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A
NEW PARADIGM
FOR R&D
TO IMPLEMENT NEW
ENERGETIC MATERIALS
IN MUNITIONS

Technical Paper

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Introduction:

The future position of our Nations and their well-being in the world will be challenged on many fronts in the coming decades and perhaps the foreseeable future. There are several current issues that may or will bring about changes in the world in the near future, from what we know today. These include: (1) the economic development of the third world, (2) the global competition for energy and natural resources, (3) the tensions between societies with different ethnic and cultural histories, (4) the tensions between several different cultures as we move towards a more interconnected and global world, (5) the potential stark realities and tensions of an effectively ever smaller world brought about by an increasing human population, (6) the tensions that can result from global climate changes whether warming or cooling, and (7) the resulting environmental and social positive and negative effects of these issues.

While addressing these issues does not directly involve a military component, history suggests that societies will develop military capabilities that may be used to influence the global balance of power on many of these issues. Much as all of our Nations and all world powers have done since World War II and are continuing to do. A cornerstone of the U.S. military strength of the last half of the twentieth century, and it continues today, was the development and superiority of U.S. munitions. These munitions encompass both conventional and nuclear ordnance. Superiority ranging from advanced chemical propulsion systems for rockets motors and guns to advanced nuclear warheads provided superpower status for the U.S. in the twentieth century. As larger fractions of the world's population moves into the modern technically interconnected world, both global and regional balances of power will surely change. Whether for the positive or negative is to be debated in the political arena, not in the domain of engineering and science. As such, this paper does not advocate, endorse, or support any specific political viewpoint or agenda. We are here to address technology and the improvement thereof.

In this paper, we attempt to address the issue of how to maintain technologically viable munitions in the 21st century from strictly the point of view of the energetic materials used for the propellants and explosives in those munitions. In attempting to address these issues; one must ask: Will maintaining the status quo be sufficient?, Will using technology developed in the years following WWII be sufficient for providing energetic materials, propellants and explosives, for future munition/weapon needs to meet new threats and provide for defenses?, Will investment in new sensors and electronics be sufficient or will new energetic materials be required?, Will the existing paradigm used for the development of energetic materials be sufficient, or will a new paradigm be required?

History of R&D and EM Developments:

This section provides a thorough description of energetic materials research and development history and concludes with a philosophical/policy discussion of the importance of developers, among other things, to implement new design concepts that enable systems to meet new military requirements. Historical statements regarding the degree that emerging military requirements resulted in new propellant and explosive material could reveal an important limitation in the current development process and another basis for a shift in strategy. The modern development of energetic materials for chemical propulsion and warheads can be traced back to the mid to late 19th century and beginning of to the middle of the 20th century with the development of nitroglycerine, nitrocellulose, and other energetic organic nitrate/nitramine compounds such as RDX, HMX, TATB, etc.

Most sophisticated plastic bonded explosives and propellants were developed just before and during the WWII timeframe. A great majority of “new” solid rocket motor propellants were developed during the first two decades of the cold war. Most of the developments after those timeframes are in essence follow-on work to the earlier research and development. A large part of that development can be characterized as; trial and error or what is commonly referred to as “Edisonian”, although, that characterization disfavors Edison.

The current paradigm of an empirical “Edisonian” approach to develop new propellants and explosives is perceived by some as being too slow (lacking time responsiveness), largely unsuccessful, or

providing limited successes and is thus considered high risk and unworthy of significant investment. In some circles, it is disparagingly referred to as “tweaking molecules”. Given the large number of different requirements that must be satisfied to make a new propellant or explosive that meets very high performance goals while being as intrinsically safe and as stable as possible; i.e., insensitive, it is not surprising that the slow empirical “Edisonian” approach has not been as successful as most would desire. Similar challenges are encountered in the development of new drugs. This paper considers the pharmaceutical industries’ approach to addressing similar research and development issues and how that approach may serve as a guide for the development of a new paradigm for energetic material R&D. We considered the pharmaceutical industries’ approach not only because of their similar research and developmental issues but also the fact that many of their precursor compounds are, or can be, very energetic in nature and they test to identify and exclude¹, where we desire to identify and include via test.

To circumvent the perceptions and/or limitations associated with the current “Edisonian” approach will require the development of a new R&D paradigm that can facilitate the creation of new propellants and explosives much more rapidly, with orders of magnitude less material, and at the same time providing new data that can be used to guide the design of new compounds, composite materials, and applications. The paper also addresses the requirement or need for new experimental methods and diagnostics tools. The primary objective being to provide the material scientist/engineer with the experimental tools needed to design new formulations required to meet the system requirements of the future.

