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DEVELOPMENT OF INERT SIMULANTS FOR CASTABLE PLASTIC BONDED EXPLOSIVES

By
Wayne L. Elban

18 NOVEMBER 1971

NAVAL ORDNANCE LABORATORY, WHITE OAK, SILVER SPRING, MARYLAND

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ABSTRACT: This report describes the development and evaluation of inert simulants for two new castable explosives developed by NOL, namely, PBXW-106 and PBXN-103. The simulants closely duplicated the loaded density, processability, machinability, ultimate tensile strength and cured hardness of each explosive. Each simulant has a binder system consisting of an oil extended, hydroxyl-terminated polybutadiene resin that reacts with toluene diisocyanate to form a solid polyurethane polymer. Glass beads were the primary filler ingredient but a small amount of zinc powder was incorporated in the PBXN-103 simulant to attain the high density and low casting viscosity requirements. Using the basic solids-loaded polymer system selected for this work it is possible to formulate a simulant with a density that would closely match the density of most explosives of military interest.
Development of Inert Simulants for Castable Plastic Bonded Explosives (U)

This report describes the development of inert simulants for two explosives developed by NOL, namely, PBXW-106 and PBXN-103. This work was supported under Task ORD-332-001/091-1/UF17-354-313.

ROBERT WILLIAMSON II
Captain, USN
Commander

ALBERT LIGHTBODY
By direction
CONTENTS

1. INTRODUCTION ............................................. 1

2. MATERIALS ................................................. 1
   2.1 Simulant Composition .................................. 1
   2.2 Polymer System ....................................... 2
   2.3 Filler Materials ...................................... 2

3. EXPERIMENTAL ............................................... 2
   3.1 Processing ............................................. 2
   3.2 Simulant Properties Determination .................... 3
      3.2.1 Density .......................................... 3
      3.2.2 Density Distribution ............................. 3
      3.2.3 Viscosity ........................................ 3
      3.2.4 Workable Pot Life ................................ 3
      3.2.5 Mechanical Properties ............................ 4

4. RESULTS AND DISCUSSION ................................. 4

5. SUMMARY .................................................... 5

ACKNOWLEDGEMENTS ........................................... 6

REFERENCES ................................................... 7

APPENDIX A ................................................... A-1

APPENDIX B ................................................... B-1

APPENDIX C ................................................... C-1

TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Comparison of PBXW-106 and Simulant Properties</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>Comparison of PBXN-103 and Simulant Properties</td>
<td>9</td>
</tr>
<tr>
<td>3</td>
<td>Composition and Properties of PBXW-106 Simulants</td>
<td>10</td>
</tr>
<tr>
<td>4</td>
<td>Composition and Properties of PBXN-103 Simulants</td>
<td>11</td>
</tr>
</tbody>
</table>
1. INTRODUCTION

A program was undertaken at the Naval Ordnance Laboratory (NOL), White Oak, Maryland, to develop inert simulants for the castable, plastic-bonded explosives PBXW-106 (Refs. (1) and (2)) and PBXN-103 (Refs. (3) and (4)). Both PBX's are based on elastomeric polymer binders filled with various powdered explosives, oxidizers, and fuels. The testing and evaluation of weapons systems for characteristics other than explosive performance, sensitivity, and lethality are usually conducted with inert-loaded warheads. The use of explosive simulants simplifies certain phases of a warhead test program by greatly reducing safety requirements. Ordnance devices loaded with energetic materials make costly facilities and precautions essential for handling explosives; the same warhead, inert-loaded, may be tested without such limitations.

The properties that the weapon designer may specify for a given explosive simulant are many and varied. They include:

a. Density
b. Mechanical properties
c. Magnetic properties
d. Acoustic properties
e. Coefficient of thermal expansion
f. Resistance to temperature extremes
g. Thermal conductivity and specific heat
h. Pot life and viscosity of uncured simulants
i. Machinability of cured material

As a practical matter only those properties desired for a particular application are simulated.

The most important properties of both PBXW-106 and PBXN-103 which were to be simulated are given in Tables 1 and 2. Other important properties were homogeneity, good processing and casting characteristics, and machinability.

