	Literature value for Q_{tnt} 1.10 [66] [384]
Lead Azide	Sodium Azide Lead Nitrate	0.39	Literature value for Q_{tnt} 0.39 [385]

As can be seen from this table, the calculator determines the products of detonation based on stoichiometry and provides an accurate determination of TNT equivalence.

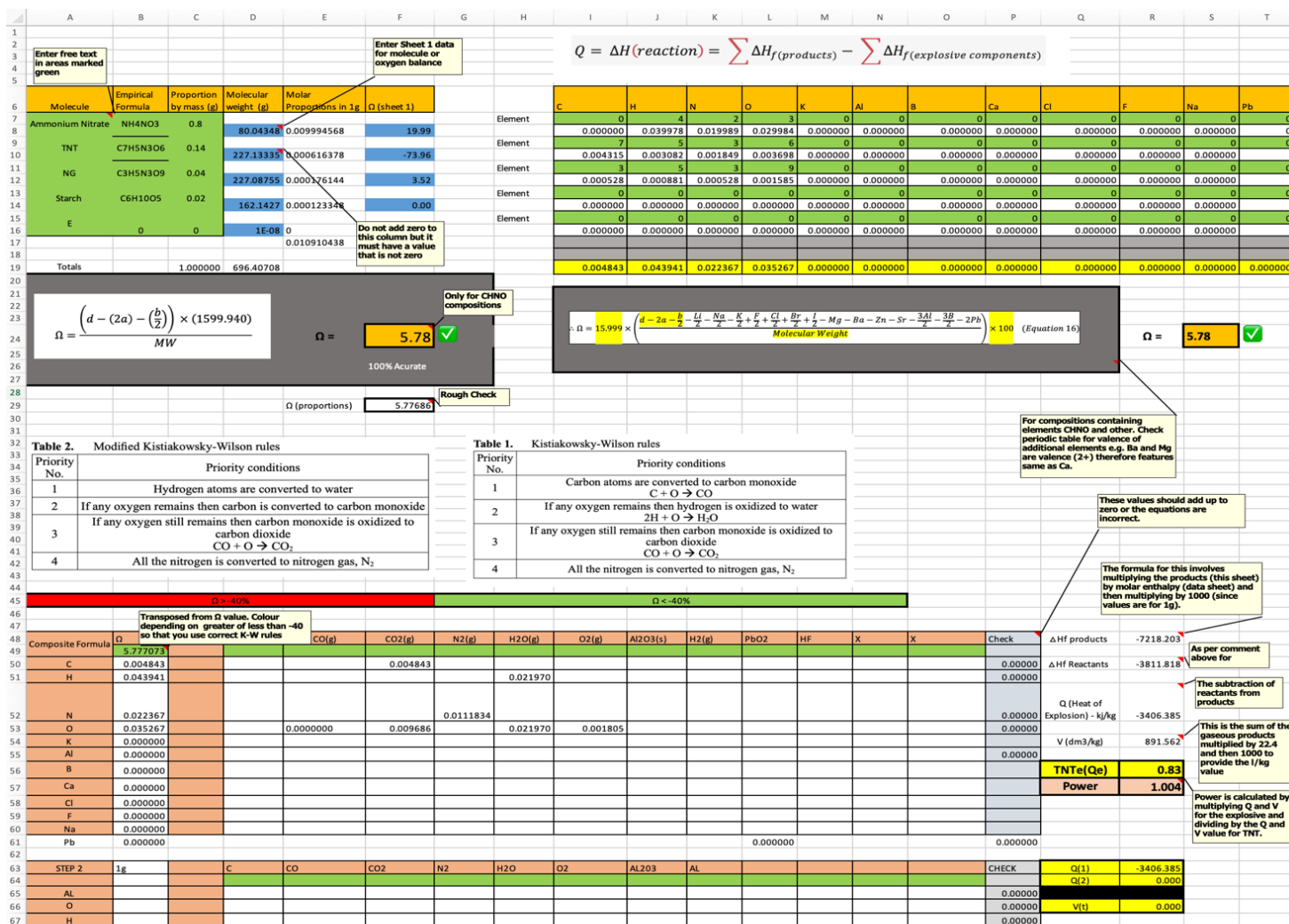


Figure 7-2: Excel Version of HME Performance Calculator – Donarite (available at DOI: 10.17862/cranfield.rd.25053614)

Explosive	Chemical Precursors	Molecular Formula	Molar Mass	C	H	N	O	X	Y	Ω
Ammonium Nitrate	NH4NO3		80.043	0	4	1	3		0	19.99
Ammonium Perchlorate	NH4ClO4		117.489	0	4	1	4		35.453	27.24
Barium Nitrate	Ba(NO3)2		261.340	0	0	2	6		137.3300	36.73
EGDN	C2H4N2O6		152.064	2	4	2	6		0	0.00
Hydrogen Peroxide	H2O2		34.015	0	2	0	2		0	47.04
Lead Azide	Pb(N3)2		291.240	0	0	6	0		207.2	-5.50
Nitroglycerine	C3H5(ONO2)3		227.088	3	5	3	9		0	3.52
Sodium Nitrate	NaNO3		84.995	0	0	1	3		22.9898	56.47
Potassium Nitrate	KNO3		101.103	0	0	1	3		39.0983	47.47
Nitromethane	CH3NO2		61.040	1	3	1	2		0	-39.32
Nitrostarch	C6H7N3O9		265.136	6	7	3	9		0	-39.22
PETN	C5H8N4O12		316.138	5	8	4	12		0	-10.12
Picric Acid	C6H3N3O7		229.106	6	3	3	7		0	-45.39
Potassium Chlorate	KClO3		122.550	0	0	0	3		39.0983	39.17
Potassium Perchlorate	KClO4		138.549	0	0	0	4		39.0983	46.19
Potassium Permanganate	KMnO4		158.034	0	0	0	4		39.0983	54.94
RDX	C3H6N6O6		222.117	3	6	6	6		0	-21.61
Sodium Chlorate	NaClO3		106.441	0	0	0	3		22.9898	35.45
TNT	C7H5N3O6		227.133	7	5	3	6		0	-73.96
Urea Nitrate	CH5N3O4		123.069	1	5	3	4		0	-6.50
TATP	C9H18O6		222.239	9	18	0	6		0	-151.18
Charcoal	C7H4O		104.108	7	4	0	0		0	-230.52
HMTD	C6H12N2O6		208.171	6	12	2	6		0	-92.23
Icing Sugar	C12H22O11		342.301	12	22	0	11		0	-112.18
Nitrobenzene	C6H5NO2		123.111	6	5	1	2		0	-162.45
Sawdust	CH1.35O0.617		23.243	1	3	0	0		0	-141.66
Coffee	C8H10N4O2		194.193	8	10	4	2		0	-156.54
Fuel Oil	C16H34		226.447	16	34	0	0		0	-346.20
Vaseline	C12H32		176.387	12	32	0	0		0	-362.82
Paraffin Wax	C25H52		436.851	25	52	0	0		0	-278.35
Kerosene	C12H26		170.339	12	26	0	0		0	-347.53
Glycerol	C3H8O3		122.039	3	8	0	3			-108.97
Diesel	C12H23		167.311	12	23	0	0			-339.49
Lead Styphnate	PbC6H3N3O9		468.310	6	3	3	9		207.2	-18.79
MFTNB	C6H12N3O6F		231.100	6	12	3	6			-34.70
Woodmeal	C1.41H2.66N2.54O2		102.424	1	3	3	3		0.07 0.09	
	C5OH72O33		1201.104	50	72	0	33			-137.20

PbO

Atomic Number	Symbol	Name	Atomic Weight	Ω	Oxide
1	H	Hydrogen	1.0080		
2	He	Helium	4.0026		
3	Li	Lithium	6.9410		
4	Be	Beryllium	9.0122		
5	B	Boron	10.8110		
6	C	Carbon	12.0110	-266.41	CO2
7	N	Nitrogen	14.0067		
8	O	Oxygen	15.9994		
9	F	Fluorine	18.9984		
10	Ne	Neon	20.1790		
11	Na	Sodium	22.9898		MgO
12	Mg	Magnesium	24.3050	-65.83	
13	Al	Aluminum	26.9815	-88.92	Al2O3
14	Si	Silicon	28.0855		
15	P	Phosphorus	30.9738		
16	S	Sulfur	32.0660	-99.81	SO2
17	Cl	Chlorine	35.4530		
19	K	Potassium	39.0983		
18	Ar	Argon	39.9480		
20	Ca	Calcium	40.0800		
21	Sc	Scandium	44.9559		
22	Ti	Titanium	47.9000		
23	V	Vanadium	50.9415		
24	Cr	Chromium	51.9960		
25	Mn	Manganese	54.9380		
26	Fe	Iron	55.8470		
28	Ni	Nickel	58.7000		
27	Co	Cobalt	58.9332		
29	Cu	Copper	63.5460		
30	Zn	Zinc	65.3800	-24.43	ZnO
31	Ga	Gallium	69.7200		
32	Ge	Germanium	72.5900		
33	As	Arsenic	74.9216		
34	Se	Selenium	78.9600		
35	Br	Bromine	79.9040		
36	Kr	Krypton	83.8000		
37	Rb	Rubidium	85.4678		
38	Sr	Strontium	87.6200		
39	Y	Yttrium	88.9059		
40	Zr	Zirconium	91.2240		
41	Nb	Niobium	92.9064		
42	Mo	Molybdenum	95.9400		
43	Tc	Technetium	98.0000		
44	Ru	Ruthenium	101.0700		
45	Rh	Rhodium	102.9055		
46	Pd	Palladium	106.4000		
47	Ag	Silver	107.8680		
48	Cd	Cadmium	112.4100		
49	In	Indium	114.8200		
50	Sn	Tin	118.6900		
51	Sb	Antimony	121.7500		
53	I	Iodine	126.9045		
52	Te	Tellurium	127.6000		
54	Xe	Xenon	131.3000		
55	Cs	Cesium	132.9054		
56	Ba	Barium	137.3300	-11.63	BaO

c7h4o
250kj/kg

Compound	ΔHf (kJ/mol)
AgO(s)	-30.60
CuS(s)	-48.50
CuSO4(s)	-769.90
AgBr(s)	-99.50
AgCl(s)	-127.00
Fe3O4(s)	-1120.90
H2O(g)	-241.80
H2O(l)	-285.80
Al2O3(s)	-1669.80
BaCl2(s)	-860.10
BaCO2(s)	-1218.80
BaO(s)	-548.10
BaSO4(s)	-1465.20
Ca(OH)2(s)	-986.60
CaCl2(s)	-795.00
CaCO3(s)	-1207.00
CaO(s)	-635.50
CaSO4(s)	-1432.70
CCl4(l)	-139.50
CH3OH(l)	-238.60
CH4(g)	-74.80
CHCl3(l)	-131.80
C2H2(g)	226.70
C2H4(g)	52.30
C2H2O(l)	-277.60
C2H6(g)	-84.70
C3H8(g)	-103.80
n-C4H10(g)	-124.70
n-C5H12(l)	-173.10
CO(g)	-110.50
CO2(g)	-393.50
CoO(s)	-239.30
C2O7(s)	-1128.40
Cu2O(s)	-166.70
CuO(s)	-155.20
Charcoal(s)	
Diesel	-249.66
Sugar(s)	-2221.20
Coffee(s)	-243.20
Sawdust	-80.50
Glycerol	-669.60
Woodmeal	-945.80
MFTNB	-242.67
Barium Nitra	-991.90
Paraffin Wax	-2460.50