Many of the ideas presented and discussed in this report are based on ideas and discussions from the Joint Army, Navy, NASA, and Air Force (JANNAF) and the Chemical Propulsion Information Analysis Center (CPIAC) sponsored workshop on “R&D Required to Implement New Energetic Ingredients in Munitions”. The workshop was held at the Battelle Conference Center, Aberdeen, MD from 29-31, August 2006. Fifty-five individuals from various DoD (Army, Air force, and Navy) and DOE (Sandia, LLNL, and LANL) laboratories, US energetics and munitions industry, and academia participated in the workshop. The backgrounds of the participants were broad: with expertise in basic research, formulation development, manufacturing, systems development, and program management.

The primary objective for the workshop was to create a plan for R&D investment strategies that would enable the rapid implementation of new energetic ingredients (e.g., high nitrogen compounds energetic binders, and ionic liquids) needed to reach new munition goals, while meeting insensitive munition (IM), aging, quality assessment and cost requirements. To construct strategies for future R&D investments, we discussed many aspects concerning future requirements for new munitions, the role for new ingredients, and the R&D required for their development. Discussions focused on two themes: (1) the requirements for munition systems of the future, and (2) scientific and technical issues that will enable the rapid development of new energetic materials that can be used for the development of new munition systems. By the end of the workshop the following was achieved: (1) developed a strategy for assessing future munition requirements; (2) reviewed the current state of capabilities used for munition development; (3) identified gaps in our R&D capabilities that limit the development of new energetic materials; (4) initiated discussions on research approaches that can be used to develop technology that will close these gaps and enable rapid development of new energetic materials.

One theme, that was repeatedly discussed, was the perceived high degree of risk, by individuals inside this field, of investing in energetic materials R&D in a national environment of limited funding, which in effect also self limits funding in this area. Limited funding, also in turn, restricts the development of new tools needed to understand and design new materials. Thus, a self-fulfilling feedback cycle that limits the development of new energetic materials is created. The immediate ramifications of this situation are (1) a lack of excitement and enthusiasm about future science and engineering directions, (2) the lack of state of the art tools and instruments, (3) the inability to attract some of the best and brightest students to the field, and (4) a growing disparity between the availability of new technology and the need for increased functionality and preparedness.

A NEW PARADIGM FOR R&D TO IMPLEMENT NEW ENERGETIC MATERIALS IN MUNITIONS

This limited funding, in part, has been addressed by the US Department of Defense, OSD (AT&L), in the development and programming of a budget line for the Joint Insensitive Munitions Technology Program (JIMTP). As good an advance as this development of a budget line is, and it is a good advance, the overall funding picture is still quite limited in real dollar and in historical terms.

This lack of investment of R&D dollars in research on energetic materials, which is resulting in the current downward spiral in the U.S. capabilities to develop new energetic materials for propulsion systems and warheads, may simply be seen as a prudent investment decision by some individuals and corporations. However, it may also be a shortsighted investment decision based on a lack of knowledge, resulting in the inability to foresee future requirements and opportunities. In this paper, and the report of the August 2006 JANNAF meeting, we provide our assessment of the requirements for energetic ingredients for future munitions and the research and development opportunities that may enable the U.S. to maintain viable munitions to support our military responsibilities throughout the 21st century. The main themes addressed in the JANNAF report are: (1) Why should any individual, nation, or corporation invest in energetic material R&D, (2) A brief history of energetic material development, (3) Assessment of a need for a new paradigm, (4) Technical opportunities, (5) Implementation strategy, (6) Why investing in energetic material R&D is a sound future policy?

Some of the answers proffered to the first and main question above; “Why should anyone individual, nation, or corporation invest in energetic material R&D?” were: (a) World societies, friendly and not friendly, will continue to invest in military technology, (b) Other societies may develop threats using new propellants and explosives, as well as new defenses, even with today’s limit R&D tool set, (c) Other societies may have more manpower to devote to these efforts, (d) These efforts may provide marginal improvements in materials that will translate into significant military advantage vis-à-vis our current capabilities.

If other nations or international groups develop offensive or defensive capabilities using new propellants or explosives, how will our advantages be maintained with conventional munitions? How does one conduct or advance R&D in conventional ordnance that will facilitate quick responses to actual or perceived threats? To stay competitive will require the agility to design, develop, and consistently (reproducible cost and quality) produce new materials rapidly. This must be coupled together with tight integration to implement those new energetic materials in new system designs. A scientific approach is therefore needed to design those energetic materials to meet new insensitive munition (IM), safety, aging, quality, health, and environmental compliance issues.