2. MATERIALS

2.1 Simulant Composition: The basic composition chosen to simulate the non-explosive properties of both explosives consisted of a commercially-available polyurethane binder filled with solid glass spheres.

2.2 Polymer System: The binder was made by reacting hydrocarbon oil extended-poly bd*hydroxyl-terminated liquid resins (Refs. (5) and (6)) with curing agents such as conventional di and polyisocyanates. The butadiene backbone of Poly bd resins is structurally similar to solid, general purpose diene rubbers; hence polymers formulated with these resins respond to solids reinforcement in an analogous manner.

*Trademark
propeller mixer to stir the ingredients until homogeneous. Most critical during this operation is adequate dispersion of the finely-divided, solid catalyst; mixing should be continued until agglomerates are no longer visible.

A typical batch mixing procedure was as follows:

The glass spheres were added to the premix in several increments and mixed until homogeneous. If more than one particle size was used, the fine material was added first. Then TDI was added and thoroughly mixed. Typical mixing cycles were 20 minutes in a one quart (500 cc maximum mixing capacity) Atlantic Research Corporation (ARC) vertical mixer operating at 50 r.p.m. and 25 ± 2°C. Mixing under vacuum was unnecessary because the viscosity was sufficiently low so that entrapped air was easily removed during vacuum casting. The material was cured at 50 ± 5°C for 24 hours.

3.2 Simulant Properties Determination

3.2.1 Density: The density sample was vacuum cast into a 5 cm I.D. cylindrical split mould. Once cured, the specimen was removed and machined to a nominal height of 2.5 cm. The density was calculated from the measured dimensions and weight of the sample.

3.2.2 Density Distribution: A two-fold approach was taken in determining the extent of solids settling. Initially, indentation hardness of opposite faces of the density sample was measured using a Shore durometer (Ref. (12)). Any appreciable density gradient should manifest itself as a measurable difference in the Shore hardness of the top and bottom faces. A second technique involved determining the density of a series of slabs sectioned from a 15 cm diameter by 30 cm long cylinder of material. Density data for various sections of the casting gave a clear indication of the degree of solids settling.

3.2.3 Viscosity: In view of the large emphasis on the compositions' processability, a Brookfield viscometer (Model HAO) placed on a Helipath stand was utilized to determine viscosity. The Helipath stand with accompanying bar-type spindles served to minimize the channeling effect as the spindle was rotated and translated in a helical path. Measurements were made at room temperature (25 ± 2°C) approximately 30 minutes after the addition of TDI; the viscometer operated at a constant 1 r.p.m. for all compositions. Readings were taken as the spindle was lowered and then reversed.

3.2.4 Workable Pot Life: Workable pot life is the time duration that the viscosity of a ready-to-cast composition remains sufficiently low to allow acceptable processability. A Sunshine Scientific gel time meter was used to evaluate the time from the addition of TDI to the time when the viscosity reached 10,000 poise, at the casting temperature (25 ± 2°C). Although chosen arbitrarily, material with a 10,000 poise viscosity is still castable and hence considered to be completely manageable.
3.2.5 Mechanical Properties: The mechanical properties of PBXW-106 and PBXN-103 desired to be most closely simulated were ultimate tensile strength, elongation and elastic modulus. These properties were determined in accordance with American Society for Testing and Materials (ASTM) procedure D 638-67T using Type I specimen dimensions (Ref. (13)). All testing was conducted using a Baldwin Universal Testing Machine operating at a crosshead speed of 5 cm per minute.

4. RESULTS AND DISCUSSION

A single lot of R-45M resin was used in all formulations for this program. The analysis accompanying this material listed a Brookfield viscosity at 30°C of 52 poise and a hydroxyl value of 0.73 meq/gm. The formulations for the inert simulant of PBXW-106 are given in Table 3, along with pertinent physical properties. The measured densities of these compositions were close to theoretical and followed the relation:

\[ \sum \frac{\varphi_i}{\rho_f} + \frac{1}{\rho_b} = \frac{1}{\rho_s} \]  

(1)

where: \( \varphi_i \) = solids loading weight fraction of the \( i \)th filler component  
\( \rho_f \) = density of the \( i \)th filler component  
\( \rho_b \) = binder density  
\( \rho_s \) = simulant density

The density and processability of the selected simulant composition closely match PBXW-106. No measurable difference in indentation hardness was detected for the opposite faces of the simulant density sample; it was concluded that solids settling didn't occur in this material. In addition to being homogeneous, no voids were observed in any of samples of this material.

