(2)

AD

AD-E402 217

Technical Report ARAED-TR-91013

AN EXPLOSIVES PRODUCTS THERMODYNAMIC EQUATION OF STATE APPROPRIATE FOR MATERIAL ACCELERATION AND OVERDRIVEN DETONATION: THEORETICAL BACKGROUND AND FORMULATION

Ernest L. Baker

July 1991

US ARMY
ARMAMENT MUNITIONS
& CHEMICAL COMMAND
ARMAMENT RDE CENTER

U.S. ARMY ARMAMENT RESEARCH, DEVELOPMENT AND ENGINEERING CENTER

Armament Engineering Directorate
Picatinny Arsenal, New Jersey

REPORT DOCUMENTATION PAGE

Form Approved
OMB NO. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	July 1991	

4. TITLE AND SUBTITLE

AN EXPLOSIVES PRODUCTS EQUATION OF STATE APPROPRIATE FOR MATERIAL ACCELERATION AND OVERDRIVEN DETONATION: THEORETICAL BACKGROUND AND FORMULATION

5. FUNDING NUMBERS

6. AUTHOR(S)

Ernest L. Baker

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

ARDEC, AED
ATTN: Energetic Materials and Warheads Div.
ATTN: SMCAR-AEE-WW
Picatinny Arsenal, NJ 07806-5000

8. PERFORMING ORGANIZATION REPORT NUMBER

Technical Report ARAED-TR-91013

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

ARDEC, IMD
STINFO Br
ATTN: SMCAR-IMI-I
Picatinny Arsenal, NJ 07806-5000

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release, distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

Many modern explosive applications require modeling of both overdriven detonation and lower pressure detonations products expansion. Common thermodynamic equations of state used for warheads design have been demonstrated to provide poor representations of overdriven detonation. The Jones-Wilkens-Lee-Baker (JWLB) has been formulated to provide a more accurate representation. This report provides a detailed theoretical background and equation of state formulation for JWLB.

14. SUBJECT TERMS	15. NUMBER OF PAGES
	17
	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	SAR

CONTENTS

BACKGROUND

Many modern explosive applications require finite element and finite difference modeling of both overdriven detonation and lower pressure detonation products expansion. Large detonation wave shaping and multiple point initiation are typical overdriven detonation applications. Lower pressure detonation products expansion is required for material acceleration applications, such as explosively formed penetrators and shaped charges. Current thermodynamic equation of states used in dynamic finite element and finite difference programs are either parameterized to give agreement with thermochemical calculations [1] or experimental copper cylinder explosive expansion experiments [2,3]. Thermochemical calculations have proven to be very useful for the prediction of explosive products properties, particularly near and above the Chapman-Jouguet state [4,5]. Unfortunately, they do not reproduce the products expansion behavior accurately enough for typical warheads design. Currently, thermodynamic equations of state (JWL, Wilkens) [2,3] used for warheads design are normally calibrated to give agreement with copper cylinder explosive expansion experiments. These equations of state have not been calibrated for high pressures above the Chapman-Jouguet state. Experimentation [6] and comparison with thermochemical calculations (Figures 1,2, and 3) have demonstrated that a poor description of the high pressure region exists. In order to achieve a suitable equation of state for both overdriven and lower pressure products expansion, an appropriate equation of state form has been derived. A previous preliminary report [7] briefly describes the equation of state and parameterization methodology, but does not include details. This report provides a detailed theoretical background and equation of state formulation. A forthcoming report will provide a detailed description of the parameterization methodology.

