Environmental Impact of Munitions Life Cycle: A case study using Composition B

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Abstract

Munitions and their impact on the environment has become an ever increasing topic of interest and research. Short and long-term effects upon environments, ranging from atmospheric effects to aquatic life to mammals, has to be considered when choosing an energetic material for a munitions or pyrotechnic. New materials are being used within munitions and ordnance to comply with National, regional and REACh legislation/policy.

As part of this renewed attention into the environmental impact of munitions, MSIAC has carried out a review of the literature and work being performed within the nations and NATO. To aid the review process, a case study was developed using two energetic material compositions; Composition B and PBXN-109. The life cycle of these materials were reviewed from manufacture through to disposal. At each stage the potential environmental impact, including pristine and reacted material, was considered.

Using the Composition B data from the review, this paper will discuss the range of physical, mechanical, chemical and toxicological parameters that are needed to describe the complex problem. A number of models related to toxicity will be discussed and evaluated against the composition.

Recommendations are made as to how to use the models and parameters to assess energetic materials with regards to their potential environmental impact.

1. Introduction

Over the last 20 years, the environmental and toxicological impact of munitions over their life cycle has become more important to the nations and the international community. The life cycle of a munition, including the environmental impact, has been discussed within NATO and is covered by two STANAGs: STANAG 7141 – Joint NATO Doctrine for Environmental Protection During NATO Led Military Activities (NATO, 2006) and STANAG 4518 – Safe Disposal of Munitions, Design Principles and Requirements, and Safety Assessment (NATO,

2001). A reviewed of STANAG 4518 was carried out by MSIAC (Archambault, 2007) which described how the STANAG refers to the potential environmental impact of munitions and that this should be considered at the planning stage as well as at the point of disposal. A number of nations have implemented their own systems of environmental management to capture these requirements, for example the UK uses Project Orientated Environmental Management System (POEMS) whilst the US uses Programmatic Environmental, Safety, and Health Evaluation (PESHE).

In 1994 NATO became interested in the potential environmental impact that munitions could have and held an AGARD symposium on the topic (AGARD, 1994). In 1999 an RTO meeting was held that investigated the environmental pollution at military bases (RTO, 1999). In 2002 another RTO meeting (AVT-089) was held that investigated the advances in rocket performance life and disposal (RTO, 2002). Subsequent AVT meetings and workshops have produced reports on the Environmental Impact of Munitions (AVT-115) (RTO, 2010), Munition and Propellant Disposal (AVT-177), Design for Disposal (AVT-179) and Munitions Related Contamination – Source Characterization, Fate and Transport (AVT-197).

Within STANAG 4518 it states that design, demilitarization and disposal plans must be reviewed with time and if changes occur to environmental policy or national legislation.

Research carried out by CRREL and DRDC have shown that the method of disposal for a munition and the type of energetic material present within will have a profound difference in the explosive residue that can be transferred to the environment (Walsh, et al., 2013). Experimental results have also shown the transfer into the soil of propellant residue at gun positions (Diaz, et al., 2008). Some of the materials used within energetic materials have been shown to be toxic both to humans and to other species.

This information on the increased awareness for energetic materials to be transferred to the environment, and the change in the European legislation on the registration of chemicals has provided an increased impetus to understand how energetic materials will impact the environment. The Registration, Evaluation, Authorisation and Restriction of Chemicals (REACh) (EC, 2006) aims to improve human health and protect the environment by restricting or banning the use of chemicals/substances of high or very high concern (SHC/SVHC). These materials are defined by their availability to the environment through persistence, bio-accumulation and toxicity.

The REACh legislation and the potential increased deposition of energetic materials caused MSIAC to carry out another review of the literature associated with the environmental impact

of energetic materials (Stonhill, 2015). The aim was to examine the experimental data associated with determining environmental fate of energetic materials and propose a methodology for assessment. A life cycle study was carried out using two energetic materials as the means to focus the work; Composition B and PBXN-109 (Stonhill, 2015). Some of the findings for Composition B are presented within this paper.