Compound	ΔHf (kJ/mol)
CuS(s)	-48.50
CuSO4(s)	-769.90
Fe2O3(s)	-822.20
Fe3O4(s)	-1120.90
H2O(g)	-241.80
H2O(l)	-285.80
H2O2(l)	-187.60
H2S(g)	-20.10
H2SO4(l)	-811.30
HBr(g)	-36.20
HCl(g)	-92.30
HF(g)	-268.60
HgO(s)	-90.70
HgS(s)	-58.20
HI(g)	25.90
HNO3(l)	-173.20
KBr(s)	-392.20
KCl(s)	-435.90
KClO3(s)	-391.40
KF(s)	-562.60
Mg(OH)2(s)	-924.70
MeCl2(l)	-641.80
MeCO3(s)	-1113.00
MeO(s)	-601.80
MeSO4(s)	-1278.20
MeO(s)	-384.90
MnO2(s)	-519.70
NaCl(s)	-411.00
NaF(s)	-569.00
NaOH(s)	-426.70
NH3(g)	-46.20
NH4Cl(s)	-315.40
K2O(s)	-363.17
KNO3(s)	-494.00
Nitrobenzene	67.50
NaClO3(s)	-365.40
NaNO3(s)	-467.00
Na2O(s)	-416.00
PbO2(s)	-277.00
KNO2(s)	-369.80
PbO(s)	-219.00

Compound	ΔHf (kJ/mol)
NH4NO3(s)	-367.50
NiO(s)	-244.30
NO(g)	90.40
NO2(g)	33.90
Pb2O4(s)	-734.70
PbBr2(s)	-277.00
PbCl2(s)	-359.20
PCl3(g)	-306.40
PCl5(g)	-398.90
SiO2(s)	-859.40
SnCl2(s)	-349.80
SnCl4(l)	-545.20
SnO(s)	-286.20
SnO2(s)	-580.70
SO2(g)	-296.10
SO3(l)	-395.20
ZnO(s)	-348.00
ZnS(s)	-202.90
Lead Azide	468.61
Lead Styphnate	-836.80
Mercury Fulminate	267.99
Tetrazine	189.12
DDNP	321.00
DADP	-598.50
TATP	151.40
HMTD	-363.00
Nitroglycerine	-370.70
Nitrocellulose (14.14)	-652.66
EGDN	-249.37
PETN	-499.27
PETN	-530.53
RDX	70.29
HMX	75.02
Nitroguanidine	-92.05
Picric Acid	-214.35
TNT	-62.07
Nitromethane	-74.76
Urea Nitrate	-562.79
Potassium Perchlorate	-430.12
Baritol	-295.00
Lead Styphnate	-836.80
Cheddite	-278.80
Ammonium Perchlorate	-290.60

Figure 7-3: Data Sheet for HME Calculator

Explainer: TOP LEFT CALCULATOR The top left table can accommodate up to 5 compositions (A, B, C, D and E). The table is used to calculate the molar proportion of each atom in 1 mol for the combined mixture. For example, AN-AI at 88/12 would display the molar proportions in 1 g. The data for empirical formula, molecular weight and oxygen balance is linked to the data sheet by [NAME] of molecule. Column D (molecular weight) MUST NOT have a value of zero in rows where there is no molecule or atom present. In this case the figure 0.0000001 is entered TOP RIGHT CALCULATOR This calculator is automatic and determines the proportions of each atom in the overall molecular composition of the HME. All that is required is for the user to enter the number of atoms of C, H, N, O, X, Y etc MIDDLE LEFT CALCULATOR This calculator is AUTOMATIC. DO NOT TOUCH. If the explosive composition is only CHNO based, then this formula automatically calculates the oxygen balance in CELL F24. By way of checking a degree of accuracy, column F in table 1 is averaged by percentage composition in CELL F29. Reference is Cooper. MIDDLE RIGHT CALCULATOR This calculator is AUTOMATIC, DO NOT TOUCH. It works on the oxygen balance formula derived for non-ideal explosives. To confirm accuracy, if the explosive were just CHNO based then the value in CELL S24 should be the same as the calculator and CELL F24. If it is not then the data in the TOP LEFT or TOP RIGHT tables have been entered incorrectly. If the explosive is non-ideal and of structure CHNOXYZ etc, then the oxygen balance derived in this table should not be the same as the MIDDLE LEFT calculator. TABLE 1 & TABLE 2 These are the K-W and modified K-W rules applied to the bottom table, dependent upon the oxygen balance and molecular formula derived in the TOP RIGHT and MIDDLE RIGHT calculators. BOTTOM TABLE - PULLING IT ALL TOGETHER The oxygen balance and molecular formula are AUTOMATICALLY transposed to CELLS B49 - B60. DO NOT TOUCH THOSE CELLS. The products of detonation are calculated based on the oxygen balance and the sequence that would be followed under the K-W or modified K-W rules. Based on the values in the cells, the CHECK column (column P50 - 60) should be ZERO. If values are not zero then STAGE 2 and STAGE 3 reaction are to be followed. ANAEROBIC and AEROBIC respectively. Column B on STAGE 2 will fill up with the associated check of unreacted product showing in column P. If there is anything left then STAGE 3 column B will show values to react with atmospheric oxygen. Up to end STAGE 2 is the determination of HEAT OF EXPLOSION Q. Any energy release under STAGE 3 would be classed as 'AFTERBURN'. TNTe The YELLOW BOX (CELL R56) shows the HEAT OF EXPLOSION FOR STAGES 1 and 2, divided by the HEAT OF EXPLOSION OF TNT.
--

Figure 7-4: Excel Calculator User Guide

For the first responder, calculations allow the determination of likely outcomes based on HME discovery, the types of ECP present, and to plan cordon and evacuation distances. This is important in pre- and post-blast bomb scene management [386], with Chapter 6 also facilitating blast injury and building damage prediction based on container geometry and crater size. This latter chapter has huge potential for further work, which will be discussed in Chapter 8 as cratering determination shall remain an Achilles Heel for some time to come.

7.3 Academic Underpinning

Academic underpinning has been required for three specific chapters given that mathematical, thermochemical and statistical concepts were developed. Chapter 3 introduces Bayesian belief updating to the C-IED process to better define the complexity of human beings in illicit diversion and how international efforts could be better applied at point of need. Chapters 5 and 6 introduce simple and effective calculations to determine the heat of explosion and TNT equivalence of HME compositions, addressing the worst-case outcomes for whatever fuel and oxidiser is used. In all cases, the academic underpinning has improved understanding and introduced concepts to new fields of study.

7.3.1.1 Determining Performance from Heat of Explosion

As recently as 2023 [387], attempts have continued to characterize non-ideal explosives in terms of performance and security threat, focusing on precise compositions. The reality is that HME recipes are not precise and are ‘cooked’ by criminals from the internet, where yield, purity, loading density, particle size, crystal habit, critical diameter, critical density and nature of confinement are seldom perfect. For example:

- the Parson Green bombing on 15th September 2017 failed to function as intended due to an issue with the explosive train [388].
- In December 2009, AQAP (Richard Reid) attempted to bring down an airliner travelling from Amsterdam to Detroit. The HME used was able to

slip through security checks, but the IED explosive train was of sub-optimal design given his choice of materials [389].

Richard Reid epitomises the quantity, type and ingenuity of HME formulations that can be devised, but that their non-ideal characteristics (see Chapter 5) require appropriate loading density, critical diameter, fuel particle size and specific stoichiometry to become detonable from an SII. As such, HME is complex, expensive and resource intensive to characterise with so many variables at play and the large-scale tests that would be required to make sense of them.

This aspect of the thesis therefore attempted to reduce an expensive UK-based trials burden, but still had to contend with three principal problems:

- understanding TNT equivalence;
- obtaining credible data on explosive performance; and
- generating a formula that could interpret HME compositions that may contain several fuels and oxidisers dependent upon supply chain availability.

7.3.1.1.1 TNT Equivalence

In terms of TNT equivalence, Chapter 5 highlighted the vagaries of experimental and theoretical values, dependent upon whether the value was applicable to brisance, heave, or heat output for example. A paper by Locking [281] proved pivotal since it brought together numerous values of TNT equivalence across decades of research and highlighted errors as high as 35% compared to one another for a myriad of testing regimes. As such, scientific rigour could only really apply within a calculator using heats of explosion, since the products of detonation could be determined from theory as opposed to experimental measurements. Having designed this calculator, TNT equivalence can now be determined within $\pm 10\%$ for HME compositions based on the three-stage process of anoxic detonation, anaerobic combustion and aerobic combustion.

7.3.1.1.2 Data capture of Explosive Performance

Obtaining data on explosive performance of non-ideal compositions is also difficult given that most HME are not listed at open source for obvious security

reasons. However, it was possible to obtain data for non-ideal explosives that had been manufactured or tested as explosives of interest in World Wars 1 and 2. It is from the following publications (references [31] [390] [391] [392] [393] [394] [395] [396] [397] [398] [399] [400] [401] [402]), and the work of Federoff and Sheffield [50], that a small number of explosives of known composition and heats of explosion could be used to test the validity of the formulae generated in Chapter 5. It must also be conceded that criminal entities likely obtained their manufacturing methodology from similar references and continue to monitor for improvement today.