Environmental compliance issues or the development and fielding of “green” energetic materials raises additional questions such as; what is the measure of “green”, by what/whose definition, how much is enough or too much, and at what cost in terms of resources (money and time) and in terms of safety and performance? These issues must be addressed by any energetic materials development paradigm. The second theme noted above from the JANNAF report was; “A brief history of energetic material development” and its relation to where the state of the art is today. That theme is tightly coupled with the third theme “Assessment of a need for a new paradigm”. Current methods for development of new propellants and explosives are based on an empirical “Edisonian” approach developed in the early decades of the cold war. This approach requires large quantities of materials for tests, provides little insight beyond “go/no go” results, and takes several years to go through one testing cycle. An honest assessment is this approach has provided very limited successes in implementing new ingredients in the last 60 years. The results of using this approach has created the current perception that investing in the further development of new energetic material is fraught with risk and warrants little, or no, investment.

New instruments, new experimental methods, and new computational capabilities (theme of “technological opportunities” noted in the JANNAF report) will allow and facilitate the investigation of complex reactive systems that heretofore have not been available for use in investigating energetic materials. These tools have been applied to address complex issues in biological & biochemical systems and have revolutionized opportunities in these areas. These tools have not been applied in our overall

industry; remember the “black art” philosophy, to address the complex reaction issues that underlie the behaviors of propellants and explosives. Our “Implementation strategy” has to be a new paradigm whereby we not reject, but minimize, trial and error and maximize our current “technological opportunities” while continuing to develop new instruments, methods, and capabilities.

The ultimate goal of the scientific and engineering communities is to understand, measure, model, and predict the forces; i.e., the quantitative and qualitative mechanics that act upon the bonds between independent atoms, between intra-molecular atoms, and between molecules of complex molecular formulations. If these forces (chemical, mechanical, and electrical) can be understood and modeled from the molecular/atomic to macroscopic spatial scales (Fig. 1), the future performance or behavior of macro sized, orders of magnitude, infinitely more complex systems have the potential to be modeled with the advanced computational capabilities now available and perhaps understood and predicted².

The answer to the question/theme; “Why investing in energetic material R&D is a sound future policy” is the sustainment of leading edge capabilities in chemical propulsion systems and warheads. The table below projects the major payoffs that can be expected as additional focused research is accomplished.

Table 1: R&D Expectations

<i>Research Area</i>	<i>Energetic System</i>	<i>Major Payoff Projected</i>
Propulsion		
	Rocket Motors	Enhanced energy in heavy lift systems.
		Energetic binders to increase I_{sp} .
	Guidance Systems	Tailorable burn rates to provide in flight control resulting in more precise target interdiction.
	Guns	Tailorable burn rates to permit reduced gun weight, erosion, corrosive products, and extended gun life.
Warheads	Micro-propulsion	Programmable on-board micro-propulsion devices to steer warheads for increased accuracy/lethality.
	Energetic Payload	Use of controlled payload output utilizing different types of energetic material to permit a desired type of reaction with a particular target.
High Energy IM Systems	Propulsives & Warheads	Enhanced energetics knowledge to optimize tradeoffs between insensitivity and system requirements
	Propulsives & Warheads	Enhanced IM knowledge to provide safer- high performance systems that are less costly to transport, store and maintain.
Surveillance (Aging)	Propulsives & Warheads	New evaluation methods that can provide a better means for understanding aging behavior to optimize the life expectancy, assure safe continued performance and overall lowest life cycle cost.

Propulsion & Warhead Development:

If one reflects on the state of other technologies, such as optical and mass spectrometers and computers, which are ubiquitous and commonplace in our present-day laboratories, it is apparent that these tools were not available to the scientists and engineers who developed our original propulsion and warhead systems. To develop these energetic materials and their application articles at the time, testing protocols were created to enable engineers to develop safe munitions. Those tests typically provided limited information and for the most part simply provided an assessment of whether or not an energetic formulation would meet limited, and in most cases gross, laboratory and/or production line, safety and handling specifications. Further, in many cases the formulation, configuration, and subsystem specifications were based not on system requirements or the quest for optimum performance but merely on preproduction/production test results.

For example, drop or fall hammer tests were developed to assess impact sensitivity and various types of card gap tests (it seems most laboratories have their own favorite) were developed to assess shock sensitivity. This methodology continues in use today in the development of new formulations. Through extensive testing on a limited number of ingredients and formulations, an *art* (not a science) has been practiced in the design of new rocket motors and warheads using a well characterized, but limited set of ingredients. Thirty plus years ago when quite a number of current practitioners entered this business propellant development was referred to as a “black art”. The bad news is that these methods are basically still used today to design “new” propellants and explosives.

To help shift focus from antiquated methods still in use to what will be required in the future, a detailed description/list of the various “things that matter”, which was developed at the JANNAF meeting, is provided below as Table 2. These are all things, items, or issues that should frame any discussion of a new energetic material. Thus, it is important to recognize that experimental tools must focus on providing an understanding of reactivity over a wide range of conditions. The use of tools must also provide an understanding of this reactivity that can be used to design new compounds and materials.