EQUATION OF STATE FORMULATION

The equation of state form was chosen so as to adequately describe the high pressure regime produced by overdriven detonation, and yet retain the low pressure expansion behavior required for standard material acceleration modeling. To this end, the derived form is based on the Jones-Wilkens-Lee (JWL) equation of state [1] due to its computational robustness, and asymptotic approach to an ideal gas at high expansions. Additional exponential terms and a variable Gruneisen parameter have been added to adequately describe the high pressure region above the Chapman-Jouguet state. The resulting equation of state form, named Jones-Wilkens-Lee-Baker (JWLB), is

$$P = \sum_i A_i\left[1 - \frac{\lambda}{R_i V}\right]e^{-R_i V} + \frac{\lambda E}{V} + C\left(1 - \frac{\lambda}{\omega}\right)V^{-(\omega+1)} \qquad (1)$$

where,

$$\lambda \equiv \sum_i (A_{\lambda i}V + B_{\lambda i})e^{-R_{\lambda i}V} + \omega \qquad (2)$$

For consistency with the JWL equation of state, V is defined as a specific volume ratio, $V \equiv$

ρ_o/ρ and E is defined as $E \equiv \rho_o e$ where e is the specific internal energy. The JWLB equation of state form is based on a first order expansion around the principal isentrope:

$$P_s = \sum_i A_i e^{-R_i V} + C V^{-(\omega+1)}. \qquad (3)$$

Using the Gruneisen Parameter,

$$\lambda \equiv V \frac{\partial P}{\partial E}\bigg|_V, \qquad (4)$$

the isentropic identity,

$$P = -\frac{\partial E}{\partial V}\bigg|_S \qquad (5)$$

$$\Rightarrow E_s - E_{cj} = \sum_i \frac{A_i}{R_i} e^{-R_i V} + \frac{C}{\omega} V^{-\omega} - \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} - \frac{C}{\omega} V_{cj}^{-\omega}, \qquad (6)$$

and the Chapman-Jouguet condition,

$$E_{cj} = E_o + \frac{1}{2}(P_{cj} + P_o)(V_o - V_{cj})$$

$$= \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} + \frac{C}{\omega} V_{cj}^{-\omega}, \qquad (7)$$

the final form may be derived

$$P = \frac{\lambda}{V}(E - E_s) + P_s$$

$$= \frac{\lambda}{V}\left(E - \sum_i \frac{A_i}{R_i} e^{-R_i V} - \frac{C}{\omega} V^{-\omega}\right) + \sum_i A_i e^{-R_i V} + C V^{-(\omega+1)} \qquad (8)$$

$\Rightarrow$ Final Form.

Some important characteristics of the equation of state are that the Gruneisen Parameter λ, is represented as an analytic function of specific volume, V. $\lambda + 1$ approaches a constant adiabatic gamma, $\frac{V}{P}\frac{\partial P}{\partial V}\Big|_S = \omega + 1$ for large V, so that ideal gas behavior is asymptotically approached. The principal isentrope description is essentially identical to JWL, with the exception of an increased number of exponential terms. It has been found that for most explosives, three exponential terms (instead of two in JWL) are adequate to describe the principal isentrope over both the high pressure region above the Chapman-Jouguet state and the lower pressure expansion region. It is important to note that the internal energy referencing is defined by (7). The value of E_o must be consistent so that,

$$E_o = \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} + \frac{C}{\omega} V_{cj}^{-\omega} - \frac{1}{2}(P_{cj} + P_o)(V_o - V_{cj}) \,. \tag{9}$$

Normally, the equation of state parameters are chosen so that E_o has the value $E_o = \rho_o \Delta H$, where ΔH is the heat of detonation. This is consistent with the initial internal energy of the unreacted material having a value of zero.

SPEED OF SOUND

The generalized speed of sound is often required for implementation into a finite element or finite difference program. The speed of sound may be easily derived as follows,

$$\begin{aligned}\frac{\partial P}{\partial V} = {} & \sum_i A_i \left[\frac{\lambda}{R_i V^2} - \frac{\frac{\partial \lambda}{\partial V}}{R_i V}\right] e^{-R_i V} - \sum_i A_i \left[1 - \frac{\lambda}{R_i V}\right] R_i e^{-R_i V} \\ & + C\left(-\frac{\frac{\partial \lambda}{\partial V}}{\omega}\right) V^{-(\omega+1)} - C(\omega + 1)(1 - \frac{\lambda}{\omega}) V^{-(\omega+2)} \\ & - \frac{E\lambda}{V^2} + \frac{\lambda}{V}\frac{\partial E}{\partial V} + \frac{E}{V}\frac{\partial \lambda}{\partial V}\end{aligned} \tag{10}$$