For example, Favier first patented the detonative properties of AN with a fuel such as dinitro-naphthalene in 1885 [391] at weight percentages of 88% and 12% respectively. Kelso discussed precise ANFO compositions involving 96% AN and 4% diesel [403], citing previous works in his literature review. PIRA began to use ANFO in the early 1970's, thereby provoking diluent regulation in 1972 [130]. Diluent regulation using calcium ammonium nitrate (CAN) was defeated shortly thereafter by PIRA based on Naoum's discussion on diluents in 1924 [132]. Bohanek et al inform readers on the importance of prill size, loading density and nitrogen content associated with AN [87]. The most recent research [387] provides information on the need of a critical diameter in AN above 77 mm to obtain detonation, which can be reduced to 25 mm if Al is added.

As such, the values obtained for this research centre principally on the AMATOLS, ALUMATOLS, AMMONALS, BARONALS, BARATOLS, BURROWITES, CHEDDITES, DYNAMITES and MINOLS (whose original uses are described in the glossary), but also some primary compositions such as LA, LS, MF and the PEROXIDES of ACETONE such as DADP and TATP. They provide a good sample size from which to determine a generic formula, which is representative of criminal manufacture. And if the formula works for compositions comprising barium, aluminium, potassium, lead and mercury, then the academic rigour is adaptable for numerous fuel/oxidiser compositions.

7.3.1.1.3 Determining a reliable source of Heats of Formation

The next problematic step was to identify the enthalpies of formation for the explosives themselves, and standardised enthalpies of formation for the products of detonation. Again, it was possible to identify robust values (see Table 5-5) and to generate an excel spreadsheet that fed the calculator.

Whilst it was possible to determine the heats of formation for the oxidisers, many of the fuels (specifically the hydrocarbons) used by criminal entities offered no information, or significant variations in heats of formation. It is in this aspect (the fuels) that Chapter 5 determined that errors may be present, but which could be mitigated using bomb calorimetry. However, the results of calculator use identified that errors were within 10% of literature Q values, and favoured over-compensation as opposed to under-compensation. This scientific rigour therefore presented calculation risk as ALARP.

7.3.1.2 Determining Mass of HME Used from Crater Size

Academic underpinning was achieved in this part of thesis by focusing on numerous eminent literature publications on crater calculation [315] [323] [324] [325] [326] [328], and using the measurement methodology for crater dimensions promoted by Cooper [327], which has been used in those subsequent publications (see **Figure 6-2** for crater dimensions). This provided commonality in both measurement and terminology. However, Mandal, Goel and Agarwal [404] determine that there is such an elevated presence of complexity and non-linearity involved during crater formation, that the development of any analytical model is difficult. It is therefore necessary in this part of our understanding to develop empirical and semi-empirical formulae from experimental data. This is because the dimensions of a crater formed by a detonation is dependent upon so many variables, which Moorthy et al place into two main parameters – environmental and explosive [405]. A non-exhaustive list of environmental and explosive parameters can be seen in Table 7-3:

Table 7-3: Environmental and Explosive Parameters Associated with Crater Formation

<i>Environmental Parameters</i>	<i>Explosive Parameters</i>
<i>Soil density and composition</i>	Quantity of explosive used
<i>Strength and compaction</i>	Type of explosive used
<i>Moisture content</i>	Charge geometry of the charge
<i>Layering of soil medium</i>	Charge orientation (buried, surface, above surface),
<i>Atmospheric conditions</i>	Type of container housing charge
<i>Altitude.</i>	

These parameters associated with crater formation are so complex within literature that only those of potential significance to a terrorist were examined as part of this thesis [406]:

- explosive type;
- charge size;
- charge dimensions;
- charge position relative to the surface;
- the soil medium itself (alluvial soil in this instance); and
- the crater dimensions produced.

The author chose these criteria from the ICCT guidance [406] based on the data obtained by Rook, Carnes and Davis in 1974 [407], which considered data from British, American and Russian cratering trials between 1950 and 1970. The data described the contributory nature of explosive type, charge size, charge dimension, and charge position to crater formation.

As for soil conditions, current methodologies are limited by the lack of data from well-controlled tests that involve the full gamut of soil types, density and water content. This is, however, now in the process of being collated [408], but until

such improved data is published, soil criteria will remain within the realm of comparison.

Chapter 6 also focused on **surface explosions**, that is charges in contact with the ground (see Figure 7-5), and which can be visibly identified. As such, a comparison on crater size could not necessarily be used accurately for buried charges, above surface explosions, or free-air explosions [409]. For example (see Figure 7-6), buried charges are difficult to find by first responders, and if discovered, the depth of burial and point of detonation would be required to progress any effective crater calculation.

In the case of this figure, the EOD operator is unaware that the main charge is a cylinder approximately 60 cm in diameter and 90 cm in length ($L:D = 1.33:1$). He can only observe the top of the IED charge container (within the red ellipse) from a very light finger-tip search of the soil surface. The power source and point of initiation are at the base of the charge, some 100 cm below the soil surface, which the EOD operator cannot see.

To determine the precise location of the power source, interaction from the first responder with the IED would be required, thereby falling into the realms of positive EOD action [410]. In such a scenario, a cordon and evacuation would normally be required, with the EOD operator having to discount command and time devices in their threat assessment before any manual approach [318]. It is likely that the first responder would simply use semi-remote means in a complex case like this (such as placing a donor charge to detonate the IED *'in situ'*), with the crater dimensions being measured thereafter to *'guesstimate'* charge size.



Figure 7-5: Example of a 10 kg surface-laid main charge (PCFO) with switch © BCL



Figure 7-6: Example of a 40 kg buried main charge (PCFO) © BCL

A free-air explosion is not a credible scenario for the first responder either, since this involves blast waves interacting with structures from height before being reflected from the ground. If the first responder has got their threat assessment correct then they would not be in a position where free air bursts were a reality.

An example of such representative scenarios is shown below (Figure 7-7), where H_c is the height of the charge (W) above the ground, and R_c the horizontal distance of the charge from the base of the structure:

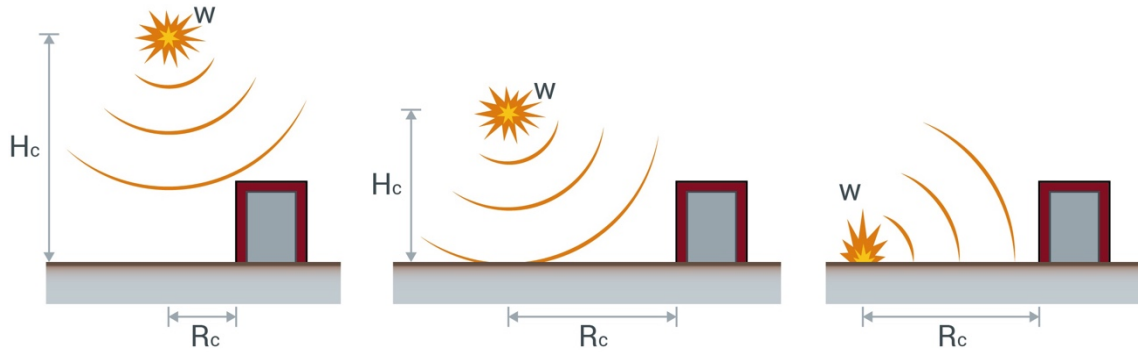


Figure 7-7: A diagrammatic representation of external explosion and blast loading orientation; (left) free-air burst, (middle) air burst, (right) surface burst.

However, if research were to improve such areas, then other equations/methods must be considered, and are available [404] for non-ideal explosions based on such scenarios. For buried charges, Chabai [411] reports that scaling laws neglect the effects of gravity and as such an exponent of $1/3.4$ as opposed to $1/3$ should be used. This is further refined by Westine [412] and Baker et al [413] for buried charges, where $\frac{R}{d}$ becomes a function of the following five variables:

$$\frac{R}{d} = f\left(\frac{W^{7/24}}{\rho^{7/24}g^{1/8}c^{1/3}d}\right) \quad (7-3)$$

Where W is the charge weight, R the crater radius, d the burial depth of the explosive, ρ the soil density and c the seismic velocity of the soil. Mandal et al [404] suggest that equation (7-3) works well when:

$$\frac{W^{7/24}}{d} > 0.3 \quad (7-4)$$

but can be hugely sensitive to variable changes when:

$$\frac{W^{7/24}}{d} < 0.3 \quad (7-5)$$

And finally, Ambrosini and Luccioni [414] provide a buried spherical charge assessment of the variation of crater diameter with scaled distance. The medium in this instance is described as brown clayey silt of low plasticity:

$$\log\left(\frac{D}{2d}\right) = 0.2993 \left[\log\left(\frac{W^{\frac{7}{24}}}{d}\right) \right]^3 + 1.8562 \left[\log\left(\frac{W^{\frac{7}{24}}}{d}\right) \right]^2 + 4.4913 \log\left(\frac{W^{\frac{7}{24}}}{d}\right) + 4.7946 \quad (7-6)$$

Where W is the charge weight [kg], D the crater diameter [m], and d [m] the depth of burial of the explosive in the soil.

Overall, this research has found crater prediction from many practical tests to be somewhat elusive given the lack of data pertaining to container shape. Whilst a comparison between hexahedral charges and spherical charges has been attempted in two media (asphalt and alluvial soil), there will remain a large disparity in crater parameter predictions from calculation and those observed in practical tests. As such, the first responder must continue to rely on support from theory and practical experience whilst further work is conducted.

7.3.1.3 Determining the Impact of Detonation on Human Beings

Academic rigour was achieved in this part of the thesis by using Hopkinson-Cranz scaling laws [311] [312] and validated blast parameters from Kinney & Graham [315], Kingery [313] and Kingery & Bulmash [314]. Hopkinson is important because his calculations state that:

“similar blast waves are produced at identical scaled distances when two explosive charges of similar geometry and the same explosive composition, but of different size, are detonated in the same atmosphere” [311].

As Chapter 6 demonstrates, similar charge geometries and identical compositions are used, thereby facilitating determinations of scaled distance (7-7), scaled time (7-8) and scaled impulse (7-9) as follows:

$$Z = \frac{R}{W^{1/3}} \quad (7-7)$$

$$\tau = \frac{t}{W^{1/3}} \quad (7-8)$$

$$I_{ss} = \frac{I_s}{W^{1/3}} \quad (7-9)$$

Using these equations within the automation of Bulson [356] and Vasilis [357], provides accurate data for the first responder, which can also be validated in simple graphical format using Bass' new standard for reflected and free field blast waves (Figure 6-8). It must be remembered, however, that HME does not behave in an ideal fashion. Density, charge shape, charge confinement, stoichiometry and blast reflections from surfaces all affect the performance [256] [268]. As such, the shape of the Friedlander blast wave may be recognisable, but energy release is retarded, leading to lower peak pressures, and longer positive and negative impulse durations. Such variation in overpressure and blast duration for non-ideal explosions is presented in two recent papers:

- graphically by Figuli et al [415], who compared blast wave propagations in air from charges of RDX and ANFO; and
- in tabular format by Gao et al [416] for PBX-1 and PBX-1 mixed with boron and aluminium (see Table 7-4, where Stages 1 – 3 refer to those discussed in Chapter 5 as anoxic detonation, anaerobic combustion and aerobic combustion).