Table 4 lists the compositions and properties of simulants for PBXN-103. Again, measured densities closely approached maximum theoretical given by Eq(1). Processing characteristics of the chosen composition would allow this material to be made in the same equipment used for PBXN-103. Density values for a number of slabs sectioned from a 15 cm diameter by 30 cm high right cylinder ranged from 1.89 to 1.88 gm/cm³ from top to bottom. Hence, in addition to offering excellent agreement with explosive density and viscosity, no solids settling was evident.
Machining characteristics of the cured simulants were very similar to those of their respective explosive. Both materials were easily cut with standard machining tools and had about the same surface finish as either explosive.

Excellent reproducibility was obtained between Shore hardness values of each simulant and respective explosive. However, examination of tensile properties revealed some disparity. While there was good agreement between ultimate tensile strength, elongation at break was low by approximately a factor of four for each simulant. Also erratic stress-strain behavior made evaluation of the elastic modulus of the simulants impractical. It is concluded, however, that the modulus of each simulant is considerably higher than the corresponding explosive. A comparison of the properties of the selected simulants with PBXN-106 and PBXN-103 properties is given in Tables 1 and 2 respectively.

5. SUMMARY

Inert Simulants for the castable plastic-bonded explosives PBXN-106 and PBXN-103 have been developed and tested yielding compositions which have a number of non-explosive properties closely corresponding to those of the explosive. In addition to similar processing characteristics, both simulants closely conformed to the loaded density, machinability, ultimate tensile strength, and Shore hardness of their respective explosives. The simulant for PBXN-106 consisted of 73.60% glass beads and 26.40% polyurethane binder. Using the same binder system, the PBXN-103 simulant contained 77.59% of a bimodal blend of glass beads and 5.00% zinc powder.
ACKNOWLEDGEMENTS

The able work of Edward T. Dyer in performing the mechanical property tests is gratefully acknowledged. The numerous helpful and enlightening discussions with Vernon D. Ringbloom is also gratefully acknowledged.
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2. NOL ltr 233:HH:job Ser 0645 of 31 Mar 1971 to NOSC


4. NOL confidential ltr 233:MJS:ba Ser 0193 of 5 Feb 1971 to NOSC

5. ARCO Chemical Company Product Bulletin BD-1: "Poly bd Liquid Resins"

6. ARCO Chemical Company Product Bulletin BD-2: "Reinforcement of Urethane Elastomers Based on Poly bd Liquid Resins"


12. 1968 Book of ASTM Standards, Part 27, ASTM Designation D2240-64T

**TABLE 1**

Comparison of PBXW-106 and Simulant Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>PBXW-106</th>
<th>Simulant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, gm/cm(^3)</td>
<td>1.65</td>
<td>1.65 ± 0.01</td>
</tr>
<tr>
<td>Ultimate Tensile Strength, kg/cm(^2) (psi)</td>
<td>2.81 (40)</td>
<td>2.97 (42.29)</td>
</tr>
<tr>
<td>Elongation at Break, %</td>
<td>13</td>
<td>3.3</td>
</tr>
<tr>
<td>Shore Hardness, A/1 sec dwell</td>
<td>25 Minimum</td>
<td>32</td>
</tr>
<tr>
<td>Workable Pot Life, hrs at 25°C</td>
<td>4-6</td>
<td>8</td>
</tr>
<tr>
<td>Viscosity, poise at 25°C</td>
<td>2,000-4,000</td>
<td>200</td>
</tr>
</tbody>
</table>
TABLE 2