$$\begin{aligned}(5), (10) \Rightarrow \left.\frac{\partial P}{\partial V}\right|_S = {} & \sum_i A_i \left[\frac{\lambda}{R_i V^2} - \frac{\frac{\partial \lambda}{\partial V}}{R_i V} - R_i + \frac{\lambda}{V}\right] e^{-R_i V} \\ & - C\left((\omega+1)(1-\frac{\lambda}{\omega}) + V\frac{\frac{\partial \lambda}{\partial V}}{\omega}\right) V^{-(\omega+2)} \\ & - \frac{E\lambda}{V^2} - \frac{\lambda}{V}P + \frac{E}{V}\frac{\partial \lambda}{\partial V}\end{aligned} \tag{11}$$

$$c^2 = \frac{\partial P}{\partial \rho} \Rightarrow \rho_o c^2 = -V^2 \left.\frac{\partial P}{\partial V}\right|_S \tag{12}$$

$$\begin{aligned}\Rightarrow \rho_o c^2 = {} & \sum_i A_i \left[V\frac{\frac{\partial \lambda}{\partial V}}{R_i} - \frac{\lambda}{R_i} + R_i V^2 - \lambda V\right] e^{-R_i V} \\ & + C\left((\omega+1)(1-\frac{\lambda}{\omega}) + V\frac{\frac{\partial \lambda}{\partial V}}{\omega}\right) V^{-\omega} + E\lambda + \lambda V P - EV\frac{\partial \lambda}{\partial V}\end{aligned} \tag{13}$$

$$\frac{\partial \lambda}{\partial V} = \sum_i A_{\lambda i} e^{-R_{\lambda i} V} - \sum_i (A_{\lambda i} V + B_{\lambda i}) R_{\lambda i} e^{-R_{\lambda i} V} \tag{14}$$

ADIABATIC GAMMA

Another useful quantity is the generalized adiabatic gamma. The adiabatic gamma may also be easily derived,

$$\gamma \equiv -\left.\frac{\partial \ln P}{\partial \ln V}\right|_S = -\frac{V}{P}\left.\frac{\partial P}{\partial V}\right|_S \tag{15}$$

$$(11),(15) \Rightarrow \gamma = \frac{1}{P}\sum_i A_i\left[\frac{\frac{\partial\lambda}{\partial V}}{R_i} - \frac{\lambda}{R_i V}\frac{\frac{\partial\lambda}{\partial V}}{R_i} + R_i V - \lambda\right]e^{-R_i V}$$

$$+\frac{C}{P}\left((\omega+1)(1-\frac{\lambda}{\omega}) + V\frac{\frac{\partial\lambda}{\partial V}}{\omega}\right)V^{(\omega+1)} + \frac{E\lambda}{VP} + \lambda - \frac{E}{P}\frac{\partial\lambda}{\partial V} \tag{16}$$

$$(14) \Rightarrow \frac{\partial\lambda}{\partial V} = \sum_i A_{\lambda i}e^{-R_{\lambda i}V} - \sum_i (A_{\lambda i}V + B_{\lambda i})R_{\lambda i}e^{-R_{\lambda i}V}.$$

PRINCIPAL ISENTROPE PROPERTIES

Often, properties along the isentrope that passes through the Chapman-Jouguet state are of particular interest. The Gruneisen parameter is given by (2). The adiabatic gamma is given by,

$$(3) \Rightarrow \frac{\partial P_s}{\partial V} = -\sum_i A_i R_i e^{-R_i V} - C(\omega+1)V^{(\omega+2)} \tag{17}$$

$$(3),(15) \Rightarrow \gamma_s = \frac{V\sum_i A_i R_i e^{-R_i V} + C(\omega+1)V^{(\omega+1)}}{\sum_i A_i e^{-R_i V} + CV^{(\omega+1)}}. \tag{18}$$