Table 7-4: A comparison of ideal and non-ideal explosive detonation rates

Explosive	Thickness of DDZ (mm)	P _{cj} (GPa)	Energy Released (kJ kg ⁻¹)	Energy Release Rate (ms)		
				Stage 1	Stage 2	Stage 3
PBX-1 (HMX/Binder) (95/5)	0.3	32.67	5249	0.000044	0.0001	0
PBX-1+B/Al+Binder (64/10/10/16)	0.7	24.93	6184.9	0.000102	0.1 - 20	140

The pressure-time curves for Figuli demonstrate that HME compositions provide a retarded energy release, with blast propagating over a greater distance. Romero and Williams [417] contribute this to lack of oxygen balance, which causes energy to be released after the shock wave has transmitted into the surrounding air, and later reactions of detonation products with oxygen in the atmosphere as Table 7-4 demonstrates.

This thesis accounts for all phases of the blast wave from initiation (Stages 1 and 2) through to afterburn (Stage 3), thereby allowing rapid decision making on the likely effects of HME should they be discovered.

In this fashion the performance of any HME composition made from ECP could be determined whether it be buried, on the surface, or a free air burst. Based on the container or enhancements (such as '*shipyard confetti*') it would also be possible to determine fragment velocity using Gurney [418]. Fragmentation has not formed part of this research although it would be a logical follow-on step.

7.3.2 Products to Assist First Responders and Security Agencies

This thesis has identified three specific products that can be developed within user-friendly applications to assist in the regulation of ECP, determining human factors behind support and use, and the prediction of hazard. These three

products have all used extensive literature review, the application of theory, and practical trials for their underpinning and therefore present an academic as well as vocational tool for those required to use/implement them.

8 Conclusions

Non-state actors shall continue to exploit explosive chemical precursor risk strategies in the manufacture of home-made explosives. Real success in mitigation can only be achieved through advocacy and cooperation between governments, industry, suppliers, retail outlets and law enforcement, combined with the development and application of information management systems.

This thesis provides four pivotal mechanisms to assist in the identification of ECP that may have utility in IEDs and to assist the first responder in mitigation.

Firstly, this thesis has established a methodology for a global risk reduction system to prioritise chemical precursors to ensure that the ones most readily available chemically and commercially are effectively managed through standardisation. In doing so, it has already contributed to international policy at the highest level and the identification of one ECP (Urea Hydrogen Peroxide) that is not regulated, yet has utility in main charge explosive compositions.

Secondly, this thesis has used the concept of Bayesian Networks to identify the causal factors behind the illicit diversion of ECP in failed and failing states, thereby **introducing belief updating as a methodology to be applied to any part of the C-IED process**, military or humanitarian, thereby refining cost-benefit analysis and resource mobilisation. Coupled with strategic advocacy, this approach tackles both ends of the supply chain, thereby constraining opportunity for criminals.

Thirdly, this thesis has looked at how assistance can be provided to the first responder when faced with HME manufactured from ECP. It has **created a simple process for predicting the heat of explosion for both $C_aH_bN_cO_d$ explosives, and explosives comprising mixtures or organic, inorganic and organometallic compounds.** This method is useful to the first responder since an in-depth knowledge of the chemical or thermochemical properties of explosives is not required. Compared to TNT equivalence criteria published in literature, this procedure combines accuracy and simplicity to predict the

performance of numerous energetic materials based on the valence of the atoms that exist within any composition, and at what stage reactions take place. Variance from reported literature does exist, but at a scale much reduced from other methods of TNT equivalence (no more than $\pm 10\%$ in the examples provided as opposed to $\pm 30\%$).

Fourthly, calculation of HME performance is often based on spheres and hemispheres, not the actual geometry of the IED main charge container, or the warhead used. This thesis has determined the cratering performance of hexahedral charges (the most used container shape) **and**, based on crater size and volume in alluvial soil, determined **parameters that could be applied in other soil types** such as asphalt, **thereby allowing the first responder to determine the potential impact of blast waves on people and structures** using well-established Kingery-Bulmash, Bowen and Bass curves.

9 Data Availability

Technical data supporting this PhD thesis is available from CORD at:

- Chapter 5 - DOI: [10.17862/cranfield.rd.25047764](https://doi.org/10.17862/cranfield.rd.25047764); and
- Chapter 6 - DOI: [10.17862/cranfield.rd.25053614](https://doi.org/10.17862/cranfield.rd.25053614)

10 Future Work

10.1 Continuing Predictive Threat Analysis for ECP Identified

The oversight of chemical precursors appears to be devolved to several disparate Regulations or Acts. Using UHP as the example, commercially available carbamide peroxide is governed within the Cosmetic Products (Safety) (Amendment) Regulations 2012 [419], whilst urea, hydrogen peroxide and sulphuric acid are governed by the Deregulation Act 2015 [112]. Knowledge of both Acts was required for total visibility. In terms of the UK, the Deregulation Act 2015 combines poisons and ECP, and the link to the Cosmetic Regulations appears to work (the HP concentration in carbamide peroxide being changed to <12% for example), thus providing an approach much clearer than other countries. Therefore, future work must consider simplifying regulation in regions where there is a significant disconnect in information management. It is hoped that this function will be carried out globally by the UNCCT. For the UK, the Control of Explosives Precursors and Poisons Regulation 2023 will use predictive threat analysis to determine those precursors catching the eye of criminals.

10.2 Developing App-Based Systems

It is not appropriate to rely on excel-based systems to determine the heat of explosion of HME, or to aid first responders in safety and hazard assessment. The systems described in Chapters 5 and 6 should be simplified and provided as App-based technologies. Applications such as this can then exploit other available data for ECP such as GHS classification to determine the non-explosive hazard such as toxicity. The author has worked on the latter with GICHD, but this book is only available as a downloadable reference [64].

10.3 Continuing Bayesian Belief Updating

Given that the relevance of Bayesian belief updating has been proved by an expert panel and focus groups, its effective implementation within a DAG can now be refined by statisticians and mathematicians. In the meantime, its applicability can be considered by C-IED enablers and offered as part of theoretical 'good practice' on Defence & Security platforms [420].

10.4 Developing Crater Efficiency Criteria for All Soil Mediums

There is a clear need for further research to be conducted on determining the quantity of explosive used in post-blast scenarios dependent upon soil type, charge dimensions and placement (above surface, surface or buried).

Aside the equations derived in this thesis, and those presented in Table 6-1, it may be that the intelligent use of penetration equations, such as those produced by Young [421], could be adapted to consider penetration as depth of burial for a variety of charge shapes and container material. This is logical if one considers that the explosive train must survive to get to that depth. Young uses cylinders of varying L:D ratio to gain predictions of crater diameter to within 15% for soil media ranging from rock, concrete, ice, dense, dry, cemented sand, to soils of very low shear strength such as clay marine sediments. He also considers geometric scaling laws and how the average cross-sectional diameter of non-cylindrical shapes can be determined. There are then the more exotic and numerical simulations of buried explosions and crater size which could be reviewed, although most focus on one fixed variable such as charge size [422], soil medium [423] or charge shape [424], which does not underpin a broader understanding.

As such, future work in this arena is required since it has application in both the humanitarian and security sector. Most importantly, it is hugely pertinent in the reconstruction process following current conflicts such as Yemen, Syria, the Ukraine and Gaza, allowing first responders to determine the likely effects of positive EOD action on infrastructure close by, or for business interruption insurance to be accurately assessed within the insurance industry. It is therefore suggested that such research focus on surface and buried charges of hexahedral and cylindrical dimensions, which are more representative of the menace posed by non-state actors and ERW of the 21st century.

It is believed that the following equations (Table 10-1), when used in conjunction with Figure 2-1, shall provide an effective strategy for ECP risk mitigation.

Table 10-1: Summary of pivotal equations calculated in this thesis

Chapter	Equation	Remarks
2	$\therefore \Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} - \frac{Li}{2} - \frac{Na}{2} - \frac{K}{2} + \frac{F}{2} + \frac{Cl}{2} + \frac{Br}{2} + \frac{I}{2} - Mg - Ba - Zn - Sr - \frac{3Al}{2} - \frac{3B}{2} - 2Pb}{molecular\ weight} \right) \times 100$	Oxygen balance formula for a non-ideal explosive – by atom
2	$\therefore \Omega = \frac{15.999 \left(d - 2a - \frac{b}{2} + (2 \sum Valence(\pm 4) + \frac{3}{2} \sum Valence(\pm 3) + \sum Valence(\pm 2) + \frac{1}{2} \sum Valence(\pm 1) + \dots) \right)}{molecular\ weight} \times 100$	Oxygen balance formula for a non-ideal explosive – by valence
6	$V_e^{1/3} = 0.1687M^{1/3}$	Experimental apparent crater volume in asphalt for hexahedral charges (surface detonation L:H ≤ 1.5).
6	$V_c^{1/3} = 0.175M^{1/3}$	Theoretical apparent crater volume for the same spherical mass of explosive (surface detonation).
6	$V_b = 0.339V_c$	Comparison of the apparent volume of a crater from a hexahedral charge on asphalt, to that of a spherical charge in the same medium.

Chapter	Equation	Remarks
6	$V_a \approx 3V_b$	The relationship between craters from surface explosions of hexahedral charges on asphalt and alluvial soil.
6	$R_a = (0.46 + 0.027P_{cj})(2E_{CR}M)^{1/3}$	The relationship between craters from surface explosions of spherical charges in any medium if the cratering efficiency factor of that medium (E_{CR}) is known.
7	$\frac{R}{d} = f\left(\frac{W^{7/24}}{\rho^{7/24}g^{1/8}c^{1/3}d}\right)$	The relationship of apparent radius and depth for spherical charges buried in alluvial soil, which could be adapted for hexahedral charges.
7	$\log\left(\frac{D}{2d}\right) = 0.2993 \left[\log\left(\frac{W^{7/24}}{d}\right) \right]^3 + 1.8562 \left[\log\left(\frac{W^{7/24}}{d}\right) \right]^2 + 4.4913 \log\left(\frac{W^{7/24}}{d}\right) + 4.7946$	The relationship of D/d to W for buried charges in brown clayey silt of low plasticity. E_{CR} could, perhaps, be introduced here.

