Use of JMP for High Explosive Formulation, Testing, and Data Analysis

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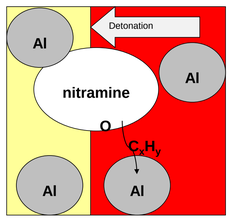
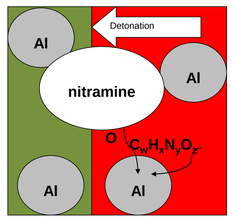
TECHNOLOGY DRIVEN. WARFIGHTER FOCUSED.

Introduction

Until recently, the formulation of explosives was an iterative "one factor at a time" process. By utilizing a mixture design in JMP, in conjunction with thermodynamic code, the design space of a formulation can be visualized and efficient trade-offs made. Further exploration of PAX-30, an explosive that combines both high blast and high metal pushing energy for fragmentation [1], will be shared. The explosive is unique in that it reduces the logistical needs of a soldier to possess multiple ammunition types for anti-personnel, through-wall, and anti-materiel targets. Early studies hypothesized that oxygen balance is the primary driver of early aluminum reaction [2], but other studies contradicted such evidence [3]. Since detonation calorimetry has been shown to directly correlate with gas expansion energy of cylinder expansion [4], an effort was undertaken so to resolve the factors that contribute to early aluminum reaction in the detonation process. Because the factors are confounded (oxygen balance, explosive/Al/Binder loading, amount of oxygen in the binder), a statistical DOE was used to resolve the primary factors. These included aluminum particle size, type of binder system, aluminum loading, and explosive loading. The type of binder, whether inert hydrocarbon or energetic with nitrate groups, was the primary driver of early aluminum reaction.



Composition w/ Inert Hydrocarbon Binder



Composition w/ Energetic Binder

Methods

JMP Analysis

A statistical mixture design of experiments was created using JMP Software (SAS Institute, Cary, NC, USA). The design consisted of two binder types (inert = polystyrene/dioctyl adipate, PS/DOA; energetic = bisdinitropropyl acetyl-formal/cellulose acetate butyrate, BDNPAF/CAB), three aluminum particle sizes (size 1, 2, and 3), and various loadings of nitramines (explosives), binder, and aluminum. Cheetah 5.0 Thermochemical code was used to calculate the theoretical heats of detonation assuming 100% and 0% aluminum reaction with the exp6.3 library. The design is shown in Table 1.

Detonation Calorimetry

The compositions were prepared in a pint Baker-Perkins (BP) vertical mixer by evaporation of the solvated binder system from a mixture of solids. Once sufficiently granulated, the powders were dried and fifteen gram detonation calorimeter samples were uniaxially pressed in a 2.38cm diameter die. Pressed densities ranged from 98.2% to 99.4% TMD for the BDNPAF/CAB compositions and 97.1% to 97.9% TMD for the PS/DOA compositions. The finished pellets were loaded individually into standard alumina crucibles and detonated in the detonation calorimeter with a 5.5g C4 booster charge and an RP-80 exploding bridgewire detonator (EBW) as previously reported [5]. Samples were tested in duplicate to obtain average detonation energies for each composition. The results are listed in Table 2 with the respective formulations. **Green**, **Red**, and **Blue** markers denote size 1, 2, and 3 aluminums, respectively, while X and O markers denote energetic and inert binders, respectively.

Table 1. Mixture DOE of the calorimeter shots and the respective oxygen balance.

Composition	% Nitramines	% Al	% Binder	Binder Type*	Al Particle Size	Composition %OB	Marker
PAX-30-2	77%	15%	8%	Energetic	1	-38%	X
PAX-30-3	73%	15%	12%	Energetic	1	-41%	X
PAX-30-4	72%	20%	8%	Energetic	3	-41%	X
PAX-30-5	68%	20%	12%	Energetic	3	-44%	X
PAX-30-6	77%	15%	8%	Inert	3	-54%	O
PAX-30-7	68%	20%	12%	Inert	1	-68%	O
PAX-30-8	73%	15%	12%	Inert	3	-64%	O
PAX-30-9	72%	20%	8%	Inert	1	-57%	O
PAX-30-10	72.5%	17.5%	10%	Energetic	2	-41%	X
PAX-30-11	72.5%	17.5%	10%	Inert	2	-61%	O