The speed of sound along the principal isentrope is given by,

$$(12) \Rightarrow \rho_o c^2 = \sum_i A_i R_i V^2 e^{-R_i V} + C(\omega+1)V^{\omega}. \tag{19}$$

REACTED PRODUCTS HUGONIOT

Another often used state space locus is the reacted products Hugoniot. Assuming the initial pressure to be zero, conservation gives,

$$\text{Mass: } \rho_o D = \rho(D-u) \tag{20}$$

$$\text{Momentum: } P = \rho_o D u \tag{21}$$

$$\text{Energy: } \frac{D^2}{2} + \frac{E_o}{\rho_o} = \frac{P}{\rho} + \frac{(D-u)^2}{2} + \frac{E}{\rho_o} \tag{22}$$

$$(20) \Rightarrow u = \frac{\rho - \rho_o}{\rho} D = (1-V)D \tag{23}$$

$$(23),(20) \Rightarrow P = \rho_o(1-V)D^2 \Rightarrow D^2 = \frac{P}{\rho_o(1-V)} \tag{24}$$

$$(22),\ (24) \Rightarrow \frac{P}{2\rho_o(1-V)} + \frac{E_o}{\rho_o} = \frac{P}{\rho} + V^2\frac{P}{2\rho_o(1-V)} + \frac{E}{\rho_o} \tag{25}$$

$$\Rightarrow E = E_o + \frac{P}{2(1-V)} - V^2\frac{P}{2(1-V)} - PV$$

$$= E_o + \frac{P}{2(1-V)}(1-V^2-2V+2V^2) = E_o + \frac{P}{2(1-V)}(V^2-2V+1)$$

$$= E_o + \frac{P(1-V)}{2} \tag{26}$$

$$(1),\ (26) \Rightarrow E\left(1 - \frac{\lambda(1-V)}{2V}\right)$$

$$= E_o + \left(\sum_i A_i\left[1 - \frac{\lambda}{R_i V}\right]e^{-R_i V} + C\left(1 - \frac{\lambda}{\omega}\right)V^{-(\omega+1)}\right)\frac{(1-V)}{2} \tag{27}$$

$$\Rightarrow E = \frac{E_o + \left(\sum_i A_i\left[1 - \frac{\lambda}{R_i V}\right]e^{-R_i V} + C\left(1 - \frac{\lambda}{\omega}\right)V^{-(\omega+1)}\right)\frac{(1-V)}{2}}{\left(1 - \frac{\lambda(1-V)}{2V}\right)} \tag{28}$$

CONCLUSION

An advanced thermodynamic equation of state applicable to problems involving overdriven detonation and material acceleration has been developed and calibrated for several explosives. This manuscript has presented a theoretical background and formulation for the new equation of state. A forthcoming report will describe the parameterization methodology. The new equation of state maintains required low pressure expansion behavior while providing a better high pressure description applicable to overdriven detonation. Typical applications of the new equation of state include wave shaped and peripherally initiated munitions. Finally, the equation of state asymptotically approaches the constant gamma equation of state at high expansions. It is therefore believed that the equation of state will be applicable to extremely large volume expansion applications, such as blast, without a loss of accuracy in the higher pressure regions. In order to use the equation of state for very large expansions, proper calibration to very large volume expansion experimentation will be required.

SYMBOLS

$P \equiv$ Pressure

$\rho \equiv$ Density

$V \equiv$ Ratio of Specific Volume to Initial Specific

Volume

$E \equiv$ Specific Internal Energy divided by Initial Specific Volume

$\lambda \equiv$ Gruneisen Parameter

$\gamma \equiv$ Adiabatic Gamma

$c \equiv$ Sound Speed

$D \equiv$ Detonation Velocity

$u \equiv$ Mass Velocity

$\Delta H \equiv$ Heat of Detonation

$A_i, R_i, C, A_{\lambda i}, B_{\lambda i}, R_{\lambda i}, \omega \equiv$ Equation of State Constants

$_s \equiv$ Isentropic

$_{cj} \equiv$ Chapman-Jouguet State

$_o \equiv$ Initial Conditions

REFERENCES

1. C.L. Mader, *Numerical Modeling of Detonations*, University of California Press, 1979.

2. M.L. Wilkens , "The Equation of State of PBX 9404 and LX04-01", Lawerence Radiation Laboratory, Livermore, Rept. UCRL-7797, 1964.