For each process within the life cycle of an energetic material there is the potential, as with any other chemical, for it to be transferred to air, water, and soil and subsequently expose human, flora and fauna. The additional complexity that occurs with energetic materials is that they are designed to change form upon function (generation of gas, smoke, light, etc).

During the review, it was determined that a number of chemical and physical parameters are used to aid in the classification of chemicals for REACh and that Life Cycle Assessment (LCA) methodologies are being used to provide the User with information on the likely fate of chemicals in a process (EPA, 2014). LCA is a technique that assesses the environmental impact and potential impacts associated with a process or product by compiling, evaluating and interpreting factors such as material inputs, energy use, and environmental release. This type of assessment requires extensive knowledge of all processes within a system.

In the case for one type of munition this requires breaking down the life cycle (Figure 1) from the synthesis of the raw ingredients, each stage of manufacture to produce the formulation, filling and associated processes in manufacturing the round, proofing, through to storage and then the operations of in-service use and demilitarization. For the environmental release each stage has to be assessed against the potential for release and what will occur. From manufacturing through to storage analysis of this data could be carried out on ingredient information, as one moves through the life cycle so the analytical problem becomes more complex (decomposition products from reaction).

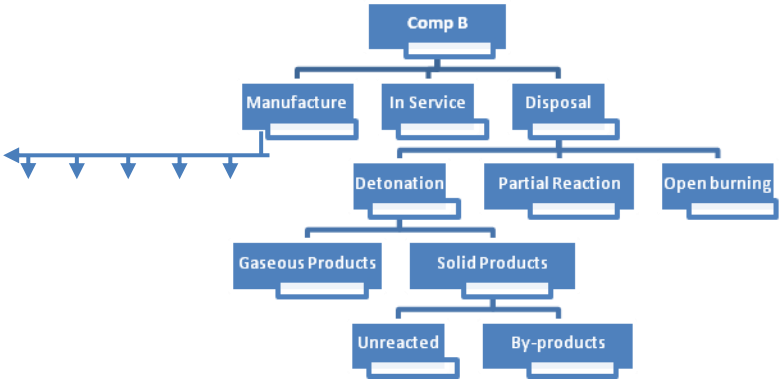

Figure 1 Part of the life cycle for a munition focusing on the energetic material

These techniques have been used in a number of industries (Arena, et al., 2003) (Henrickson, et al., 2006) and across many different chemicals including civil explosives (Ferreira, et al., 2015). It was considered that USETox covers the required output of the LCAs that would provide the energetic material user with the potential environmental fate data. The USETox method calculates the potential toxicity impacts, both to humans and eco-system, based on the physico-chemical properties of a compound within a defined environment (Rosenbaum, et al., 2008).

This paper covers the physical, chemical and toxicological parameters required to carry out an assessment using USETox. By way of example, data for Composition B was collated and an assessment performed to compare the toxicological impact of its ingredients (Table 1).

Table 1 Compositional information for Composition B

Composition B	Weight (%)	CAS #
RDX	59.5	121-82-4
TNT	39.5	118-96-7
Paraffin Wax	1.0	593-45-3

2. Methodology

The following sections describe the proposed life cycle for the energetic formulation, the role that REACh has in requesting and holding information on toxicological parameters and the additional parameters required for a USETox assessment.

2.1. Life Cycle for Munitions

The UK CADMID procurement cycle was used as the basis for the assessment with the following stages being considered: manufacturing, in-service use (training and operational), storage and finally disposal or demilitarisation. At each stage the hazards and possible routes into the environment were identified (Stonhill, 2015). From this assessment it became clearer which physical parameters would be required to describe the process.

The parameters could be identified by the process or, of more use to this work, by the route of exposure.