Comparison of PBXN-103 and Simulant Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>PBXN-103</th>
<th>Simulant</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density, gm/cm$^3$</td>
<td>1.89</td>
<td>1.89 ± 0.01</td>
</tr>
<tr>
<td>Ultimate Tensile Strength, psi</td>
<td>7.31 (104)</td>
<td>7.49 (106.59)</td>
</tr>
<tr>
<td>Elongation at Break, %</td>
<td>11</td>
<td>2.9</td>
</tr>
<tr>
<td>Shore Hardness, A/1 sec dwell</td>
<td>83</td>
<td>71</td>
</tr>
<tr>
<td>Workable Pot Life, hrs at 25°C</td>
<td>48</td>
<td>5.5</td>
</tr>
<tr>
<td>Viscosity, poise at 25°C</td>
<td>350-1250</td>
<td>380</td>
</tr>
</tbody>
</table>
# TABLE 3
Composition and Properties of PBXW-106 Simulants

| Identification | Glass Spheres | | | | | | | |
|----------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|---------------|
|                | PBI 2429 Wt % | PBI 3000 Wt % | R-45M Wt % | Tufflo 100 Wt % | TDI | \( \rho \text{(gm/cm}^3) \) | \( \sigma \) | \( \epsilon_b \) | SH | PL | \( \eta \) | Remarks |
| Trial 1        | 59.25         | 15.75         | 12.05       | 12.05          | 0.90 | 1.67          | -             | -             | -- | 6  | 1600       | Density Too High |
| Trial 2        | 59.25         | 15.75         | 8.13        | 16.27          | 0.60 | 1.71          | -             | -             | -- | 8  | 120        |               |
| Trial 3        | 75.00         | --            | 8.13        | 16.27          | 0.60 | 1.70          | -             | -             | -- | 8  | --          |               |
| Trial 4        | 79.60         | --            | 6.63        | 13.27          | 0.50 | 1.80          | -             | -             | -- | 8  | --          |               |
| Trial 5        | 73.60         | --            | 8.58        | 17.16          | 0.66 | 1.65          | (42.29)       | 3.3           | 32 | 8  | 200        | Selected Composition |

FeAA constitutes 0.37 Wt % premix in Trial 1 and 0.03% in remainder of the Trials.
<table>
<thead>
<tr>
<th>Identification</th>
<th>Glass Spheres</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PBI 2429 Wt %</td>
<td>PBI 3000 Wt %</td>
<td>Z-5 Wt %</td>
<td>R-45M Wt %</td>
<td>Tufflo 100 Wt %</td>
<td>TDI Wt %</td>
<td>ρ</td>
<td>σ</td>
<td>e_b</td>
<td>SH</td>
</tr>
<tr>
<td>Trial 1</td>
<td>84.50</td>
<td>--</td>
<td>5.04</td>
<td>10.09</td>
<td>0.37</td>
<td>12000</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial 2</td>
<td>67.60</td>
<td>16.90</td>
<td>--</td>
<td>5.04</td>
<td>10.09</td>
<td>6</td>
<td>5500</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial 3</td>
<td>56.50</td>
<td>--</td>
<td>20.00</td>
<td>7.64</td>
<td>15.29</td>
<td>2.5</td>
<td>100</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial 4</td>
<td>62.07</td>
<td>15.52</td>
<td>5.00</td>
<td>5.66</td>
<td>11.31</td>
<td>0.44</td>
<td>1.89</td>
<td>7.49</td>
<td>(106.59)</td>
<td>71</td>
</tr>
</tbody>
</table>

FeAA is 0.03 Wt % premix for each Trial.
APPENDIX A

Glossary of Symbols

\( \rho \)  
Density, \( \text{gm/cm}^3 \)

\( \sigma \)  
Ultimate tensile strength, \( \text{kg/cm}^2 \) (psi)

\( e_b \)  
Elongation at break, %

\( E \)  
Elastic modulus, \( \text{kg/cm}^2 \) (psi)

\( \text{SH} \)  
Shore hardness, A/1 sec dwell

\( \text{PH} \)  
Workable pot life, hrs at 25°C

\( \eta \)  
Viscosity, poise at 25°C
Guidelines for Formulating Simulants with Different Densities

With the solids loaded polymer system chosen for this work, it is possible to produce a simulant whose density would closely match the density of almost any explosive of military interest. To determine the amount of filler needed to obtain a simulant of desired density one uses Eq(1). A sample calculation is given below for a simulant utilizing the same ingredients in the PBXW-106 simulant and having a density of 1.75 gm/cm³.