References

[1] Balas, W.; Anderson, P.; Cook, P.; Nicolich, S.; Capellos, C.; Pincay, J.; Stiel, L. *Development, Optimization and Application of Combined Effects Explosives,* Proceedings of the 2009 Insensitive Munitions Energetic Materials Technology Symposium, Tucson, AZ, May 11 – 14, 2009

[2] . Volk, F. Schedlbauer. "Products of Al Containing Explosives Detonated in Argon and Underwater". *Proceedings of the 10th International Detonation Symposium,* July 12 – 16, 1993, Boston, MA.

[3] .D. Gilev, V.F. Anisichikin. "Interaction of Aluminum with Detonation Products". *Combustion, Explosion, and Shock Waves,* Vol. 42, 107 – 115, 2006.

[4] I.B. Akst. "Heat of Detonation, the cylinder test, and performance munitions". 9th Symposium on Detonation, Portland, OR Aug 28, 1989.

[5] A.R. Davis, et al. "Anaerobic Detonation Behavior of Selected Enhanced Blast and Combined Effects Explosives". *Proceedings of the JANNAF 43rd Combustion Subcommittee Meeting,* December 7 – 11, 2009, La Jolla, CA

Results

The results from the calorimeter shots are shown graphically as a function of oxygen balance and energy output compared to theoretical output in Figures 1 and 2.

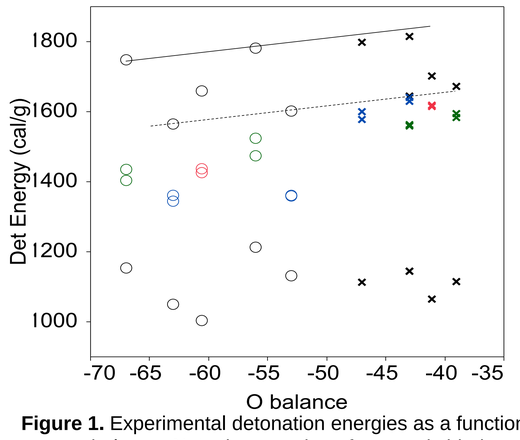


Figure 1. Experimental detonation energies as a function of oxygen balance. Note the grouping of energetic binder systems. —— is 8% binder, ----- is 12% binder, and two other points in between are 10% binder (centerpoints). Bottom points are 0% Al reaction, top are 100% Al reaction.

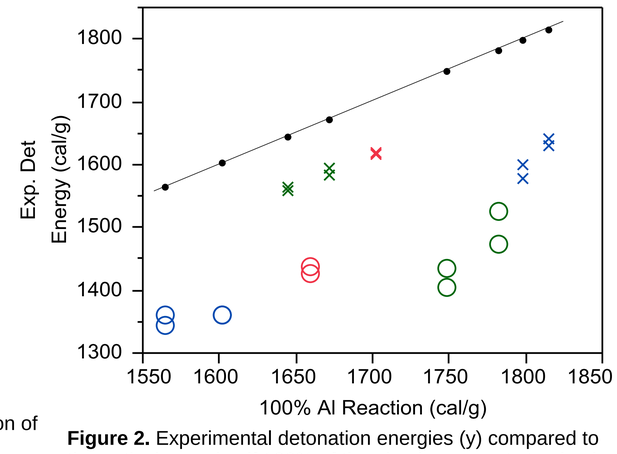


Figure 2. Experimental detonation energies (y) compared to theoretical energies if 100% of the aluminum reacts to aluminum oxide (x). Note all BDNPAF/CAB systems are closer to the 100% line.

