What Makes a Useable New Energetic Material?

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ABSTRACT. In the last 50 years, very many new energetic compounds have been made as potential ingredients for explosive, propellant and pyrotechnic formulations. Of these compounds very few have come to be used in military munitions. To obtain a better understanding of why this has been the case and to help address the discrepancy, the NATO Insensitive Munitions Information Centre (NIMIC) held a workshop in June 1994 open to representatives from government and industry within NIMIC member nations, to study what it is that makes a new energetic material useable. Issues that were addressed included:

- what is currently being used from the current understanding of detonics and molecular modelling in the targeting and preparation of new energetic materials;
- what use is made by the energetic materials designer of present capabilities to predict the performance and safety of new compounds and formulations;
- what do the users require of predictive resources and molecular modelling in order to target more potentially useful new energetic materials;
- what are the user's requirements for useful new energetic materials and can these be interpreted as quantitative properties of energetic molecules.

This paper presents a short summary of those conclusions of this NIMIC workshop that are relevant in the field of the understanding and modelling of detonation at a molecular level.

1. INTRODUCTION

One way of attempting to improve the performance of munitions without compromising safety is to make changes to the energetic materials with which they are filled. A study of the current literature on programmes for research into new ingredients and formulations reveals an apparent lack of an overall, logical and systematic approach to their development, qualification, and assessment of their safety and suitability for use in munition systems. This means that there are significant characteristics missed or overlooked in assessing materials, there are materials discarded when they meet current needs, and there is unnecessary testing. This adds up to time and resources being inefficiently used in the complex route from the conception of a new molecule to the acceptance of a weapon system.

Prediction and modelling of the properties of energetic materials are logically the first steps in the route from the conception to the realisation of energetic materials. However, it is not obvious which attributes of a compound or composition should be modelled in order to try to anticipate whether it is likely or not to be useful in service. One of the purposes of the recent NIMIC workshop was to look at what is available and being used from the current understanding of detonics and molecular modelling in the targeting and preparation of new energetic materials by synthesis and formulation chemists. A further aim was to determine whether what is being predicted coincides with what the users really require of predictive resources and molecular modelling in order to target more potentially useful new energetic materials. In the NIMIC workshop, this followed on from studying the users requirements for new energetic materials and how these can be interpreted as quantitative properties of energetic molecules.

2. PROPERTIES OF ENERGETIC MATERIALS

2.1 Performance

The driving force behind the development (or at least the funding for development) of any new materials for defence use is, and almost certainly always will be, performance. This is readily apparent from almost all recent papers proposing or describing new energetic compounds. An example is found in Olah and Squire [1], where discussion throughout compares performance of new compounds to the current highest energy density materials. This is reasonable, as munition performance requirements are continually increasing, but, however attractive and apparently obvious performance indicators are as a guide to the

most promising materials, there are challenges to this approach that must be considered. These challenges include:

- a) what is the most relevant performance indicator to use?
- b) will increased 'performance' in a compound lead to increased available performance in a useable composition?
- c) will the promotion of new materials on grounds of performance mean that compounds that could be used to give the levels of performance now available but with increased safety be overlooked?

Looking at these points in turn, the first, the question of suitable performance indicators has rarely been addressed. It is common to see lists of detonation velocity or pressure, or theoretical Isp from which conclusions about the highest performance materials are made. However these are not necessarily suitable figures to compare as they oversimplify the estimation of performance [2]. The effect of shaped charges for instance is not solely dependent on detonation velocity, but also on the composition on the product gases and the detonation energy [3]. In fact for widely differing compositions the detonation velocity figures can be completely misleading. A recent example of this came from the study of a LAX112, a new explosive with a very high density and detonation velocity. Comparison of detonation velocities with HMX, RDX etc. implies that this relatively insensitive compound could have wide application because of its high performance, however, comparison of Gurney energies indicates that it will perform relatively poorly in metal accelerating warheads [4]. The situation is at least as complex for propellants, where comparisons can only sensibly be done through the medium of the Isps of optimised compositions containing the compounds of interest. However, optimised compositions may be very dissimilar for different compounds, it is not satisfactory or reasonable to take a baseline formulation and simply replace one oxidiser with the same proportion of another. In comparing nitrate ester and azide containing energetic binders as propellant ingredients for example, there is the possibility of obtaining over-oxidised compositions with nitrate ester binders, which is most unlikely with azide containing ones [5]. In addition, the burning rate, burning rate exponent, and temperature sensitivity etc. are crucial in determining the utility of propellants. There is clearly no single figure that will tell the whole story concerning performance of either explosives or propellants.