- Air contamination (manufacture, detonation, partial reaction):
    - Vapour pressure (Pa, 25ºC), an indication of a liquids evaporation rate (at equilibrium)
    - Particle size (µm), physical parameter that determines inhalable fraction

- Soil contamination (manufacture, partial reaction):
    - K_{ow} (-), ratio of the solubility of a compound in n-octanol and water, with high values (log K_{ow} > 4.5) relating to the tendency for adsorption in soil
    - K_{oc} (L kg^{-1}), soil organic carbon to water partition coefficient used to determine the transport of a compound through soil
    - $t_{1/2\ soil}$ (day), half life in soil relates to the time taken for a compound to decompose by 50%
- Water contamination (manufacture, partial reaction):
    - K_{ow} (-), as above
    - K_H (Pa.m^3 mol^{-1}), Henry's law constant that relates the solubility of a gas in liquid (at equilibrium)
    - $Solubility_{H2O}$ (mg L^{-1}, 25ºC), the degree that a compound will dissolve into water
    - $t_{1/2\ water}$ (day), half life in water relates to the time taken for a compound to decompose by 50%

In addition to these physical parameters are the toxicological parameters that enables one to determine how the chemical will affect human, flora and fauna.

2.2. REACh regulations

The purpose of REACh is to improve the protection of human health and the environment by the early identification of chemicals (either mixtures or single compounds) with the potential to be persistent, bio-accumulative and toxic (PBT) or very persistent and very bio-accumulative (vPvB). This identification is achieved through the submission of a dossier containing chemical, physical, toxicological and ecotoxicological data. The following table (Table 2) shows the information that is submitted as part of the registration dossier and used in the chemical safety assessment.

Table 2 Physicochemical and ecotoxicological data required by REACh submission (Postle, et al., 2011)

Property	Units	Property	Units
Physicochemical			
Physical state	20ºC/101325Pa	**Melting Point**	ºC
Boiling point	ºC	**Density**	g cm^{-3}
Vapour pressure	Pa	**Surface tension**	mN/m
Water solubility	g L^{-1} (*x* ºC)	**K_{ow}**	--
Flash point	ºC	**Flammability**	20ºC/101325Pa
Explosive Properties	ºC or kPa	**Self ignition temperature**	ºC
Oxidising Properties	--	**Dissociation constant**	mol L^{-1}
Viscosity	Pa s		
Ecotoxicology			
Aquatic toxicity	LC_{50}, LD_{50}, NOEC as mg L^{-1}	**Degradation**	Half life in water/soil/air
Fate and behaviour	Adsorption/desorption and bioaccumulation	**Effects on terrestrial organisms**	LC_{50}, LD_{50}, NOEC as mg kg^{-1}
Long term toxicity to sediment organisms	e.g. $EC(L)_{50}$ as mg kg^{-1}	**Long term reproductive toxicity to birds**	e.g. $EC(L)_{50}$ as mg kg^{-1}

The physical parameters in Table 2 were similar to those identified by Stonhill as well as the toxicological parameters needed for assessment. To carry out this assessment limits were required to determine which compounds have a high risk of effecting the environment. SHC and SVHC are determined by assessing the provided data against limits that are set out in the REACh regulations (EU, 2011) . These limits are shown in Table 3.

Table 3 Limits defined by REACh for PBT parameters

Parameter	P (vP)	B (vB)	Toxicity	CMR1	CMR2
$t_{1/2\ fresh\ water}$ (days)	>40 (>60)		**$LD_{50\ ing}$ (mg kg^{-1})**	<25	25-200
$t_{1/2\ sediment/soil}$ (days)	>120 (>180)		**$LC_{50\ inh}$ (mg L^{-1})**	<0.25	0.25-1.0
BCF (L kg^{-1})		>2000 (>5000)	**$LC_{50\ inh}$ (mg L^{-1})**	<0.5	0.5-2.0
Log K_{ow} (-)		>3 (>4.5)	**$EC_{50\ (daphnia)}$ (mg L^{-1})**	<1.0	1-10

The evidence that is submitted is assessed against the strength of experimental data and when not available the quantitative grouping approaches or structure-activity relationships ((Q)SAR).