Table 2: Things That Matter

<i>Item</i>	<i>Prop?</i>	<i>Exp?</i>	<i>Category</i>	<i>Reactive?</i>
Long-term stability	Y	Y	C	Y
Response in fires	Y	Y	S	Y
Response to impact – low rate mechanical energy input	Y	Y	S	Y
Response to shock -- high rate mechanical energy input	Y	Y	S	Y
Response to electrical stimuli	Y	Y	S, PF	Y
Coupling of mechanical/thermal in fire. Thermally induced changes alter response to mechanical energy.	Y	Y	S	Y
Toxicity & environmental compliance	Y	Y	S	N
Specific impulse	Y	N	PF	N
Pressure exponent	Y	N	PF	Y
Pressure oscillations	Y	N	PF	Y
Propellant or explosive integrity	Y	Y	PF, S	Y
Erosivity (guns)	Y	N	PF, C	Y
Tailor-able thrust	Y	N	PF	Y
Detonation velocity, detonation pressure	N	Y	PF	N
Processibility	Y	Y	M	Y
Dispersal of active compounds at target	Y	Y	D	Y
Response to Environmental Stressors (T, H, V, & S)	Y	Y	S, PF	Y

C - Compatibility; S - Safety; PF- Performance; M - Manufacturing; D - Disruptive technology Issues

Energetic Materials Research:

Modern experimental and computational methods have been brought to bear to understand reaction processes in energetic materials starting in the early 1980s. New research methods using laser-based optical diagnostics and mass spectrometers were developed to probe details of the reaction chemistry in propellants and explosives. Recent reviews of articles have shown how these instruments were used to probe the flame chemistry of propellants^{3,4} and reactions in shocks^{5,6}. The elementary reactions associated with processes that occur in flames have been probed experimentally and insight has been developed on the details of reactions at the atomic and molecular levels^{7,8}. Theoretical methods have also been used to calculate reaction pathways in both the gaseous⁷ and condensed phases^{10,11}. Much of this information has been used to construct mathematical representations of the combustion processes in solid propellants¹³⁻¹⁵.

These review articles provide excellent summaries of the application of state-of-the-art methods of physical chemistry and chemical physics to understand these relatively complex gas-phase processes. The articles also point to the relative lack of understanding of reaction processes in the condensed phase. Much of the research has focused on developing a deep understanding of the reaction processes of a few energetic compounds commonly used in explosives and propellants. The application of these methods to a wide range of different types of energetic compounds has been limited to an extensive set of flame chemistry work⁴.

While this research has provided a great deal of new understanding, there are two broad areas where our understanding remains quite limited. The first is how to connect the behaviors of *energetic materials* to their *molecular properties*. Brill has addressed this issue through extensive work examining the rapid thermolysis of many different types of energetic compounds. This work and those of others in this area has been summarized and general empirical correlations of behavior to different molecular properties developed¹⁵. As pointed out by Brill, “correlations between molecular properties and macroscopic bulk behavior are risky because of the myriad of processes taking place may defeat the simple fundamental connections with the parent molecule.” This leads to the second area in which we lack understanding: the reaction of energetic materials in the condensed phase at low and moderate temperature. The response of energetic materials at low and moderate temperature to thermal, mechanical and electrical energy stimuli underlie their safety and aging characteristics. A myriad of reactions control their behavior.

The response of new energetic materials to thermal and mechanical stimuli at low and moderate temperatures is the leading cause of failure to introduce new energetic ingredients into propellants or explosives. As Brill indicates there are a myriad of process taking place in the response of a bulk sample. In other words, the reaction processes involve complex reaction mechanisms, which take place in systems that may be considered to have disordered kinetics. This concept of examining the means to determine complex reaction mechanisms has been examined quite extensively outside the field of energetic materials. Ross, Schreiber and Vlad have recently published a book summarizing the issues, terminology, ideas, and approaches associated with determining complex reaction mechanisms in chemical, biological and genetic systems¹⁶. While many of the concepts currently used to characterize complex reaction mechanisms in chemical and biological systems are applicable to investigations of reaction processes in the condensed phase of energetic materials, it must be recognized that most of the complex chemical and biological systems deal with reactions in dilute solutions, or low density gases, where the concepts of elementary reactions and the role of stochastic variations in disordered kinetics are fundamental features of these systems. In contrast, reactions of energetic materials in response to thermal or mechanical stimuli take place in concentrated solutions, or solids, that have localized reaction environments on a range of different spatial scales.

The successful development of new energetic materials will require using methods to identify, understand, and characterize the reaction process in the various reactive environments that may be formed within a bulk energetic material. The various types of reactive environments may be characterized by spatial scales that are intrinsic properties of a material, or develop during the course of reaction. The possible spatial scales that need to be considered and various means to address reaction environments on these spatial scales are illustrated by the magenta lines in Figure 1 (see following page).