The second challenge raised above, that of a compound's performance relative to a useable composition containing that compound, can be illustrated by HMX compositions. The maximum percentage of HMX that can be used in a main charge composition for small warheads is approximately 96% [6]. There is a need for a binder for all HMX compositions to give them some mechanical properties and to make them tolerably safe to use throughout their intended life. Larger warheads need more binder so that they are processable and adequately safe. Some known compounds cannot be processed without using considerably more binder because of the morphology e.g. nitroguanidine, and others need more binder to make them safe enough to process and handle, e.g. PETN. Comparisons of simple performance parameters do not allow for the amount of binder required in different applications to obtain acceptable mechanical, processing or safety properties.

The third difficulty with promoting new compounds on the grounds of performance is that it will miss those materials that might give similar performance when in compositions to those compositions in use today with increased safety. Similarly it will miss those that have intrinsically less performance but, by virtue of the physical and safety properties, might be useable in higher proportions in compositions. A theoretical example might be 'super-TNT', a melt castable compound that has performance less than HMX but that can be used neat like TNT or melt cast with HMX. Its performance when compared to neat HMX would not be attractive, but it could lead to compositions of higher performance.

2.2 Cost

A search of the literature provides scant evidence that cost per se has ever stopped the development of an otherwise suitable new material. However, it may severely limit its application in large or widely used munitions. TATB is an example of this, where its insensitivity and performance have meant that it has found application in a limited range of munitions but its cost prohibits widespread use. Unfortunately this is not necessarily in the best interests of systems costs. Cost/benefit on large rocket systems have

suggested that due to the very high cost of the payloads, relatively small increases in propellant Isp brought about even by using expensive 'exotic' ingredients can reduce the system cost. Cost is strongly related to quantity produced and can frequently be reduced significantly if demand warrants investments to obtain economies of scale.

2.3 Safety

Both explosive and environmental safety issues may prevent the widespread use or even the development of an energetic material. For instance, the concern (however unfounded) about HCl emission from composite rocket motors together with concerns about plume signature for tactical missile motors has led to a considerable effort to find alternative oxidisers to replace ammonium perchlorate [7]. Regarding material safety, the recent and growing interest in less sensitive munitions and explosives can be seen from the development of national and international insensitive munition policies [8], and additions to UN transport regulations [9]. A significant point about safety in terms of sensitivity, is that unlike performance, it is not a fundamental and unalterable property of most materials. The most insensitive materials can be made to appear relatively sensitive to some stimuli, and conversely sensitive materials can sometimes be made acceptably insensitive. An example of this being HMX, which in certain crystal forms is unusably sensitive to impact, in the normal beta form is less sensitive but still too sensitive to use by itself, and when mixed with a suitable binder is acceptable. Note that the increase of safety is not in this case related to performance [10]. The least sensitive crystal form of HMX is also the one with the highest energy density.

Discussion of compatibility and stability is often noticeably absent in papers presenting new energetic materials. Yet in the literature there are reports on several materials that have appeared very promising in early studies, but after some development have had to be dropped because of compatibility or aging problems. The classic example of this is picric acid which is a more powerful explosive than TNT and was used extensively in WWI, but is not now because of its incompatibility with acid sensitive materials (particularly in the forming of sensitive picrate salts with metals) [11]. More recently, a number of high density compounds containing 2-carbonyl-1,3-dinitramino groups were proposed as high performance explosives until studies highlighted their tendency to hydrolyse in the presence of moisture [12], [13]. One of the most promising materials for high performance low signature solid rockets is ammonium dinitramide, but after several years of research into its synthesis and performance, it has been found relatively unstable (although the reason for this is unclear as yet and it may not be an insoluble problem) [14]. Whatever its performance, it will not be widely used unless it can be used in formulations with a reasonable life expectancy.