2.3. USETox

USETox is an environmental model for characterisation of human ecotoxicological impacts that was developed by multiple researchers under the UNEP-SETAC Life Cycle Initiative. The USETox model calculates characterisation factors for chemical emissions to air, water, and soil and human toxicity. The model defines the units of ecotoxicity as PAF.m^3.day kg^{-1}, where PAF is Potentially Affect Fraction, and the units of human toxicity as cases $kg^{-1}_{emission}$. These factors were described by the team (Rosenbaum, et al., 2008) as ecotoxicity "provides an estimate of the potentially affected fraction of species integrated over time and volume per unit mass of a chemical emitted" and human toxicity being "the estimated increase in morbidity cases in the total human population per unit mass of a chemical emitted".

In order for USETox to calculate the aforementioned factors the model requires input to allow it to calculate how the chemical will be transferred from one compartment to another (Huijbregts, et al., 2010).

The following Figure (Figure 2) describes how the factors interrelate:

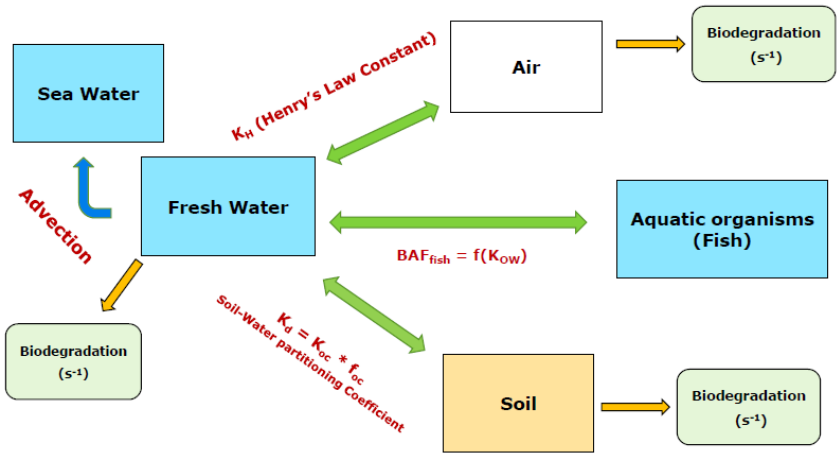

Figure 2 Fate and transport model highlighting the role of the physico-toxicological parameters for assessing environmental impact (Mehrkesh & Karunanithi, 2013)

The information gathered in the fate and transport model will then be cross referenced to each stage in the life cycle model for Composition B (Figure 1).

3. Results and Discussion

Composition B was chosen as the compound as it has been heavily researched and a significant body of data exists within the open literature both on the raw ingredients and the composition.

3.1. Parameters for Composition B

When performing searches for information on the ingredients for Composition B it was found that the CAS[1] number was the most important search parameter and easiest to use (Table 1). All the chemical databases, ECHA registration site, and regulatory bodies use this unique numerical identifier in their databases. It was also noted that several of the chemical databases also allow searches via the SMILES[2] string which can be useful if the string for the compound has already been generated.

It has been noted by the authors that not one database is complete with all the necessary data therefore time must be spent searching for reliable sources. The compiled dataset for Composition B ingredients can be found in Table 4. For TNT, RDX and Wax experimental data was available for K_{ow}, solubility in water (@ 25ºC), and vapour pressure (Pa). Experimental data was found for the Henry's coefficient (K_H) for TNT but not for RDX and Wax. No K_{oc} data was found for all three ingredients.

The degradation experimental data for both TNT and RDX was supplied in the ECHA registration documentation. It was found though that for REACh/PBT evaluation the RDX assessment was carried out on analogous data (HMX soil degradation) and whether the compound was still present after a set period of time (120 days), which for HMX varied depending upon soil type. The type of soil effecting degradation rate was also found to be true for other materials (Stonhill, 2015). So half life data in air, soil, water and sediment was not always available therefore for consistency the PBT Profiler modelling data was used in the USETox assessment for TNT, RDX and Wax. EPI Suite output could also be used as similar estimates for half life were also calculated.