Both experimental and modeling & simulation methods must be developed to investigate reaction processes of energetic materials at these various spatial scales. New instruments, experimental protocols, and modeling & simulation methods to probe complex reaction mechanisms and the associated reaction kinetics of energetic materials in response to thermal stimuli have been developed by Behrens and summarized in a recent review article¹⁷. This type of approach also needs to be developed to investigate the complex reaction mechanisms and associated reaction kinetic of energetic materials in response to other types of energetic stimuli.

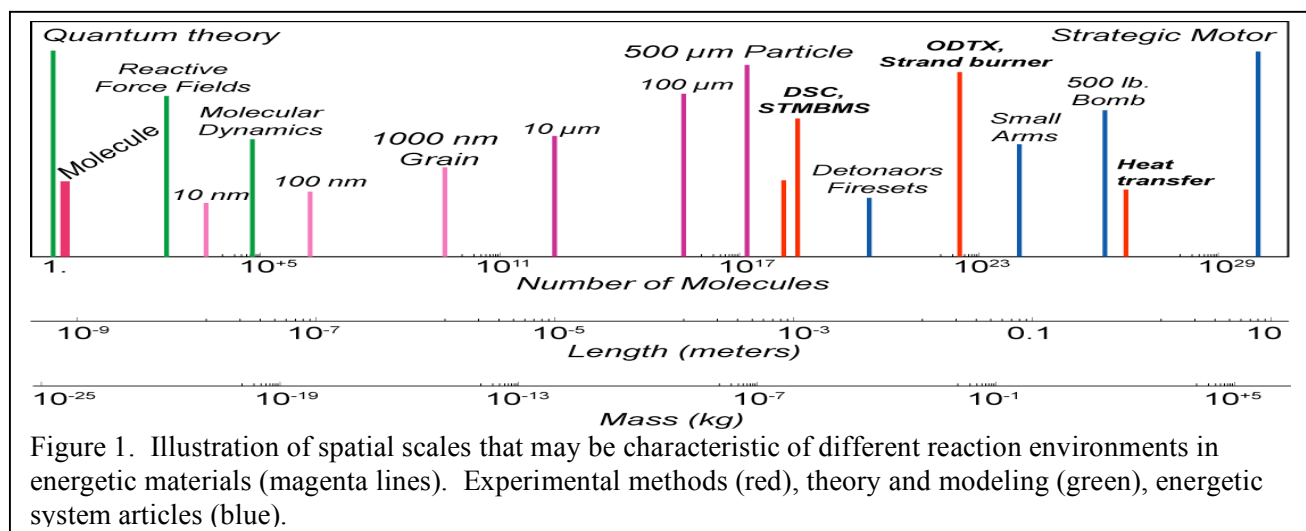


Figure 1: Scale of Issues

Ties between Research and Development:

The ties between research and development within the DoD in the area of propellant and explosive development have been limited. The development of new energetic materials for propulsion and warheads still relies on the empirical “Edisonian” approach of synthesizes, scale up, and test. No new experimental methods for research have been implemented in development venues. What is limiting the transfer of methods from the research community to the development community? First, most of the research has focused on the understanding elementary chemical reactions and the role that they play in combustion under propellant burning and explosive detonation conditions. While this provides valuable insight for connecting the properties of small energetic molecules to their behavior in combustion, to evaluate the burn rate or detonation velocity of new ingredients during the development process only requires a simple measurement. Thus, knowledge of the complex reaction processes that underlie combustion of a new propellant or detonation of a new explosive does not, in general, provide significant benefit in developing new ingredients by itself. In terms of performance, the development process requires the means to develop ingredients to tailor the burn rate of propellants as a function of pressure or make insensitive explosives. Research methods that can be transformed into development tools that will provide guidance for the development of new ingredients that meet these requirements would be beneficial.

It is also informative to consider the type of information that is required to develop new propellants and explosives. The developer needs to satisfactorily address the following issues: (1) Satisfactory burn rates and pressure exponents for propellants and detonation velocity and pressure for explosives, (2) Design materials to have the lowest impact and shock sensitivity, (3) Design materials to respond to slow and fast heating in a non-violent and relatively benign manner, (4) Design materials that are insensitive to electrostatic discharge, (5) Design materials that do not degrade with time, or degrade with time in a predictable and acceptable manner, (6) Provide a means to manufacture the material and not introduce any new features that may affect the material’s performance, safety or aging behaviors, (7) Provide a means to assess the state of the munition in a relatively inexpensive, but thorough manner. (8) Not present health or environmental compliance issues, (9) Disposal in an inexpensive and environmentally benign manner, (10) Implement new design concepts that enable systems to meet new military requirements.