As with sensitivity, apparent instability is not always a fundamental property of the material under study. Investigation may show that removable trace impurities may catalyse an otherwise slow decomposition. It is the impurities in low grade TNT that predispose it to decomposition and exudation [15]. In addition the development of polymer microencapsulation where reactive materials can be shielded from moisture and air may make it possible to use materials found too unstable in the past [16].

Another factor with aging and stability is the possible development of stabilisers. It is well known that nitrate ester containing materials usually require stabilisers to prevent autocatalytic decomposition that by reacting with NO₂ radicals give them adequate service lives. Similarly, many synthetic polymers require anti-oxidants.

2.4 User requirements

The conclusion from energetic material users at the NIMIC workshop was that for any material (NB this is the composition and not necessarily the individual ingredients) to be useful it must have:

- a) delivered performance at least comparable to materials it might replace;
- b) safety characteristics no worse than a compound such as PETN (except possibly within explosive trains of fuze systems);
- c) a reasonable shelf life in a finished article, e.g. 10 years or more.
- d) a production cost not significantly greater than TATB, unless a significant cost-benefit can be

- demonstrated or it is the only suitable/allowed material for an application;
 e) no concerns about its effect on its manufacturing or the global environment.

3. CODES AND METHODS AVAILABLE TO PREDICT ENERGETIC MATERIAL PROPERTIES

3.1 Performance

Unfortunately, it appears from the NIMIC workshop that the methods used by energetic materials designers in many laboratories do not predict well the attributes required of the energetic materials by their eventual users. The main codes and methods available for the calculation of performance parameters are given in table 1.

Type	Name	Function	pros	cons
Ab initio	Gaussian 8x [17]	Geometry optimisation, Hf, total electronic energy, nuclear repulsion energy, ionisation potential, etc.	No parameterisation necessary.	CPU and memory intensive
	BAC-MP4 [18]	Geometry optimisation, Hf, bond dissociation energies, etc.	Reliable Hf	Relatively little used
Semi-empirical (theory correlated with test data)	MOPAC [17]	Geometry optimisation, Hf, total electronic energy, etc.	Relatively rapid Well known	Accuracy depends on parameterisation
	Molecular Mechanics [19]	Geometry and energy optimisation, can also be used for density [20].	Rapid and simple	Requires parameterisation
	Blake [21]	Impetus or impulse, flame temperature, combustion products	Well known	Needs Hf and δ
	ICT [22]	Impetus or impulse, flame temperature, combustion products		Needs Hf and δ
	NASA-Lewis [23]	Specific impulse, flame temperature, average Mw of combustion products	Well known	Needs δ and Hf, ideal gas
	PEP [24]	Specific impulse, flame temperature, average Mw of combustion products	Simplified NASA-Lewis	Needs δ and Hf
	NOTS	Impetus or impulse, flame temperature, combustion products	PEP code adapted for guns	restricted to ideal gas
	Molpak [25]	Density		needs molecular structure
	Tiger [26]	Dv, Pcj	Well known	need Hf and δ
	ETARC [27]	Dv, Pcj, and other detonation properties		need δ and Hf
Correlations (empirical curve fits of test data)	Stine [28]	Density	Simple and rapid	
	Kamlet & Jacobs [29]	Dv, Pcj and other detonation properties	Well known	need δ and Hf
	Rothstein & Petersen [30]	Dv	needs only molecular formula	
	Stine [31]	Hf	needs only molecular formula	
	QSPR [32]	Hf		
	Stine [33]	Dv		needs Hf and δ
	Akst [34]	Cylinder test data		needs Hdet and δ

Table 1 - Methods for prediction of performance parameters of energetic molecules

Of the empirical curve fits, only Kamlet & Jacobs, and Akst, can be used to give parameters relevant to delivered energy of explosives, and none of them apply to non-ideal explosive compositions and perhaps also to the newer less sensitive compounds. The second drawback also applies to several of the semi-empirical methods. A recent example of this being the low sensitivity explosive NTO, where the delivered energy from detonation is significantly less than that predicted.