A comparison of experimental and modelled data of the half life of RDX in soil shows consistency in models: ECHA data: not likely to degrade in soil over based on 120 days (15 – 57%; degradation of HMX); PBT Profiler: $t_{1/2\ soil}$ 75 days; EPI Suite: $t_{1/2\ soil}$ 1800 h (75 days).

The remaining parameters associated with toxicology required further calculation in order to be in the correct format for USETox. The BAF_{fish}[3] was calculated by EPI Suite (BCFBAF Program) using the K_{ow} and experimental BCF[4] data (BCF = 2.0 L kg^{-1}), with the latter correlating to ECHA submission (BCF = 2.06 L kg^{-1}).

[1] Chemical Abstracts Service; a division of the American Chemical Society
[2] Simplified molecular-input line-entry system
[3] BioAccumulation Factor
[4] BioConcentration Factor

For the EC_{50} it was recommended that multiple sources of data covering at least three taxa be used. Calculation of the average (geometric mean) EC_{50} (mg kg^{-1}) value was then used in the USETox model. For TNT and RDX data was readily available in the literature (Sunahara, et al., 2009) covering EC_{50} for grasses, fish, worms and snails. This data corresponded to that reported in the respective MSDS. This gave confidence to the EC_{50} data in the MSDS for the Wax.

The ED_{50} (carcinogenic and non-carcinogenic) for humans was least straight forward to obtain/calculate. Little ED_{50} data is published for compounds, only one source could be found for TNT (8µg ml^{-1}) for the effective dose for an inhibition in monocytes (Scheffer, 2003). Most data for toxicity relates to acute (LD_{50}) rather than chronic or subchronic exposure which is required in determining ED_{50} values. Also not all compounds are considered to cause cancer, including TNT, RDX and Wax, therefore only non-carcinogenic factors could be considered. ED_{50} (non-carcinogenic) can be obtained by extrapolating from the No Observed Adverse Effects Level (NOEL) as determined in a specific species (*a*), over a set period of time (*t*), and exposure route (*j*) using the following equation (1) (Huijbregts, et al., 2010):

$$ED_{50_{a,t,j}} = NOEL_{a,t,j} \,.\, AF_N \qquad (1)$$

This can then be applied to the following formula (2) to convert the effect to humans (average) over their lifetime (average):

$$ED_{50_{h,j}} = \frac{ED_{50_{a,t,j}} \,.\, BW.\ LT.\ N}{AF_a.\ AF_t.\ 10^6} \qquad (2)$$

Where $ED_{50\ a,t,j}$ is the effective dose for the given test animal (*a*), over a period of time (*t*; day), and exposure route (*j*; e.g. ingestion), BW is the human body weight (70 kg), LT is the human life time (70 years), N is the number of days per year, AF_a is the conversion factor for species to human, and AF_t is the extrapolation factor for differences in time of exposure.

When experimental data was not available then the following structure-activity relationship models and tools were used: EPI Suite (EPA, 2013), PBT Profiler (Environmental Health Analysis Center, 2012), QSAR Toolbox (OECD, 2012). USETox will also use default QSAR models to estimate the following parameters: $K_{oc} = 1.26.K_{ow}^{0.81}$; $K_{h\ 25^oC} = P_{vap\ 25^oC}$ x MW/Sol_{25^oC}; $K_{oc} = 0.08.K_{ow}$; $BAF_{fish} = 0.05.K_{ow}$. USETox relies on having as a minimum parameter set: K_{ow}, vapour pressure, molecular weight and solubility in water.

The last factor considered was the units for parameters, such as vapour pressure, which are not always consistently reported; mm Hg, Pa and/or atm. The data therefore had to be converted into the units required by USETox.