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Appendices

Appendix A Ethical approval letters



2 August 2021

Dear Brig Collett ,

Reference: CURES/14300/2021

Title: Analysing the Human Environment and its Impact on the Illicit Diversion of Explosive Chemical Precursors within the Global Supply Chain.

Thank you for your application to the Cranfield University Research Ethics System (CURES).

We are pleased to inform you your CURES application, reference CURES/14300/2021 has been reviewed. You may now proceed with the research activities you have sought approval for.

If you have any queries, please contact CURES Support.

We wish you every success with your project.

Regards,

CURES Team



27 August 2021

Dear Brig Collett ,

Reference: CURES/14415/2021

Title: The use of a predictive threat analysis to propose revisions to existing risk assessments for precursor chemicals used in the manufacture of home-made explosives (HME)

Thank you for your application to the Cranfield University Research Ethics System (CURES).

We are pleased to inform you your CURES application, reference CURES/14415/2021 has been reviewed. You may now proceed with the research activities you have sought approval for.

If you have any queries, please contact CURES Support.

We wish you every success with your project.

Regards,

CURES Team



22 August 2023

Dear Brig Collett ,

Reference: CURES/20500/2023

Project ID: 23587

Title: Calculating The Heat Of Explosion For Non-Ideal Explosives

Thank you for your application to the Cranfield University Research Ethics System (CURES).

We are pleased to inform you your CURES application, reference CURES/20500/2023 has been reviewed. You may now proceed with the research activities you have sought approval for.

If you have any queries, please contact CURES Support.

We wish you every success with your project.

Regards,

CURES Team



5 September 2023

Dear Brig Collett ,

Reference: CURES/20644/2023

Project ID: 23588

Title: Understanding human survivability from ammonium nitrate and aluminium homemade explosives used in typical main charge containers

Thank you for your application to the Cranfield University Research Ethics System (CURES).

We are pleased to inform you your CURES application, reference CURES/20644/2023 has been reviewed. You may now proceed with the research activities you have sought approval for.

If you have any queries, please contact CURES Support.

We wish you every success with your project.

Regards,

CURES Team

United Nations Development Programme
برنامج الأمم المتحدة الإنمائي

To: Mr Gareth Collett CBE
PhD Student 609293
Cranfield University
Shrivenham SN6 8LA
United Kingdom



31 May 2022

Subject: Approval to use qualitative evidence from focus groups to progress PhD studies in explosive chemical precursor diversion in Yemen

Dear Gareth,

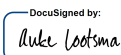
I am very pleased to hear that your multi-disciplinary PhD regarding explosive chemical precursors is progressing well, and that your first paper was published in the Heliyon Journal last year.

Regarding the second paper, which looks at applying artificial intelligence methods to refine causality behind explosive chemical precursor diversion, UNDP Yemen is content for you to use the data gathered by yourself and Responsiveness for Relief and Development (RRD). For reasons of ethics, the paper must be written in a 'stateless' fashion with no reference to Yemen or its governorates, and refer solely to focus group outcomes in a qualitative fashion. Neither the implementing partner (RRD), nor the names of the experts who assisted, are to be divulged. This is clearly intimated in your abstract and ethical proposition below.

You will be pleased to hear that under the governance and rule of law programme, funding is secured to progress focus group belief updating throughout 2023 and 2024. I sincerely hope that Bayesian network strategies will be examined by academia to determine if the application in C-IED delivers results. Whatever the outcome, this is an extremely novel and cost-effective approach and I wish you the very best of success.

Subject to the conditions above, I am therefore happy for you to proceed with this vital piece of work relating to human security, which will better inform those states faced with the manufacture and use of homemade explosives at scale.

Yours sincerely

DocuSigned by:

851F417AE3124F5...
Auke Lootsma

Resident Representative

UNDP

Yemen

Appendix B - Baseline calculations for FEFO & PBX107

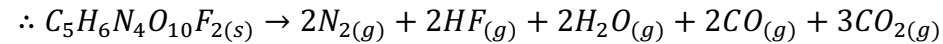
B.1 Baseline calculations for FEFO ($C_5H_6N_4O_{10}F_{2(s)}$)

$$\Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} + \frac{f}{2}}{\text{molecular weight}} \right) \times 100$$

$$\therefore \Omega = 15.999 \times \left(\frac{10 - 10 - \frac{6}{2} + 1}{320.12} \right) \times 100 = -9.99\%$$

$$\therefore \text{products of detonation} \rightarrow \frac{c}{2}N_2 + fHF + \left(\frac{b-f}{2} \right)H_2O + \left(2a - d + \frac{b-f}{2} \right)CO + \left(d - a - \frac{b-f}{2} \right)CO_2$$

$$\therefore C_5H_6N_4O_{10}F_2 \rightarrow \frac{4}{2}N_2 + 2HF + \left(\frac{6-2}{2} \right)H_2O + \left(10 - 10 + \frac{6-2}{2} \right)CO + \left(10 - 5 - \frac{6-2}{2} \right)CO_2$$



B.2 Baseline calculations for PBX 9407 ($C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09(s)}$)

$$\Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} + \frac{f}{2} + \frac{cl}{2}}{\text{molecular weight}} \right) \times 100$$

$$\therefore \Omega = 15.999 \times \left(\frac{2.69 - 2(1.41) - \frac{2.66}{2} + \frac{0.09}{2} + \frac{0.07}{2}}{102.42} \right) \times 100$$

$$\therefore \Omega = 15.999 \times (-0.0135) \times 100 = -21.58\%$$

$$\therefore C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09} \rightarrow \frac{c}{2}N_2 + fHF + clHCl + \left(\frac{b - f - cl}{2} \right) H_2O + \left(2a - d + \frac{b - f - cl}{2} \right) CO + \left(d - a - \frac{b - f - cl}{2} \right) CO_2$$

$$\therefore C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09}$$

$$\begin{aligned} &\rightarrow \frac{2.54}{2}N_2 + 0.09HF + 0.07HCl + \left(\frac{2.66 - 0.09 - 0.07}{2} \right) H_2O + \left(2.82 - 2.69 + \frac{2.66 - 0.09 - 0.07}{2} \right) CO \\ &+ \left(2.69 - 1.41 - \frac{2.66 - 0.09 - 0.07}{2} \right) CO_2 \end{aligned}$$

$$\therefore C_{1.41}H_{2.66}N_{2.54}O_{2.69}Cl_{0.07}F_{0.09(s)} \rightarrow 1.27N_{2(g)} + 0.09HF_{(g)} + 0.07HCl_{(g)} + 1.25H_2O_{(g)} + 1.38CO_{(g)} + 0.03CO_{2(g)}$$

Appendix C - Baseline Calculations for Ammonium Nitrate/Aluminium (88/12)

Appendix Table 10-1: Molecular Formula Calculation for AN-Al (88/12)

Molecule	Empirical Formula	Proportion by Mass (g)	Molecular Weight (g)	Molar Proportions in 1g	C	H	N	O	Al
Ammonium Nitrate	NH ₄ NO ₃	0.88	80.043480	0.010994	0	4	2	3	0
Aluminium	Al	0.12	26.981540	0.004447	0	0	0	0	1
TOTALS		1		0.015442	0	0.043976	0.021988	0.032982	0.004447

Note 4: Owing to the small molar proportions in 1g of explosive, up to six decimal places are used in Table 8 calculations where required.

The aluminium competes with the detonation products formed, in this case $H_2O_{(g)}$ and any excess oxygen remaining upon formation of the detonation products. As this is a non-ideal explosive, the start point is Equation 19 to determine the oxygen balance for 1 g of composition:

$$\therefore \Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} - \frac{Li}{2} - \frac{Na}{2} - \frac{K}{2} + \frac{F}{2} + \frac{Cl}{2} + \frac{Br}{2} + \frac{I}{2} - Mg - Ba - Zn - Sr - \frac{3Al}{2} - \frac{3B}{2} - 2Pb}{1} \right) \times 100$$

$$\therefore \Omega = 15.999 \times \left(\frac{d - 2a - \frac{b}{2} - \frac{3Al}{2}}{1} \right) \times 100$$

$$\therefore \Omega = 15.999 \times \left(\frac{0.032982 - \frac{0.043976}{2} - \frac{3}{2}(0.004447)}{1} \right) \times 100$$

$$\therefore \Omega = +6.92\%$$

The heat of explosion for this reaction is then determined from Hess' Law, with enthalpy values taken from Table 5-5:

$$\Delta H_{reaction}^{\theta} = \sum \Delta H_{f(products)}^{\theta} - \sum \Delta H_{f(reactants)}^{\theta}$$

$$\therefore H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447} \rightarrow \frac{c}{2}N_2 + \left(\frac{b}{2}\right)H_2O + aCO_2 + \left(\frac{2d-b}{4} - a\right)O_2 + alAl \{STAGE\ 1\}$$

$$\begin{aligned} \therefore H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447} \\ \rightarrow \frac{0.021988}{2}N_2 + \left(\frac{0.043976}{2}\right)H_2O + \left(\frac{(2 \times 0.032982) - 0.043976}{4}\right)O_2 + 0.004447Al \{STAGE\ 1\} \end{aligned}$$

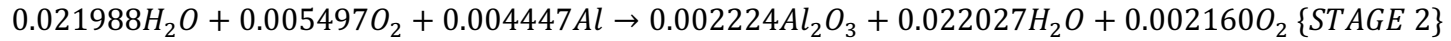
$$\therefore H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447} \rightarrow 0.010994N_2 + 0.021988H_2O + 0.005497O_2 + 0.004447Al \{STAGE\ 1\}$$

$$\therefore Q_{Stage\ 1} = \{(0.021988 \Delta H_f(H_2O(g)))\} - \{0.010994 \Delta H_f(Al(s))\}$$

$$\therefore Q_{Stage\ 1} = \{(0.021988 \times -241.8)\} - \{(0.010994 \times -365.3)\}$$

$$\therefore Q_{Stage\ 1} = -1.30\ kJg^{-1} = -1300\ kJkg^{-1}$$

At the end of Stage 1, the aluminium reacts with the product(s) of detonation as follows (see assumption 4 from Table 5-4):



$$\therefore Q_{Stage\ 2} = \{(0.022027\Delta H_f(H_2O(g))) + (0.002224 \times \Delta H_f(Al_2O_3(s)))\} - \{(0.021988 \times \Delta H_f(H_2O(g)))\}$$

$$\therefore Q_{Stage\ 2} = \{(0.022027 \times (-241.8)) + (0.002224 \times (-1669.8))\} - \{0.021988 \times (-241.8)\}$$

$$\therefore Q_{Stage\ 2} = \{-9.04\} - \{-5.32\} = -3720\ kJkg^{-1}$$

$$\therefore Q_{Stage\ 1} + Q_{Stage\ 2} = (-1300) + (-3720) = -5020\ kJkg^{-1}$$