The overall energy output and aluminum consumption is only weakly related to oxygen balance (Figure 1) despite the calculated linear relationship to detonation energy. The BDNPAF/CAB binder leads to more aluminum consumption in the detonation event than does the PS/DOA binder. This is shown by Figure 2; any points closer to the black line indicate more complete aluminum consumption. The interactive profiler generated from least squares fits of the data reveal that the categorical factor of binder type has the most effect on aluminum reaction and detonation energy (Figure 3). The least squares model possessed an R^2=0.960 with root mean square error (RMSE) = 0.028 for estimated % Al reaction, and an R^2 = 0.985 and RMSE = 15.50 (Figure 4) for the detonation energy Surprisingly, the amount of nitramines does not contribute to the overall changes in energy output. This is reflected by the relatively small slope of nitramines, binder, and aluminum amounts. However, it does possess a squared term which invokes the curvature in the response.

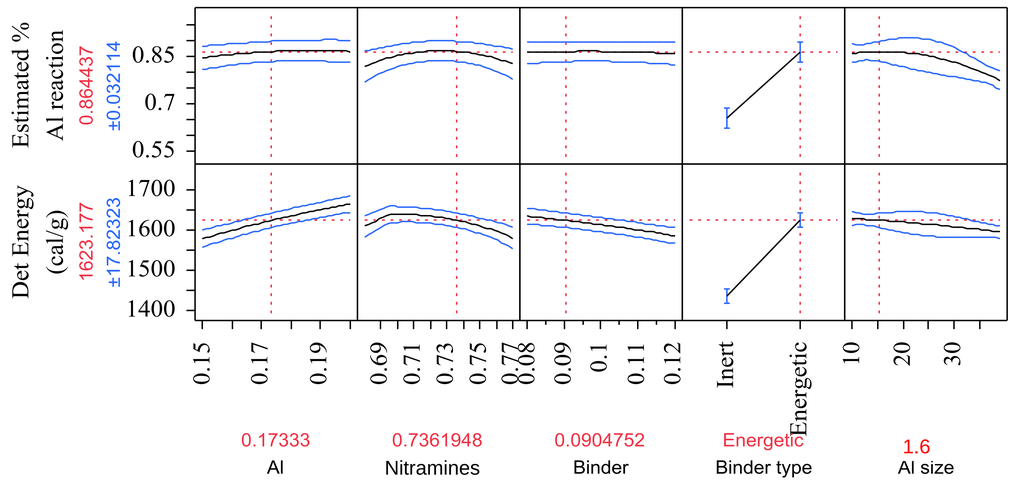


Figure 3. Optimized response curves from least squares regression fits. Note large changes in % Al reaction and detonation energies when the binder type is changed from Inert to Energetic.

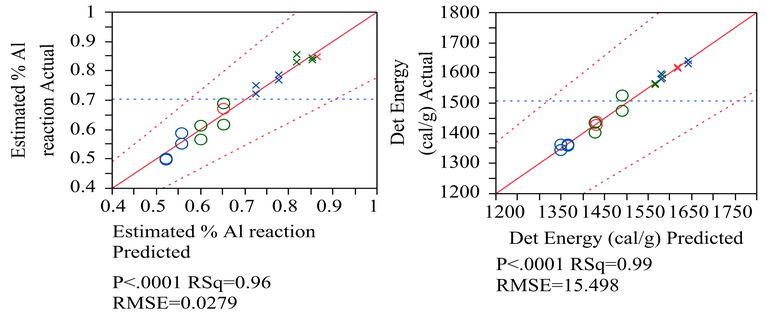


Figure 4. Actual by predicted plot of % Al reacted and Detonation energy. Due to use of the mixture design, interpretation of parameter estimates is relegated to the response profiler (Figure 3).

Conclusions

- The extent of aluminum reaction early in the detonation is *not* dependent to a significant degree on the amount of binder or up to aluminum particle size 2.
- The total energy of the system, however, is dependent upon the amount of Al, nitramines, and binder system, but the Al particle size did not have a significant impact.
- The type of binder is the primary driver behind early aluminum reaction. The data confirms the hypothesis as evidenced by the profiler that energetic functional groups on the binder promote the early reaction of aluminum. By surrounding the aluminum with oxygen rich groups, the oxygen diffusion barrier is minimized and thus the delay in reaction is minimized. This behavior leads to substantial performance gains and decreased sensitivity due to less nitramine loading.

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