3. E.L. Lee, H.C. Horning, and J.W. Kury, "Adiabatic Expansion of High Explosive Detonation Products", University of California Report No. UCRL-50422, 1968.

4. C.L. Mader, "FORTRAN BKW - A Code for Computing the Detonation Properties of Explosives", University of California Technical Report LA-3704, 1967.

5. M. Cowperthwaite and W.H. Zwisler, "TIGER Computer Program Documentation", Stanford Research Institute Publication No. Z106.

6. L.G. Green, C.M. Tarver, and D.J. Erskine, "Reaction Zone Structure in Supracompressed Detonating Explosives", University of California Report No. UCRL-101862.

7. E.L. Baker, and J. Orosz, "Advanced Warhead Concepts: An Advanced Thermodynamic Equation of State for Overdriven Detonation", Picatinny Arsenal Technical Report ARAED-TR-91007, 1991.

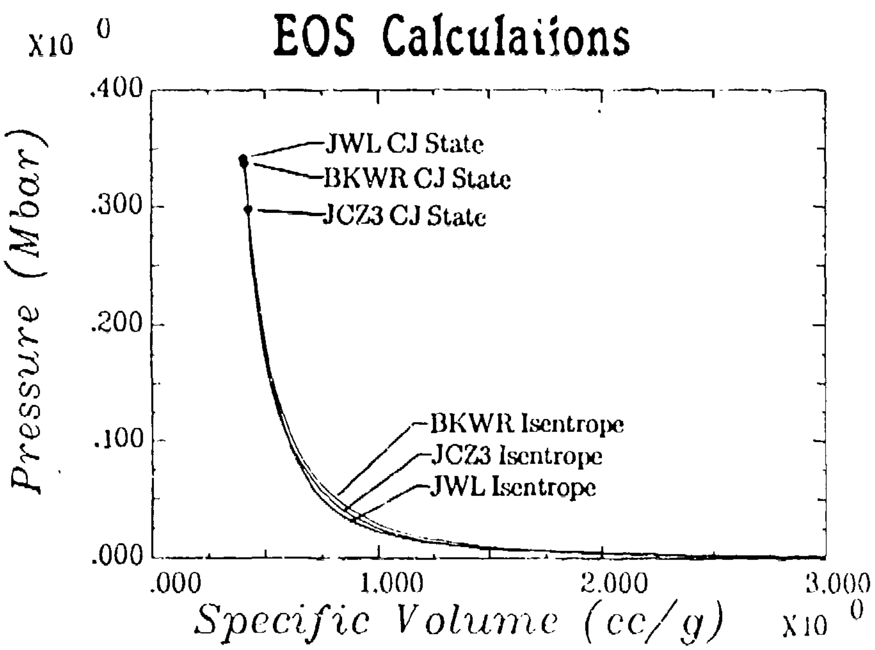

Figure 1. Pressure versus specific volume for the principal isentrope of octol 75/25 below the Chapman-Jouguet state. The thermochemical calculations (BKWR and JCZ3) agree fairly well with the standard JWL.