Table 4 Compiled physical and eco/toxicological parameters for Composition B

Parameter	TNT	Wax	RDX	PBT (vPvB)
M. W. (g mol^{-1})	227.13	254.49	222.12	--
K_{ow} (-)	39.8	1.51E+09	7.2	>1000 (>3.16E+04)
K_{oc} (L kg^{-1})	177.1	9.27E+07	*50.73*	<100 (<10)
K_h ($Pa.m^3.mol^{-1}$)	0.01	1.08E+07	0.0064	--
$P_{vap\ 25}$ (Pa)	2.65E-02	4.53E-02	5.33E-07	--
Sol_{25} (mg L^{-1})	*130*	0.006	*42*	>10 (>1000)
$t_{1/2\ air}$ (s^{-1})	9.65E-08	1.63E-05	1.73E-04	< 5.79E-06
$t_{1/2\ water}$ (s^{-1})	1.93E-07	7.72E-07	3.05E-07	< 2.89E-07 (<1.93E-07)
$t_{1/2\ sediment}$ (s^{-1})	2.14E-08	*8.27E-08*	3.40E-08	< 9.65E-08 (<6.43E-08)
$t_{1/2\ soil}$ (s^{-1})	*9.65E-08*	3.86E-07	1.54E-07	< 9.65E-08 (<6.43E-08)
BAF_{fish} (L kg^{-1})	2.92	4.36E+04	1.3	>50 (>1581)
Log_{10} EC_{50} (mg L^{-1})	*0.431*	3.473	1.630	<1 (<0)
$LD_{50\ rat\ ing}$ (mg kg^{-1})	795	5000	*71*	<200 (<25)
$LC_{50\ rat\ inh}$ (mg L^{-1})	*1.01*	--	--	<2 (<0.5)
$NOEL_{\ rat\ ing}$ (mg kg^{-1} day^{-1})	1.0	2.0	0.3	--
$ED_{50\ non\text{-}c,\ hum,\ ing}$ (kg $lifetime^{-1}$)	0.684	7.85	1.18	--
$ED_{50\ can,\ hum,\ ing}$ (kg $lifetime^{-1}$)	4.77	--	--	--

3.2. Parameter Analysis

Initial analysis of the data set (Table 4) against the REACh PBT limits can provide a first assessment of the persistence, bioaccumulation and toxicity of the ingredients. TNT has the potential to be very persistent in the environment with the degradation half lives in all areas, except soil, lower than the vPvB limits. The half life data set has been based on modelled data but information supplied to REACh agrees that TNT is poorly biodegradable (17.5% in 28 days) yet it is not considered P or B. The aquatic toxicology of TNT is recognised in the REACh assessment and in Table 4 with the low EC_{50} values.

RDX has fewer parameters that break the PBT limit and as such would not be considered PBT. REACh has assessed RDX as not PBT due to low K_{ow} and low BAF values for bioaccumulation, and that RDX biodegrades in water.

Wax, despite having a very high K_{ow} and therefore a high calculated BAF, is not considered a PBT concern due to low solubility and high degradation rates. REACh has assessed paraffin wax as not PBT.

3.3. USETox results

The dataset from Table 4 provides an output in terms of the human toxicity and the ecotoxicity potential for Composition B ingredients. Figure 3a highlights the potential for non-cancerous effect in humans being exposed to TNT, RDX and Wax via the air, water or soil. In Figure 3b the values have been normalised to the mass of the ingredients in Composition B.