In examining this list, it is apparent that performance issues comprise only a small portion of the developer’s tasks and associated issues. Research that will have the biggest impact on enhancing our ability to develop new energetic materials for propulsion and warheads will focus on addressing these

primary development issues. One current research area that can be tied into many of these development requirements are the methods that have been developed to investigate the reactions of energetic materials to thermal stimuli at low and moderate temperatures that are associated with burn rate modifiers, safety and long-term aging issues¹⁷.

A New Paradigm vs. A Shift of the Current Paradigm:

The current paradigm of an empirical “Edisonian” approach to develop new propellants and explosives is perceived as being unsuccessful and is thus considered high risk and unworthy of significant investment by today’s program managers. Given the large number of different requirements that must be satisfied to make a new propellant or explosive that meets very high performance goals while being as safe and as stable as possible, it is not surprising that the slow empirical “Edisonian” approach has not been successful.

The pharmaceutical industry often encounters similar problems of having to satisfy many different types of requirements, ranging from efficacy to safety¹ and cost. It has overcome these obstacles using and developing new scientific methods to probe the chemical, biological, and medical issues and requirements for new materials. It has developed new methods both to enhance screening methods and to develop a better understanding of diseases, in our terminology - requirements to guide the development of new drugs, vaccines and treatment therapies. When compared to the energetics product area, the pharmaceutical industry has somewhat clearer requirements statements such as the development of drugs for well-described diseases. However their quest for product improvement in efficacy, safety and cost can be seen as very similar to the need for the resolution of energetics products limitations that are well known and apparently acceptable status-quo. Table I depicts some areas of energetics performance for which successful focused R&D can result in significant product improvement.

Effective development of new energetic materials for munitions in the future will need to use a requirements-driven approach similar to that used by the pharmaceutical and biotechnology industries. This will require the development of a new paradigm that can develop new propellants and explosives much more rapidly, with orders of magnitude less material, and providing new data that can be used to guide the design of new compounds and composite materials.

Technical Opportunities:

Technical opportunities arise from addressing the technical challenges posed by future munition requirements. The technical challenges were uncovered by examining five areas at the workshop. These included: (a) Conventional methods for evaluating ingredients, (b) System requirements for new energetic materials, (c) Technical limits of implementation of new energetic ingredients in munitions, (d) New experimental concepts for evaluating performance and deleterious features of new ingredients, (e) New modeling/simulation methods for evaluating and predicting performance and deleterious features of new compounds and materials.

Material Design Parameters:

This section provides guidance to the developers of energetic material to enable them to focus on the attributes of the basic ingredients and formulations required for weapons of the future to have the desired effects on the target. However, it appears to represent a strategy very similar to the current state. Design goals are presented as incremental parameter performance improvements without regard to future weapons requirements. Goals and thresholds are represented without system performance rationale. Over 40% of the Material Design Parameters addressed indicate that the threshold parameter value, which is absolutely required for that particular parameter or application, is system or performance dependent. The objective of the Material Design Parameter Workshop Subgroup was to provide guidance to the developers of energetic molecules and materials to enable them to focus on the attributes of the basic ingredients and formulations required for weapons of the future to have the desired effects on the target.

This Subgroup would thus define the parameters of interest for ingredients for explosives, rocket and gun propellants and pyrotechnics used in DoD applications. These parameters include characteristics that contribute to energy content and release, safety, insensitive munitions (IM), service life, reliability, environmental compliance, health, processability, etc. Although difficult, due to varied Service requirements, there is a universal need to characterize energetics design characteristics and establish attainable values. Notwithstanding the differences between Services regarding energetics requirements and the difficulty in forecasting future weapons requirement, it is essential that energetics developers establish dialogue with war-planners to permit the early molding of weapons requirements based on reachable energetic material technology growth.

Experimental Methods and Diagnostics:

The primary objective is to provide the material scientist/engineer with the experimental tools needed to design new formulations required to meet system requirements of the future. The tools should provide the capabilities required to address new and different types of system requirements as the world geopolitical/military balance of power changes over long periods of time (many decades). For example, in the near term, the tools must provide the ability to design new materials to enable; (1) insensitive munitions, (2) low impact/shock sensitivity to enable earth penetrator design, and (3) tailor-able yields to enable design for asymmetric warfare scenarios. In the longer term, the tools must provide the capabilities to design weapons for (1) advanced naval conflicts and (2) space-based military encounters.

The tools must provide the nation with the capability to remain a leading world power and not be surprised by the military accomplishments of other societies on energetic technological fronts. It must be recognized that the challenge is to maintain military technologies with a smaller population compared to other emerging societies in the 21st century. This will require the ability to develop new energetic materials faster and in a smarter manner. It will also require increased efficiency in both the technical approach used to create and evaluate new materials and a more efficient and integrated use of manpower and resources, both at the national and international levels.