\[
\frac{\omega_b + \omega_f}{\rho_b} = \frac{1}{\rho_s}
\]

(1)

where

- \(\omega_b\) = Binder weight fraction
- \(\omega_f\) = Filler weight fraction
- \(\rho_b\) = Binder density
- \(\rho_f\) = Filler density
- \(\rho_s\) = Simulant density

In applying Eq. (1) the theoretical maximum density of the filler is used rather than bulk density. The unfilled cured binder whose composition is

- Wt %
  - R-45M Resin: 32.50
  - Tufflo 100 Extender Oil: 65.00
  - TDI: 2.50

has a measured density of 0.905 gm/cm³ while the reported density for the glass spheres is 2.40 gm/cm³. These values are substituted into Eq.(1) while making use of the relation

\[
\omega_b = 1 - \omega_f
\]

(2)

Hence

\[
\frac{1 - \omega_f + \omega_f}{0.905} = \frac{1}{2.40}
\]

(3)

Solving one obtains \(\omega_f = 0.78\).

Thus a simulant having a density of 1.75 gm/cm³ required 78% glass heads and 22% polyurethane binder. To process materials of this nature it is suggested that the procedure given in Section 3.1 of
this report be used as a guide. It is possible to greatly alter the processing and casting characteristics by varying the particle size distribution of the filler. The amount of hydrocarbon oil can drastically change the mechanical properties of reinforced Poly bd based elastomers. The table below gives some indication of the effect of oil-extension.

<table>
<thead>
<tr>
<th>Formulation</th>
<th>Parts by Weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-45M</td>
<td>100</td>
</tr>
<tr>
<td>TDI (-NCO/-OH=1.1)</td>
<td>7.7</td>
</tr>
<tr>
<td>Stannous Octoate</td>
<td>0.2</td>
</tr>
<tr>
<td>Tufflo 6054 Oil</td>
<td>--</td>
</tr>
<tr>
<td>Zinc Oxide</td>
<td>300</td>
</tr>
</tbody>
</table>

Physical Properties

| Ultimate Tensile Strength, kg/cm² | 72.42 | 72.73 | 35.86 |
| (psi) (1030)                     | (750) | (510) |
| Elongation at break, %           | 160   | 240   | 650   |
| Elastic Modulus, kg/cm² (psi)    | 62.57 | 40.08 | 15.47 |
| Shore Hardness, A/1 sec dwell    | 82    | 73    | 49    |
APPENDIX C

Product Identification

<table>
<thead>
<tr>
<th>Product</th>
<th>Description</th>
<th>Supplier</th>
</tr>
</thead>
<tbody>
<tr>
<td>FBI 2429</td>
<td>Glass spheres: 53-105 microns</td>
<td>Potters Brothers, Inc. Carlstadt, New Jersey</td>
</tr>
<tr>
<td>FBI 3000</td>
<td>Glass spheres: minus 44 microns</td>
<td>Potters Brothers, Inc. Carlstadt, New Jersey</td>
</tr>
<tr>
<td>Z-5</td>
<td>Zinc powder: 10 microns</td>
<td>Fisher Scientific Washington, D. C.</td>
</tr>
<tr>
<td>&quot;Merrillite&quot; *</td>
<td>Zinc powder: minus 44 microns</td>
<td>Pacific Smelting Company Torrance, California</td>
</tr>
</tbody>
</table>

*Acceptable Alternate
(U) This report describes the development and evaluation of inert simulants for two new castable explosives developed by NOL, namely, PBXW-106 and PBXN-103. The simulants closely duplicated the loaded density, processability, machinability, ultimate tensile strength and cured hardness of each explosive. Each simulant has a binder system consisting of an oil extended, hydroxyl-terminated polybutadiene resin that reacts with toluene diisocyanate to form a solid polyurethane polymer. Glass beads were the primary filler ingredient but a small amount of zinc powder was incorporated in the PBXN-103 simulant to attain the high density and low casting viscosity requirements. Using the basic solids-loaded polymer system selected for this work it is possible to formulate a simulant with a density that would closely match the density of most explosives of military interest.
Explosive Simulant

Plastic Bonded Explosive

Poly bd Hydroxyl - terminated liquid resin