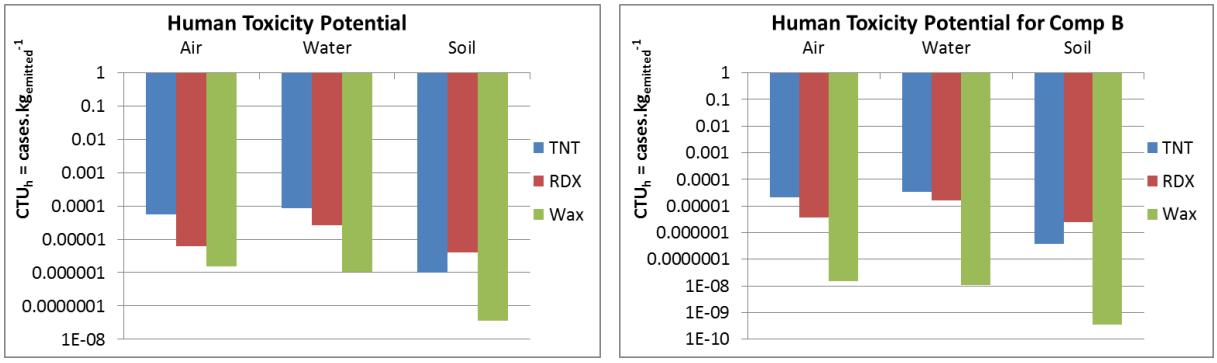

Figure 3 Human toxicity (non-carcinogenic) potential for TNT, RDX and Wax through exposure via air, water and soil (a) per kg of ingredient, and (b) per kg of Composition B

Wax is almost a factor of 10 less likely to cause an effect across all routes of exposure when compared to TNT and RDX (per kg). This increases to a factor of 100 when considering the amount of wax present in Composition B (Figure 3b). TNT is considered a greater risk to human toxicity via air and water. The latter will be affected by both its solubility, low degradation rate and toxic nature. When TNT is normalised to the mass present in Composition B the potential human toxicity remains similar at approx. 0.0001 cases kg^{-1}. RDX is considered less toxic via air, due to the low vapour pressure, and soil, with a low water solubility and low K_{oc}, than via water. This is mirrored in Figure 3b.

The ecotoxicity potential for TNT, RDX and Wax in air, water and soil is presented in Figure 4a and Figure 4b with the values normalised to Composition B.

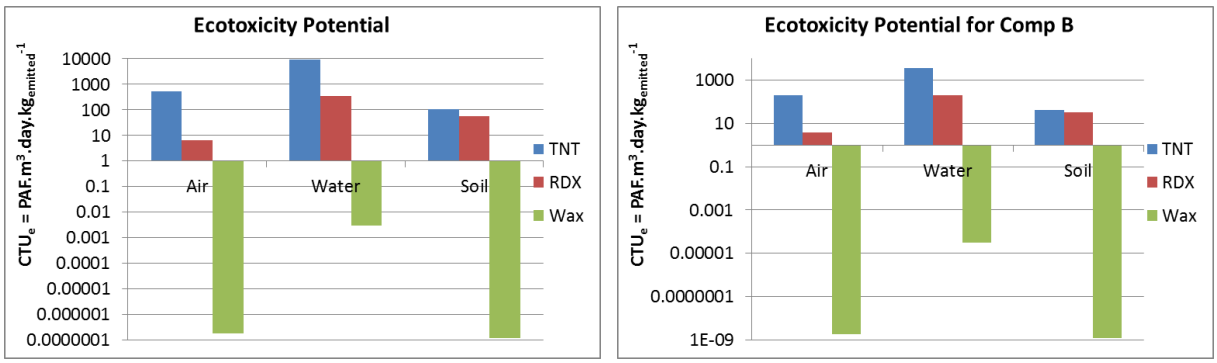

Figure 4 Ecotoxicity potential for TNT, RDX and Wax through exposure via air, water and soil (a) per kg of ingredient, and (b) per kg of Composition B

It is clear that across all three exposure routes that wax is highly unlikely to affect species living in these environments. This is more pronounced in Figure 4b with the potentially affected fraction of species in a given area and day less than $1x10^{-8}$ per kg of Composition B in the air or water. TNT has a very high ecotoxicity potential with up to 10000 affected fraction of species in water, which is slightly reduced when considering Composition B. Exposure to TNT via the air and soil is considered high and a route of concern. RDX affects species in the water to a greater extent than either the soil or the air, with the latter being a result of its low vapour pressure.

The USETox data highlights the compounds and the highest potential route of exposure to the environment. For Composition B TNT provides the greatest risk to both humans and to the aquatic water species based upon the input data to the model.