These capabilities must be maintained at a reasonable cost. This type of banal statement must be examined carefully and the underlying justification must be based on (1) a well-reasoned justification of what is a reasonable cost, and (2) what must be measured to determine if capabilities are indeed maintained. Some consideration should also be given to expandability, or elasticity, of the technical base.

By this, we mean what is the minimum level of effort or investment that will be required to provide a sustained basis for EM technology, but can be expanded rapidly to respond to potential military conflicts in the future. What is maintained as part of the nation's infrastructure? What is maintained by private industry? How can national infrastructure and private industry be efficiently integrated? The experimental tool set must allow "out-of-the-box" munition concepts to be evaluated and developed if necessary. For example, the technical basis should provide the means to address issues such as: (1) diverse interactions with a target, (2) detect and interact with selected populations, (3) benign interaction with the target (i.e., temporary disablement), (4) intelligent countermeasures, (5) miniature and tailor-able propulsion and explosive systems, (6) the ability to disable systems remotely and when desired. While implementation of many of these concepts may be undesirable, having the technical basis to rapidly implement these concepts, if necessary, may enhance future security.

Technical Challenges:

To identify, define, and develop the experimental tools needed to design energetic materials for the future requires defining how energetic materials will behave over the various environments encountered by warheads and propulsion systems during their life cycle. Conversely, as these tools are developed and the most radical capabilities and possibilities become reachable, dialogue with war-planners can be initiated to permit the early molding of weapons requirements contributing to the rapid deployment of emerging weapons. The types of things that matter were identified during the JANNAF

August 2006 meeting and presented earlier as Table 2. The items were categorized by those related to: performance (PF), safety (S), long-term aging and compatibility (C), manufacturing (M) or disruptive technology (D). Most of the important features of a propellant or explosive are dependent on the chemical reactivity of the material. As such, the success or failure of a propellant or explosive depends on its ability to meet the various criteria associated with the items listed in Table 1: Things That Matter.

Testing:

If testing or analysis results in a value above (if $<$ sign) or below (if $>$ sign) that shown, it could indicate a potential performance, safety, health or environmental issue or hazard and further testing or analysis is required. Many factors are important in estimating adverse environmental or occupational outcomes. These environmental criteria shown are intended to be used in rough screening or ranking procedures. Evaluation of environmental criteria often requires a weight of evidence approach whereby experimental data are given more weight than modeled or estimated values. An understanding of the various processes involved in environmental fate and transport are also needed since these values are not mutually exclusive in their ability to predict environmental transport or persistence.

Thus, it is important to recognize that the experimental tools must focus on understanding reactivity over a wide range of conditions. It must also provide an understanding of this reactivity that can be used to design new compounds and materials. To assess the possibility of implementing a new paradigm for the development of new energetic materials for future munition requirements, the following questions must be addressed: (a) Identify what really matters, (b) What current methods are used to address the issue, (c) What are the issues underlying reaction processes in the materials, (d) What spatial scales will play a role, (e) What is the extent of disorder, (f) What are the variations in disorder, (g) How complex are the reactions likely to be, (h) What research methods, protocols, and results are currently available and can be used to address the issue, (i) What physical and chemical phenomena are still unknown and will require more directed basic research, (j) How much material will be required to conduct a series of tests to address the issue, (k) What can be done with current state-of-the-art R&D methods, (l) What may be the smallest amount of material that could be reasonably utilized, (m) Can current research methods be developed into laboratory-scale diagnostic equipment, (n) How likely are small-scale experiments to be good predictors of larger scale munition behavior, (o) How much information will be generated by the measurements, and (p) The amount of information that will be provided for the next design cycle.

In examining each of these areas, it is important to recognize that the focus is on understanding reactivity and using this understanding to design new materials. From a very general point of view, the issue is to assess how thermal, kinetic, mechanical, or electrical energy will lead to reaction of the material. This may range from a very slow response, which would be characteristic of processes associated with aging, up to a fast response, which may be associated with performance or the response in severe abnormal environments. In examining these issues, it is recognized that there are different classes of approaches that must be used for investigating reaction behaviors in energetic materials and munitions.

These may be divided into the following categories: (1) Functional – These are typically go/no-go tests. These types of tests are used to determine whether a material meets a specified criteria or whether a device works or not. (2) Global – These tests measure a behavior that is the sum of many underlying processes. Thermal analysis tests, such as DSC, TGA or ODTX, or performance tests, such as detonation velocity, cylinder expansion, or propellant burn rates, are examples of these types of tests. These tests are often used to determine whether a new ingredient meets a set of desired “target” properties. (3) Complex reaction determination -- These tests identify local reaction environments (LRE) and characterize the reaction manifolds that control the behavior in each LRE.

These tests provide information on the actual chemical reactions that occur in a material. They provide a scientific basis for predicting the behavior of energetic materials and provide insight into how to design better compounds and materials. These types of tests may be based on (1) post-mortem analysis of

samples exposed to various energetic stimuli, or (2) real-time measurements of a localized reaction environment. These types of measurements are currently used in research laboratories. However, they have not made their way into the formulation environment.