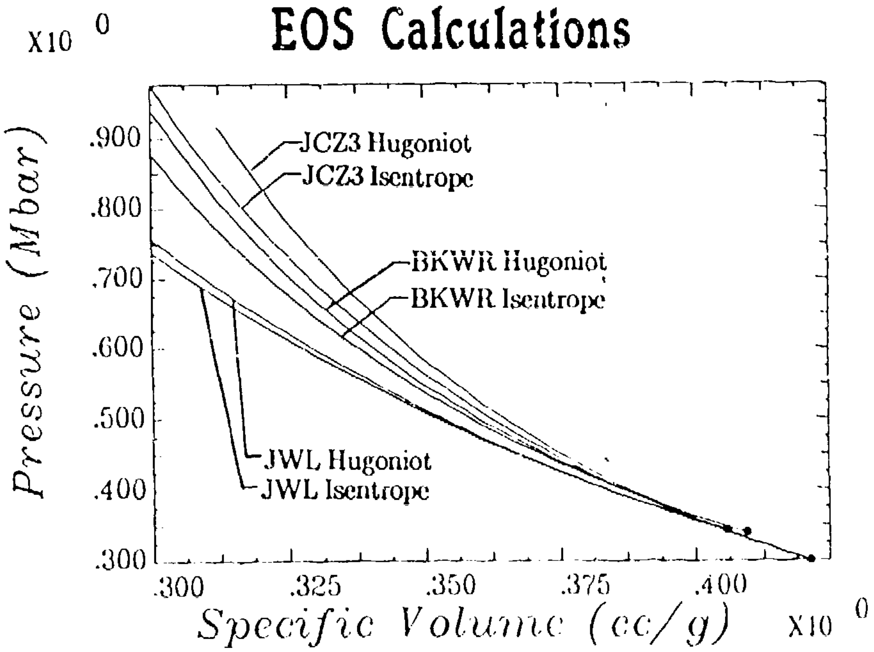

Figure 2. Pressure versus specific volume for the principal isentrope and reactive Hugoniot of octol 75/25 above the Chapman-Jouguet state. The standard JWL underpredicts the high pressure region.

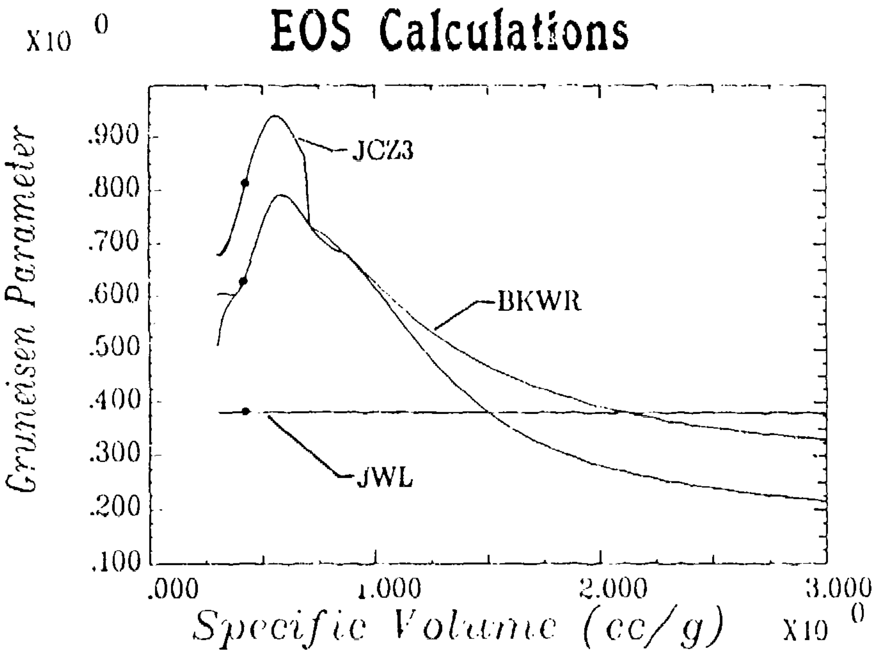

Figure 3. The Gruneisen parameter versus specific volume for the principal isentrope and reactive Hugoniot.