Relating this back to the life cycle (Figure 1) of a Composition B the USETox data give information where unreacted material is present therefore manufacturing would pose the highest risk for TNT exposure and specifically to the aqueous environment. Qualification, use and disposal would also have the potential to expose quantities of TNT to the air, water and soil. These results do not take into account the engineering measures, especially during manufacture, that are put in place to minimise the potential for unintentional release.

So where and how would the information that USETox generates be of use. Should one be carrying out a risk assessment then in a risk matrix the USETox output would be the consequence to the ecosystem/human from a release. For each stage in the life cycle an estimate or experimental data is required as to the probability of the event occurring. For example in the detonation of Composition B the probability of transferring gases into the surrounding is high whereas unreacted material is low. Research by Walsh has determined the amount of solid residue transferred to the soil, and potential water, for materials like PAX-21 and Composition B; 0.073mg (0.00002%) from a 60mm mortar (0.365kg fill) (Walsh, et al., 2013).

3.4. Discussion

The potential exists to use the values generated at face value without considering some of the approximations that have been made. Several of the parameters have been modelled/calculated which have the potential to increase or decrease the CTU outputs to levels that could be of concern, which could be the case for the TNT values. In this study the degradation half lives were calculated for all species, therefore experimental data would help to improve on the accuracy of the output. The USETox model, and the PBT Profiler have

limitation on the types of materials that can be assessed. The exceptions include gases, non-organic species such as inorganic salts and metals, high molecular weight species such as polymers and hydrolysable compounds. In the latter case materials such as isocyanates will react rapidly with water to form the amine and carbon dioxide.

RDX is known to readily degrade in water and the presence of UV light to form the nitroso and the chain scission by-products (Paquet, et al., 2011). When the by-products of a compound are known then it is possible to calculate the potential environmental impact of those species using USETox.

Many explosive compositions contain metals and polymers which may limit the use of USETox in its ability to assess these species. The model is being constantly evolved and work is ongoing into inorganic species. For polymers the potential is to use analogues of lower molecular weight species but with the caveat that key parameters such as water solubility, K_{ow} and BAF will be affected.

The gaseous decomposition products from in-service use and demil of explosives are not easy to determine either their effect to the environment (Stonhill, 2015) or to model using USETox . Although they are low molecular weight organic species (in the majority) their transfer and degradation in the surrounding media is complex. For example both carbon dioxide and ammonia will dissolve in water to produce acidic and alkaline products, therefore changing the potential interaction pathways.

USETox has been designed to provide a comparison of ingredients and to highlight those with greater environmental toxicity, yet most materials are mixtures of materials which, in some cases, have been chemically reacted to improve their properties. For explosives, composition are the norm so therefore some of the physical parameters, may be affected. The same can be said for bulk properties of the material, with a finely dispersed material having a greater surface area than a lump of the same mass, which in turn will enter the environment faster.

For new ingredients finding all the dataset may prove problematic especially for the experimentally derived EC_{50} data and NOEL. EPI Suite (ECOSAR) will allow EC_{50} estimations for fish, Daphnid and green algae

4. Conclusions

The parameters required for assessment of the potential environmental impact of Composition B were determined. These parameters have been echoed in the environmental literature to enable assessments to be performed.

A LCA environmental model was identified, USETox, and the parameters for Composition B were found in the literature. When experimental literature wasn't available the parameters were estimated using structure-activity relationships (SARs) and models such as EPI Suite, PBT Profiler and/or QSAR Toolbox.

Sources of data for Composition B ingredients included ECHA, USETox database, EPA, MSDS as well as multiple referenced papers and books, which indicates the time required to successfully complete the dataset.

Analysis of the dataset against REACh limits gave a first approximation as to the likely impact of Composition B. This suggested that TNT would have the potential to be persistent and toxic. Analysis of the USETox output showed that of the three ingredients TNT was considered the material of greatest concern, especially to the aquatic environment.

The limitations of USETox were highlighted and the work continues to improve and update both the experimental dataset and the models. The output of USETox can provide input into risk assessment models as the consequence for impact to the environment.

5. Acknowledgements

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