Summary:

There is a critical need to create a plan for national R&D investment strategies that would enable the rapid implementation of new energetic ingredients (e.g., high nitrogen compounds, energetic binders, ionic liquids, and future materials) while meeting insensitive munitions (IM), aging, quality assessment and cost requirements. There is a growing disparity between the availability of new energetic material technology and the need for increased functionality and preparedness in the future weapons arsenal.

The transition from the current Propellant and Explosive material design/development process “paradigm” requires an ability to leap ahead of war-planners and weaponeers to provide futuristic possibilities that can both elevate performance levels and provide new warfare tactics and strategies. That “leap ahead” can only be achieved with a new paradigm; one that embraces new sense, test, analyze, and design technology opportunities and developments and relies less and less on the “black art” or “Edisonian” approach of the past.

Conclusions:

We must develop near (2 year), mid (5 year) and long term (10+ year) strategies that seek to accomplish the following: (1) Establish dialogue with war-planners to permit the early molding of weapons requirements based on reachable energetic material technology growth contributing to the rapid deployment of emerging weapons, (2) Develop national initiatives to provide the material scientist/engineer with the experimental tools needed to design new formulations required to meet system requirements of the future, (3) Develop national strategies that result in a capability to design weapons for advanced land, air, and naval conflicts and space-based military encounters.

We should explore the concept of a national virtual laboratory enterprise or consortium to bring the scientific and engineering communities together to understand, measure, model, develop, and most importantly predict the actions and inter-relationships of complex energetic molecular formulations so that application developments can progress at a faster pace with greater assurances of safety, reliability, and performance.

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References:

1. Lackman, T, Screening of Potentially Explosive Substances. *Proceedings of the 13th Jan Hansson Symposium on Chemical Problems Connected with the Stability of Explosives*, Backaskog, Sweden, 6-10 June 2004 p1
2. Swanson, R. L., Inter-Relationships between U.S. Navy Insensitive Munitions, Quality Evaluation (Aging), and Explosive Safety Programs. *Proceedings of the FINNEX 2002 Seminar*, 9-11 September 2002, Levi, Kittilä, Finland. p4
3. Korobeinichev, O. P., Study of Energetic Material Combustion Chemistry by Probing Mass Spectrometry and Modeling of Flames. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 75-102.
4. Parr, T.; Hanson-Parr, D., Optical Spectroscopic Measurements of Energetic Material Flame Structure. In *Overviews of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 103-127.
5. Greiner, N. R.; Fry, H. A.; Blais, N. C. In *Detonation Reaction Steps Frozen by Free Expansion and Analyzed by Mass Spectrometry*, 10th International Detonation Symposium, Boston, Massachusetts, 1993; Boston, Massachusetts, 1993.
6. Dlott, D. D., Multi-Photon Up-Pumping in Energetic Materials. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 303-333.
7. Dagdigian, P. J., Transient Gas-Phase Intermediates in the Decomposition of Energetic Materials. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 129-160.
8. Bernstein, E. R., Role of Electronic Excited States in the Decomposition of Energetic Materials. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 161-189.
9. Thompson, D. L., Gas-Phase Decomposition of Energetic Molecules. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 241-274.
10. Fried, L. E.; Manaa, M. R.; Lewis, J. P., Modeling the Reactions of Energetic Materials in the Condensed Phase. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 275-301.
11. Rice, B. M., Applications of Theoretical Chemistry in Assessing Energetic Materials for Performance or Sensitivity. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 335-367.
12. Anderson, W. R.; Fontijn, A., Gas-Phase Kinetics for Propellant Combustion Modeling: Requirements and Experiments. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 191-239.
13. Kim, E. S.; Yang, V., Combustion and Ignition of Nitramine Propellants: Aspects of Modeling, Simulation and Analysis. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 369-417.
14. Miller, M. S., Burning-Rate Models and Their Successors, A Personal Perspective. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 419-472.
15. Brill, T. B., Connecting Molecular Properties to Decomposition, Combustion, and Explosion Trends. In *Overview of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 1-27.
16. Ross, J.; Schreiber, I.; Vlad, M. O., *Determination of Complex Reaction Mechanisms - Analysis of Chemical, Biological, and Genetic Networks*. 1st ed.; Oxford University Press: New York City, 2006.
17. Behrens, R., Thermal Decomposition Processes of Energetic Materials in the Condensed Phase at Low and Moderate Temperatures. In *Overviews of Recent Research on Energetic Materials*, Shaw, R. W.; Brill, T. B.; Thompson, D. L., Eds. World Scientific Publishing Co.: Singapore, 2005; pp 29 - 74.