Therefore, the calculated value of Q_e is 101.8% that of the reported literature value. Q_e in kJmol^{-1} has been calculated as follows:

$$1 \text{ mol } NH_4NO_3 = 80.04 \text{ g}$$

$$1 \text{ mol } Al = 26.98 \text{ g}$$

$$\therefore 1000\text{g mixture contains } 880\text{g } NH_4NO_3 = 10.99 \text{ mol}$$

$$\therefore 1000\text{g mixture contains } 120\text{g } Al = 4.45 \text{ mol}$$

$$\therefore \text{mol}\% NH_4NO_3 = \left(\frac{10.99}{10.99 + 4.45} \right) \times 100 = 71.2\% = 56.97\text{g}$$

$$\therefore \text{mol}\% Al = \left(\frac{4.45}{10.99 + 4.45} \right) \times 100 = 28.8\% = 7.77\text{g}$$

$$\therefore 1 \text{ mol} = 64.77\text{g}$$

$$\therefore Q_{Stage\ 1} + Q_{Stage\ 2} = -5020 \times \left(\frac{64.77}{1000} \right) = -325.15 \text{ kJmol}^{-1}$$

$$\therefore H_{0.043976}N_{0.021988}O_{0.032982}Al_{0.004447(s)} \rightarrow 0.010994N_{2(g)} + 0.022027H_2O_{(g)} + 0.00216O_{2(g)} + 0.002224Al_2O_{3(s)}$$

Appendix D - A comparison of precursor chemical priorities by Nation/Organisation

Appendix Table 10-2: A comparison of ECP by nation and status prepared for UNGA 77 [93] and updated to include UHP, perborates and percarbonates

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
Acetone			X		**	X		X	INDEPENDENT. Used principally in the preparation HME detonator and main charge compositions comprising TATP, HMTD, and DADP. Acetone provides one third of global solvent use. Cannot be substituted, must be controlled.
Aluminium powder	A	X	X			X		X	INDEPENDENT. Al is used as metal fuel in HME formulations. The definition of a good metal fuel is one which resists air oxidation and moisture, has a high heat output/g and is obtainable at moderate cost in a range of particle sizes. Al is therefore a cheap and available option within the metal supply chain compared to titanium, tungsten and zirconium. Used as a performance enhancer in HME, specifically thermobaric compositions at lower particle size. Must be controlled.
Ammonium	A	X	X	X	X	X	X	X	INDEPENDENT. Used widely in fertilizers (white powder or prill),

⁷ Voluntary National Code of Practice for Chemicals of Security Concern (96 chemicals of concern identified, with 15 considered priority for HME)

⁸ Explosives Act and Explosives Regulations for the safe and secure handling of explosives (Part 20)

⁹ The Environmental Pollution Control Act (2007) identifies 15 hazardous substances in HME use.

¹⁰ Explosive Substance Act 1883, Terrorism Acts 2000 and 2006, Poisons Act 1972, The Fireworks Act 2003 and Fireworks Regulations 2004, The Explosives Regulations 2014 (implementation of EU 98/2013), Pyrotechnics Articles (Safety) Regulations 2015

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
nitrate									freezing mixtures (cool packs), anaesthetics (manufacture of nitrous oxide), the manufacture of commercial explosives and as a gasifiable oxygen carrier in rocket propellants. Agreement needs to be established on a standardised % nitrogen content. Must be controlled as it is has been widely used in a variety of powerful HME compositions.
Ammonium perchlorate	C	X		X			X		INDEPENDENT. Used to make rocket propellants, explosives, pyrotechnics, as an etching and engraving agent, or in analytical chemistry When mixed with aluminium it can become a significant driving agent for blast effects and thrust. Less powerful than AN-based mixtures of comparison but makes a most effective improvised propellant explosive for projected IEDs. Must be controlled.
Antimony trisulfide	C								INDEPENDENT. Used as a fuel in detonator compositions. Surprised this is not controlled to any degree given that detonator compositions describing its role with TATP/HMTD are available on line.
Barium nitrate									INDEPENDENT. Barium nitrate is generally used in the manufacture of fireworks. In military applications it was used with TNT to form Baratol, achieving higher loading densities and higher explosive performance than the amatols. Barium nitrate can also be mixed with aluminium to form an explosive composition (commonly known as flash powder), or with thermite to form thermate, which is used in military thermite grenades. Widely available and must be controlled since HME compositions in confinement produce high blast and

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
									fragmentation.
Calcium ammonium nitrate	A		X			X		X	INDEPENDENT. Can be modified to be readily detonable with a booster. Must be controlled.
Calcium nitrate	B		X					X	INDEPENDENT. Calcium nitrate is used as an oxidizer in ammonium nitrate slurries, as a fertiliser, or as a component of fast setting concrete. Must be controlled.
Erythritol									DEPENDENT. Can be used to produce the explosive ETN through acid catalysts. The procedure is relatively simple, the explosive product being used in detonators. Must be controlled.
Ethylene Glycol									DEPENDENT. Ethylene glycol is used to make EGDN , a very powerful explosive can be synthesized by nitration. Globally available, this is a precursor that should be controlled in terms of standardization.
Guanidine nitrate							X		DEPENDENT. Guanidine is the precursor of guanidine nitrate, which in turn is the precursor to nitroguanidine. Both these are high energy explosive compositions. As such, guanidine itself should be controlled more readily than it is.
Hexamine	C		X		**			X	DEPENDENT. Widely available in retail as a camping fuel. As an explosive precursor, hexamine is used in the manufacture of RDX (hexamine plus 99% nitric acid), C-4, HMX and HMTD. Must be controlled and viable substitutes pursued.

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
Hydrazine									INDEPENDENT. hydrazine is used in various rocket fuels and to prepare the gas precursors used in airbags. With ammonium nitrate it can produce a liquid explosive of significant power. Must be controlled.
Hydrochloric acid	B								INDEPENDENT. Hydrochloric acid in the bracket of 35 – 38% w/w is commonly referred to as concentrated. It is so widely used it is extremely difficult to ban or substitute.
Hydrogen peroxide	A	X	X	X	X	X	X	X	INDEPENDENT. Used principally in bleaching applications or as rocket mono-propellants and oxidizers in the aerospace industry. Can form OPE and HPOM compositions. Upper limit concentrations vary between 12 and 65% w/w. Perpetrator has already overcome concentration issues so OPE/HPOM will endure. Pushing the concentration limit as low as practically possible is the key, or finding alternative substitute.
Magnesium powder	C		X					X	INDEPENDENT. Similar to Al
Magnesium powder	C	X	X					X	INDEPENDENT. Similar to Al
Magnesium nitrate hexahydrate			X					X	DEPENDENT. Used to produce concentrated nitric acid, essential in the nitration process for several HME compositions. Given its ability, it should be more broadly controlled.
Methyl Ethyl									DEPENDENT. Used as a precursor with hydrogen peroxide and

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
Ketone									nitric acid to form MEKP, an OPE. For use in detonators so must be controlled in retail or alternative substitutes found.
Nitric acid	A	X	X	X	X	X		X	INDEPENDENT. Upper limit concentrations vary. This is odd given that concentrated nitric acid is the proponent of nitration reaction in precursor modification.
Nitrobenzene									INDEPENDENT. Nitrobenzene is a semi-explosive liquid, being explodable by detonator, but limited in performance by a huge oxygen deficit. Extremely potent when mixed with ammonium nitrate. Must be controlled.
Nitromethane	A	X	X	X	X	X		X	INDEPENDENT. commonly used as a solvent in a variety of industrial applications such as dry cleaning, the manufacture of pharmaceuticals, pesticides, explosives, fibres, and coatings. Again, the upper limit concentration varies and needs to be standardized.
Pentaerythritol	C								DEPENDENT. The precursor for PETN explosive when nitrated. Must be controlled.
Perchloric acid				X			X		INDEPENDENT. Perchloric acid is usually sold in an aqueous solution where concentrated perchloric acid refers to concentrations of 70% by weight or more. It is used almost exclusively in the manufacture of perchlorate explosives. Must be controlled.
Percarbonates									DEPENDENT. Commonly available over the counter and a solid and stable source of hydrogen peroxide. When added to acetone and

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
									acid, it produces TATP, DADP and other OPE. There would not appear to be no control measures in place.
Perborates									DEPENDENT. As per the percarbonates.
Phenol	C								DEPENDENT. a hugely important precursor chemical in plastic manufacture, a large collection of drugs (such as aspirin) and for obtaining nucleic acids from tissues or cell cultures in medicine. Can produce picric acid, a powerful explosive, when nitrated. Must be controlled.
Phosphorus		X		X					DEPENDENT. A huge variety of uses, difficult to control, so standardization and monitoring are essential.
Potassium chlorate	A	X	X	X	X	X	X	X	INDEPENDENT. The principal component of chlorate-based explosives, incendiaries, primer formulations, pyrotechnics and matchhead compositions. Pure potassium chlorate cannot be detonated, but when a small percentage of any fuel is mixed with it, an extremely fast burning explosive is produced. Must be controlled and substitutes sought wherever possible.
Potassium nitrate	B		X	X	X	X	X	X	INDEPENDENT. Potassium nitrate is the oldest solid oxidizer used in high-energy mixtures such as black powder, pyrotechnic compositions and industrial explosives. Potassium nitrate will not undergo an explosion by itself but deflagrates and detonates when mixed with other fuels and binders. Must be controlled.
Potassium	C						X		INDEPENDENT. A strong oxidizer and preservative similar to