DISTRIBUTION LIST

Commander
U. S. Army Armament Research, Development and Engineering Center
ATTN: SMCAR-IMI-1 (5)
SMCAR-CO
SMCAR-TD
SMCAR-TDC
SMCAR-AE (3)
SMCAR-AEE (3)
Picatinny Arsenal, NJ 07806-5000

Commander
U. S. Army Armament Research, Development and Engineering Center
ATTN: AMSMC-GCL(D)
AMSMC-DSM-B(D)
Picatinny Arsenal, NJ 07806-5000

Commander
U. S. Army Materiel Command
ATTN: AMCCN-C
AMCLD,D. Vitali
5001 Eisenhower Avenue
Alexandria, VA 22333-0001

Commander
U. S. Army Armament, Munitions and Chemical Command
ATTN: AMSMC-DCG
AMSMC-DSM-A
Aberdeen Proving Ground,MD 21010-5423

Commander
U. S. Army Depot Systems Command
ATTN: AMSDS-QV
AMSDS-T
AMSDS-SM-SPA
AMSDS-CG
Chambersburg,PA 17201-4170

Administrator
Defense Technical Information Center
ATTN: Accessions Division (2)
Cameron Station
Alexandria, VA 22304-6145

Director
U. S. Army Materiel Systems Analysis Activity
ATTN: AMXSY-MP
AMXSY-RW
Aberdeen Proving Ground,MD 21005-5066

Commander
Chemical Research,Development and Engineering Center
U. S. Army Armament, Munitions and Chemical Command
ATTN: SMCCR-SPS-IL
SMCCR-CO
SMCCR-MU
SMCCR-SPS-M
SMCAR-RSP-A
Aberdeen Proving Ground, MD 21010-5423

Director
Ballistic Research Laboratory
ATTN: AMXBR-OD-ST
SLCBR-TB-EE
Aberdeen Proving Ground,MD 21005-5066

Chief
Benet Weapons Laboratory, CCAC
Armament Research,Development and Engineering Center
U. S. Army Armament, Munitions and Chemical Command
ATTN: SMCAR-CCB-TL
Watervliet, NY 12189-5000

Commander
U. S. Army Armament,Munitions and Chemical Command
ATTN: SMCAR-FSP-D
SMCAR-DS
AMSMC-IMF-L
Rock Island, IL 61299-6000

Director
U. S. Army TRADOC Systems Analysis Activity
ATTN: ATAA-SL
White Sands Missile Range, NM 88002

Commander
Naval Weapons Center
ATTN: L. Smith, Code 320
A. Amster, Code 385
R. Reed, Jr., Code 388
K. J. Graham, Code 3835
China Lake, CA 93555

Director
Lawrence Livermore National Laboratory
University of California
P.O. Box 808
ATTN: M. Finger
C. Tarver
L. Green
Livermore, CA 94550

Director
Los Alamos National Laboratory
ATTN: L. Hull
T. Bennion
J. Chapyak
J. Ritchie
Los Alamos, NM 87545

Director
Sandia National Laboratory
Albuquerque, NM 87185

Commander
Naval Surface Weapons Center
ATTN: Code G13
Dahlgreen, VA 22448

Commander
Naval Surface Weapons Center
ATTN: L. Roslund, R122
M. Stosz, R 121
Code X211, Library
E. Zimet, R13
R.R. Bernecker, R13
J.W. Forbes, R13
S.J. Jacobs, R10
C.Dickinson
J. Short, R12
Silver Spring,MD 20910

Air Force Armament Laboratory
ATTN: J. Forster, AFATL-MNW
G. Parson, AFATL-MNE
Eglin AFB,FL 32542-5434

Dyna East Corporation
ATTN: William Flis
3201 Arch Street
Philadelphia, PA 19104

Aerojet Ordnance Company
ATTN: Dan Donati
2521 Michelle Dr
Tustin, CA 92680

Applied Ordnance Technology, Inc.
ATTN: NIMIC, Eddie Norton
1000 Century Plaza, Suite 212, BX24
10630 Little Patuxent Parkway
Columbia, MD 21044

Commander
Chemical Research, Development and Engineering Center
U.S. Army Armament, Munitions and Chemical Command
ATTN: SMCCR-MSI
Aberdeen Proving Ground, MD 21010-5423

Royal Ordnance
ATTN: Dr. Peter R. Lee
Westcott, Aylesbury
Buckinghamshire, HP180NZ England