3.2 Safety

Using the safety in its broadest sense, it appears that the energetic materials designer has as yet, little assistance from predictive methods. The methods that appear in the literature for predicting some aspects of materials safety are given in table 2. However, it emerged in the NIMIC workshop that these methods

are rarely used by the majority of synthesis and formulation chemists to guide their research. This appears to be due to the fact that there is as yet no complete approach to sensitivity (to shock, impact or heat) as the causes at a molecular level are by no means fully understood [35], [36], [37], [38], [39], [40], [41], [42], [43], [44], [45], [46], [47], [48] in conjunction with the perception that all estimates of sensitivity characteristics of unknown materials tend to be unreliable when applied to unknown compounds depending as they do on the complex interplay of chemical and mechanical factors [49]. As these factors vary for every compound, it was commonly concluded that it will never be possible to find a universally reliable predictive empirical or ab initio method for solid materials. A further complication to this is the

relationship of the sensitivity of the individual ingredients of a composition to the sensitivity of the composition itself. If the sensitivity of a formulation is more dependant on the relative amounts of binder and solids and the porosity of the processed item than on the ingredients, then accurate calculations of the sensitivity of ingredients are only useful for raw material handling and not predicting usefulness.

Method	Function	Requirements	Comments
QSPR [32]	Impact sensitivity and stability used as examples	Numerous predicted or measured parameters	And empirical method for predicting any material characteristic using physical and chemical properties
Ab initio/semi empirical molecular structure (see table 1)	Bond lengths/strengths		Useful indicators, but cannot be directly correlated with any sensitivity properties
Correlation to oxygen balance (Stine) [49]	Impact, shock, critical temperature.	Oxygen balance	Cannot allow for anomalous behaviour caused by other chemical or mechanical properties
Correlation to oxygen balance (Kamlet) [50]	Impact	Oxygen balance	Cannot allow for anomalous behaviour caused by other chemical or mechanical properties
Correlation to bond length/charge distribution (Politzer) [48]	Impact	Bond lengths, atomic charges	Cannot allow for anomalous behaviour caused by other chemical or mechanical properties
Statistical/neural network [51]	Impact	Numerous predicted or measured parameters	Relatively poor correlation
Electronic structure/impact sensitivity correlation [52]	Impact	Relative variation of polarity of 'trigger bond' on excitation (from MO calculations)	Takes no account of mechanical influence on sensitivity
Electronic structure/impact sensitivity correlation [53]	Impact	HOMO and LUMO energies	Only correlated for a limited number of compounds

Table 2 - Methods for predicting the sensitivity of energetic compounds

The issue of the prediction of formulation properties based on simple analysis of the gross ingredients, was a major topic of discussion in the NIMIC workshop. It is clear that it is only possible to determine from the analysis of ingredient proportions those formulation properties that depend on the thermodynamics of the mixture, i.e. performance (with only signature being the obvious exception to this rule). It was then agreed that any formulation characteristic that was determined by the mechanical properties or the chemistry of the formulation could not be predicted simply by the proportions of major ingredients, and small proportions of additives (burn rate modifiers, processing aids etc.) could have overwhelming effects on the formulation behaviour. A significant exception to this being those formulations that are almost exclusively made from one ingredient, i.e. very highly filled, pressed, PBXs. This means that it is possible to divide formulation characteristics into three categories as illustrated in table 3. Only those properties that are directly related to ingredient proportions are amenable to prediction by present capabilities in computer modelling.

Characteristics	Detonation parameters Impulse Force Signature	Safety Hazard IM	Stability Compatibility Life Burn rate
Dominant factors in determining characteristics	Thermodynamics or products of reaction	Mechanical properties	Chemical reactivity of the formulation
Relationship to ingredient proportions	Directly related	Some relationship	Little relationship
Effect of additives	Little effect	Significant effect	Significant effect

Table 3. Effect of ingredient and additive proportions on formulation characteristics.

In addition to the above, there appears to be no systematic methods for anticipating most of the properties required of energetic materials by the users, especially important among these being sensitivity to purely thermal threats, ESD, compatibility and stability.

4. CONCLUSIONS

From the NIMIC workshop discussions, it became apparent that the targeting of new energetic materials for synthesis and formulation is in practise largely based on extrapolation from known materials. This is acknowledged not to be ideal, resulting as history shows in far more disappointing materials being made than useful ones. However, it appears that a more successful targeting strategy for the synthesis and formulation of new materials for most applications (small, highly filled, pressed explosive charges being the main exception) will not be realised until it is possible to predict the properties (thermodynamic, chemical and mechanical) of macroscopic mixtures of binders, fillers and additives.

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