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
nitrite									sodium nitrite in its properties. One would expect it to be monitored in a similar fashion.
Potassium perchlorate	A	X	X	X	X	X	X	X	INDEPENDENT. Potassium perchlorate has gradually replaced potassium chlorate as the principal oxidizer in civilian pyrotechnics . It will burn to detonation when confined and mixed with metal fuels. Must be controlled.
Potassium permanganate	B	X							INDEPENDENT. Potassium permanganate is a strong oxidising agent and medication for cleaning wounds and general disinfection. It is on the WHO's list of essential medicines . It is non-combustible but when mixed with finely divided fuels such as aluminium, the mixture may be explosive. Contact with liquid combustible materials may result in spontaneous ignition. Potassium permanganate has been mixed with aluminium to produce detonable formulations. Difficult to substitute but can be controlled.
Sodium azide		X		X					DEPENDENT. Sodium azide is commercially available and is used in the airbag mechanisms of many older generation cars, aeroplane escape slides, emergency life-rafts, a biocide in hospitals and pest control in agriculture. As such, it is widely available and inexpensive. As an explosive precursor it is used in the manufacture of lead azide. It must be controlled to restrict the manufacture of improvised detonators.
Sodium chlorate	A	X	X	X	X	X	X	X	INDEPENDENT. A less-expensive substitute for potassium chlorate and therefore readily available as a weed killer. Will produce

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
									detonable mixtures with fuels. Must be monitored.
Sodium nitrate	B	X	X		X	X	X	X	INDEPENDENT. Used in the explosives industry and is a common precursor in the manufacture of nitro starch and dynamites. Similar to potassium nitrate. Must be monitored.
Sodium nitrite	B								INDEPENDENT. Powerful oxidizer. Sits on the WHO list of essential medicines given use in dyes, pesticides and pharmaceuticals, as a food additive and as an antidote to cyanide poisoning. Difficult to monitor or substitute.
Sodium perchlorate			X	X			X	X	INDEPENDENT. Of interest as a precursor in the manufacture of ammonium perchlorate, potassium perchlorate and perchloric acid
Sulphur	B								INDEPENDENT. Broadly available, numerous applications, difficult to substitute or monitor effectively.
Sulphuric acid	B		X	X	**			X	DEPENDENT. At 98% concentration it is called concentrated sulphuric acid. Sulphuric acid is the largest manufactured chemical in the world. The addition of sulphuric acid to nitric acid intensifies the nitrating properties of nitric acid. Must be controlled but difficult to police.
Urea	B				**	X		X	DEPENDENT. A nitrogen-release fertilizer. Can form urea nitrate with nitric acid. Destructive power similar to AN. Can also produce TMDD , an amine peroxide explosive for use in detonators. Must be controlled and monitored wherever possible.
Urea								X	INDEPENDENT. Moderately available and solid source of hydrogen

Precursor	USA NAS	CFATS	EU	AUS ⁷	CAN ⁸	PGS	Singapore ⁹	UK ¹⁰	Precursor Status and Remarks
Hydrogen Peroxide									peroxide. Can be easily synthesised from chemicals that are not regulated, and which could not be substituted or standardised.
Urea ammonium nitrate	A								INDEPENDENT. See urea and ammonium nitrate. Requires stringent control.
Zinc powder	B								INDEPENDENT. Similar to Al and Mg

Notes: National Academies Committee Recommendations (NAS); Chemical Facilities Anti-Terrorism Standards (CFATS); European Union (EU); Australia (AUS); Canada (CAN); Programme Global Shield (PGS); Unregulated Watch List**

Appendix E – The Detonation of Hexahedral Surface-Laid Charges in Alluvial Soil

E.1.1 Experimental Results in Detail (available at DOI: 10.17862/cranfield.rd.25047764)

Location Firings							ELLIPTICAL				SPHERICAL									
							a	b	He	E	De	Dt	C	Hc	B					
Date	Location	Explosive	Mass ANAL (kg)	TNTe M (kg)	M ^{1/3}	Position of Charge	Crater D 1 (m)	Crater D 2 (m)	Crater Depth H (m)	Ve (m³) Apparent Experimental Elliptical	Crater Diameter Experimental De (m)	Crater Diameter Theoretical Dt (m) Ambrosini	Va (m³) spherical Cooper	Crater Depth Cooper (m)	Vb Apparent	E/C	He/Hc	E/B	C/B	
Wednesday, 18 December 2019	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.49	0.58	0.18	0.027	0.533	0.759	0.032	0.158	0.008436	85%	114%	317%	375%	
Wednesday, 18 December 2019	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.46	0.54	0.22	0.029	0.498	0.759	0.032	0.158	0.008436	90%	139%	339%	375%	
Wednesday, 18 December 2019	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.47	0.60	0.18	0.027	0.531	0.759	0.032	0.158	0.008436	84%	114%	315%	375%	
Wednesday, 12 February 2020	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.45	0.49	0.26	0.030	0.467	0.759	0.032	0.158	0.008436	94%	164%	352%	375%	
Wednesday, 12 February 2020	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.48	0.56	0.22	0.031	0.518	0.759	0.032	0.158	0.008436	98%	139%	367%	375%	
Wednesday, 12 February 2020	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.46	0.49	0.26	0.030	0.472	0.759	0.032	0.158	0.008436	96%	164%	360%	375%	
Wednesday, 24 March 2021	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.42	0.54	0.24	0.028	0.476	0.759	0.032	0.158	0.008436	90%	152%	338%	375%	
Wednesday, 24 March 2021	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.46	0.57	0.2	0.027	0.512	0.759	0.032	0.158	0.008436	87%	126%	325%	375%	
Wednesday, 21 April 2021	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.44	0.53	0.22	0.027	0.483	0.759	0.032	0.158	0.008436	85%	139%	318%	375%	
Wednesday, 21 April 2021	Mukalla	ANAL	5.68	5.907	1.81	Surface (HtL)	0.42	0.56	0.21	0.026	0.485	0.759	0.032	0.158	0.008436	82%	133%	306%	375%	
Wednesday, 21 April 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.54	0.66	0.34	0.063	0.597	1.002	0.073	0.209	0.022536	87%	163%	281%	323%	
Wednesday, 21 April 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.57	0.63	0.32	0.060	0.599	1.002	0.073	0.209	0.022536	83%	153%	267%	323%	
Thursday, 17 June 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.55	0.68	0.36	0.070	0.612	1.002	0.073	0.209	0.022536	97%	173%	313%	323%	
Thursday, 17 June 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.53	0.74	0.33	0.068	0.626	1.002	0.073	0.209	0.022536	93%	158%	301%	323%	
Thursday, 17 June 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.54	0.72	0.33	0.067	0.624	1.002	0.073	0.209	0.022536	92%	158%	298%	323%	
Thursday, 17 June 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.52	0.71	0.33	0.064	0.608	1.002	0.073	0.209	0.022536	88%	158%	283%	323%	
Wednesday, 15 September 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.57	0.68	0.35	0.071	0.623	1.002	0.073	0.209	0.022536	98%	168%	315%	323%	
Wednesday, 15 September 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.53	0.70	0.38	0.074	0.609	1.002	0.073	0.209	0.022536	102%	182%	327%	323%	
Wednesday, 15 September 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.58	0.74	0.32	0.072	0.655	1.002	0.073	0.209	0.022536	99%	153%	319%	323%	
Wednesday, 15 September 2021	Mukalla	ANAL	13.04	13.56	2.38	Surface (HtL)	0.53	0.76	0.31	0.065	0.635	1.002	0.073	0.209	0.022536	90%	149%	290%	323%	
Wednesday, 15 September 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.68	0.88	0.44	0.138	0.774	1.262	0.145	0.263	0.045107	95%	167%	305%	322%	
Tuesday, 23 November 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.64	0.85	0.46	0.131	0.738	1.262	0.145	0.263	0.045107	90%	175%	290%	322%	
Tuesday, 23 November 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.62	0.90	0.44	0.128	0.747	1.262	0.145	0.263	0.045107	88%	167%	285%	322%	
Tuesday, 23 November 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.60	0.89	0.43	0.120	0.731	1.262	0.145	0.263	0.045107	83%	164%	266%	322%	
Tuesday, 23 November 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.61	0.88	0.42	0.118	0.733	1.262	0.145	0.263	0.045107	81%	160%	262%	322%	
Tuesday, 23 November 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.64	0.86	0.44	0.127	0.742	1.262	0.145	0.263	0.045107	87%	167%	281%	322%	
Wednesday, 16 February 2022	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.68	0.85	0.43	0.130	0.760	1.262	0.145	0.263	0.045107	89%	164%	288%	322%	
Wednesday, 16 February 2022	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.70	0.82	0.42	0.126	0.758	1.262	0.145	0.263	0.045107	87%	160%	280%	322%	
Wednesday, 16 February 2022	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.61	0.83	0.44	0.117	0.712	1.262	0.145	0.263	0.045107	80%	167%	258%	322%	
Wednesday, 16 February 2022	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.61	0.86	0.46	0.126	0.724	1.262	0.145	0.263	0.045107	87%	175%	280%	322%	
Wednesday, 18 December 2019	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.64	0.84	0.48	0.135	0.733	1.262	0.145	0.263	0.045107	93%	183%	299%	322%	
Wednesday, 18 December 2019	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.63	0.88	0.44	0.128	0.745	1.262	0.145	0.263	0.045107	88%	167%	283%	322%	
Wednesday, 24 March 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.71	0.87	0.45	0.145	0.786	1.262	0.145	0.263	0.045107	100%	171%	322%	322%	
Wednesday, 24 March 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.61	0.79	0.46	0.116	0.694	1.262	0.145	0.263	0.045107	80%	175%	257%	322%	
Wednesday, 24 March 2021	Mukalla	ANAL	26.08	27.12	3.00	Surface (HtL)	0.67	0.83	0.42	0.122	0.746	1.262	0.145	0.263	0.045107	84%	160%	271%	322%	
Thursday, 14 April 2022	Mukalla	ANAL	52.16	54.25	3.79	Surface (HtL)	0.81	1.26	0.49	0.262	1.010	1.590	0.291	0.331	0.082456	90%	148%	317%	353%	
Thursday, 14 April 2022	Mukalla	ANAL	52.16	54.25	3.79	Surface (HtL)	0.85	1.16	0.48	0.248	0.993	1.590	0.291	0.331	0.082456	85%	145%	300%	353%	
Thursday, 14 April 2022	Mukalla	ANAL	52.16	54.25	3.79	Surface (HtL)	0.90	1.18	0.47	0.261	1.031	1.590	0.291	0.331	0.082456	90%	142%	317%	353%	
Wednesday, 24 March 2021	Mukalla	ANAL	52.16	54.25	3.79	Surface (HtL)	0.88	1.14	0.49	0.257	1.002	1.590	0.291	0.331	0.082456	88%	148%	312%	353%	
Wednesday, 24 March 2021	Mukalla	ANAL	52.16	54.25	3.79	Surface (HtL)	0.89	1.16	0.51	0.276	1.016	1.590	0.291	0.331	0.082456	95%	154%	334%	353%	
TOTAL NEQ (kg)			839.2	872.8												89%	156%	304%	339%	

E.1.2 Worked Example 1

If a 25 kg hexahedral charge of AN-Al (*TNTe* - 26 kg) were detonated on the surface of alluvial soil, what is the expected apparent crater volume?

$$V_a^{1/3} = 0.1687M^{1/3}$$

$$\therefore V_a^{1/3} = 0.1687M^{1/3}$$

$$\therefore V_a^{1/3} = 0.1687(26)^{1/3} = 0.4998$$

$$\therefore V_a = 0.4998^3 = 0.124m^3$$

What would be the expected crater volume if the medium were changed to asphalt?

$$V_a = 0.89V_c$$

$$\therefore \frac{0.124}{0.89} = V_c = 0.139m^3$$

$$\text{and } V_b = 0.339V_c$$

$$\therefore V_b = 0.339V_c = 0.0339 \times 0.139 = 0.047 m^3$$

Check:

$$V_c^{1/3} = 0.175M^{1/3}$$

$$V_c^{1/3} = 0.175(26)^{1/3} + 0.0033 = 0.518$$

$$\therefore V_c = 0.518^3 = 0.139m^3$$

$$\therefore V_b = 0.339(0.139) = 0.047 m^3$$

E.1.3 Worked Example 2

A 25L oil container of dimensions length 304 mm, height 444 mm and width 240 mm is filled with AN-Al of density 0.86 gcm^{-3} . Assuming a TNTe of 0.87, what is the apparent volume of the crater that would be evident in asphalt and alluvial soil?

Volume of container = 0.0324 m^3

Mass of AN-Al = $860 \times 0.0324 = 27.86 \text{ kg AN-Al}$

$$TNTe = 24.23 \text{ kg}$$

$$M_{asphalt} = 617.952 V_b^{0.794} P_k^{0.309}$$

$$\therefore 24.23 = 617.952 V_b^{0.794} P_k^{0.309}$$

$$\therefore 0.039 = V_b^{0.794} (0.304 \times 0.444)^{0.309}$$

$$\therefore \frac{0.039}{0.539} = V_b^{0.794}$$

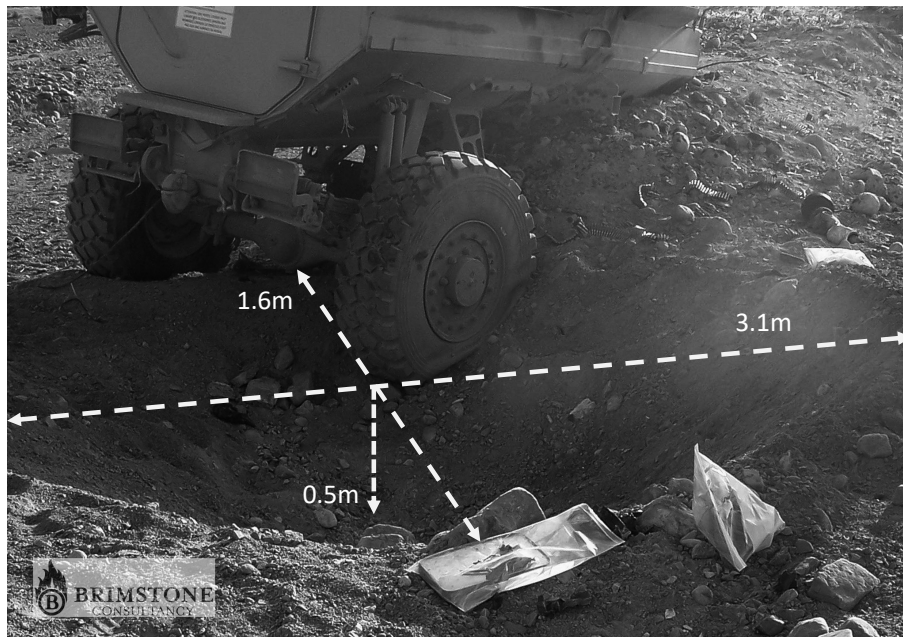
$$\therefore V_b = (0.072)^{1.259} = 0.036m^3$$

$$\therefore V_a \approx 3(0.036) = 0.108m^3$$

E.1.4 Worked Example 3

A surface-laid IED in Afghanistan badly damages a troop-carrying vehicle – see Appendix Figure 10-1. The crater dimensions are shown below, with the ground dry alluvial soil. Explosive sampling suggests an explosive comprising ammonium nitrate. The v-shaped underbelly of the vehicle is smudged with a fine grey residue amongst the soil. It is determined from intelligence within the area, and the physical evidence recovered that the likely explosive is AN-Al.

Determine the mass of the explosive used and the likely dimensions of the container based on an explosive density of 0.9 g cm^{-3} .



Appendix Figure 10-1: Crater remaining from surface IED blast

$$V_a = \frac{\pi abH_2}{6}$$

$$\therefore V_a = \frac{\pi \times 1.55 \times 0.8 \times 0.5}{6} = 0.32m^3$$

$$\therefore V_a^{1/3} = 0.687$$

$$V_a^{1/3} = 0.1687M^{1/3}$$

$$\therefore 0.687 = 0.1687M^{1/3}$$

$$\therefore M^{1/3} = 4.072$$

$$\therefore M = 67.52 \text{ kg}$$

$$V_a \approx 3V_b \therefore V_b \approx 0.106m^3$$

$$\therefore M_{asphalt} = 617.952 V_b^{0.794} P_k^{0.309}$$

$$\therefore 67.52 = 617.952(0.106^{0.794})P_k^{0.309}$$

$$\therefore P_k^{0.309} = 0.649$$

$$\therefore P_k = 0.248 \text{ m}^2$$

If the density of the AN-Al is 0.9 gcm^{-3} and its mass is 67.52 kg, then the volume of the container(s) is calculated as:

$$V = \frac{M}{\rho} = \frac{67.52}{900} = 0.075 \text{ m}^3$$

This volume therefore represents a P_k (L x H) comparable to a 40 L container (see Table 6-3) and a width (W) of up to 0.64m. This strongly suggests that the IED comprised 1 x 40 L container.

E.1.5 Worked Example 4

Urea Hydrogen Peroxide (UHP) is suspected of having been used in a bombing associated with criminality. The volume of the crater produced in asphalt is 0.028 m^3 . What is the mass of UHP likely to have been used in the attack? A man lying against a wall 10 m away from the blast has been killed, but there are no obvious signs of death from shrapnel. What is the more likely cause of death – primary blast or tertiary blast?

$$V_a \approx 3V_b$$

$$\therefore V_a \approx 3 \times 0.028 \approx 0.084 \text{ m}^3$$

$$V_a^{1/3} = 0.1687M^{1/3}$$

$$\therefore 0.084^{1/3} = 0.1687M^{1/3}$$

$$\therefore 2.596 = M^{1/3}$$

$$\therefore M = 17.5 \text{ kg TNT}$$

Given that the TNT_e of UHP is provided in literature as 0.55 for overpressure [425], this would equate to a mass of UHP in the region of 31.8 kg. At 10 m, Kingery-Bulmash provides the following data:

Appendix Table 10-3: Kingery-Bulmash Data for UHP Detonation

<i>Range (R) [m]</i>	<i>10</i>
<i>NEQ UHP (kg)</i>	31.8
<i>TNT_e (kg)</i>	17.5
<i>Peak Incident Pressure (P_s) [kPa]</i>	69.78
<i>Incident Impulse (I_s) [kPa.ms]</i>	193.55
<i>Peak Reflected Pressure (P_r) [kPa]</i>	176.99
<i>Reflected impulse (I_r) [kPa.ms]</i>	436.85
<i>Shock Front Velocity (U) [ms⁻¹]</i>	429.64
<i>Arrival Time (T_a) [ms]</i>	14.11
<i>Positive Phase Duration (T₊) [ms]</i>	8.71

Applying P_s and T_+ to the Bowen Curve for a reflecting surface (see Figure 6-8), it is unlikely that the individual would have died from primary blast injuries with a UHP charge. However, the peak reflected pressure (P_r) would have been sufficient to surpass the threshold for lung damage. It is therefore likely that the individual may have died from tertiary blast related injuries.

Appendix F – Air Blast Parameters by Distance, by NEQ and TNT Equivalence – AN/AL 90/10

AIRBLAST PARAMETERS BY DISTANCE, BY NEQ & BY TNT EQUIVALENCE

Reference Documentation is:
"Airblast Parameters from TNT Spherical Air Burst & Hemispherical Surface Burst" by
Charles N Kingerey & Gerald Bulmash, Tech Report ARBRL-TR-02555 dated April 1984.

INPUTS

Actual Stand-off Distance (D) [m]

10.00

Nett Explosive Quantity (Q) [kg]

28.00

TNT Equivalence Figure

0.87

OUTPUTS

Air

Surface

Peak Incident Pressure (Ps) [kPa]

61.7140841

86.7478333

Incident Impulse (Is) [kPa.msec]

164.8102195

237.8913889

Peak Reflected Pressure (Pr) [kPa]

153.5985705

230.8430273

Reflected Impulse (Ir) [kPa.msec]

364.0849378

553.2009279

Shock Front Velocity (U) [m/msec]

0.4196341

0.4487118

Arrival Time (Ta) [msec]

14.6023922

13.0862908

Positive Phase Duration (T+) [msec]

8.3489007

9.1056374

NOTES FOR USERS ARE BELOW - as ever make a back up copy before you start playing.

This spreadsheet program is a free calculation only, ie no cells are locked and there are no macros.

Only the cells for data input and output have been formatted.

Please only enter inputs, nothing else until you are familiar with the spreadsheet.

If inputs fall outside the applicability range of the Kingery Curves the output will read "Invalid". In cell K0 is the word "Invalid" used by the program: it shouldn't be deleted. The lower limit is when Surface Ps = 2.4kPa.

In column H are some notes and some incidental outputs.

The sub-calculations (the spreadsheet's engine) start at cell Q2 and continue to the right of Column O.

NOISE CALC

Pressure (Pa)

Range

Range 2

Final Pressure

Noise (dB)

61714

10

10000

0.061714

69.787074

GROUND SHOCK CALC

NEQ

SIGNIFICANT

GROUND SHOCK RANGE

0.87

29.8476