

AD-A148 897

12

AD-A148 897

AD

B
R
L

MEMORANDUM REPORT BRL-MR-3395

APPLICATION OF MONTE CARLO AND MOLECULAR DYNAMICS METHODS TO THE CALCULATION OF THERMODYNAMIC PROPERTIES OF MOLTEN SALTS

Richard D. Murphy

October 1984

DTIC
ELECTE
JAN 7 1985
S
B

DTIC FILE COPY

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

US ARMY BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

84 12 20 002

Destroy this report when it is no longer needed.
Do not return it to the originator.

Additional copies of this report may be obtained
from the National Technical Information Service,
U. S. Department of Commerce, Springfield, Virginia
22161.

The findings in this report are not to be construed as an official
Department of the Army position, unless so designated by other
authorized documents.

The use of trade names or manufacturers' names in this report
does not constitute indorsement of any commercial product.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER MEMORANDUM REPORT BRL-MR-3395	2. GOVT ACCESSION NO. AD-A148897	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Application of Monte Carlo and Molecular Dynamics Methods to the Calculation of Thermodynamic Properties of Molten Salts.		5. TYPE OF REPORT & PERIOD COVERED Special Report
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Richard D. Murphy *		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS US Army Ballistic Research Laboratory ATTN: AMXBR-IBD Aberdeen Proving Ground, MD 21005-5066		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 1L162618AH80
11. CONTROLLING OFFICE NAME AND ADDRESS US Army Ballistic Research Laboratory ATTN: AMXBR-OD-ST Aberdeen Proving Ground, MD 21005-5066		12. REPORT DATE October 1984
		13. NUMBER OF PAGES 16
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for Public Release: Distribution Unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES This report is based on work performed during the tenure of an ARO Summer Faculty grant. * University of Missouri at Kansas City		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Liquid Propellants Monte Carlo Liquid State Hydroxylammonium Nitrate		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report summarizes the work done during the course of an ARO Summer Faculty grant at the Ballistic Research Laboratory. The technical details will be reported elsewhere. The current state of knowledge of the structural properties of hydroxylammonium nitrate (HAN) is summarized. The possibility of determining these properties by computer simulation is discussed. The features of the Monte Carlo and Molecular Dynamics approaches to computer simulation are briefly reviewed; the former method has more promise for the present problem, and its application is explored. A formula not previously		

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

20. Abstract (Cont'd)

found in the literature was derived for the heat capacity at constant pressure for a system at given density and temperature from a single Monte Carlo run.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

TABLE OF CONTENTS

	Page
I. INTRODUCTION.....	5
II. THE MONTE CARLO AND MOLECULAR DYNAMICS METHODS.....	5
III. EXPERIMENTAL DATA ON STRUCTURE AND THERMODYNAMIC PROPERTIES.....	7
IV. PRESENT STATE OF MONTE CARLO WORK.....	8
V. RECOMMENDATIONS FOR FURTHER STUDIES.....	9
VI. ACKNOWLEDGEMENTS.....	10
REFERENCES.....	11
DISTRIBUTION LIST.....	13

S DTIC
 ELECTE
 JAN 7 1985
D
 B

DTIC
 COPY
 INSPECTED

Accession For	
NTIS GPO/NTIS	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
By	
Distribution/	
Availability Codes	
Dist. Avail. or	
Dist. Method	
A-1	

I. INTRODUCTION

The Ballistic Research Laboratory, particularly the Advanced Ballistic Concepts Branch, has been engaged for some time in the development of liquid gun propellants, one formulation of which is a concentrated aqueous solution of hydroxylammonium nitrate (HAN) and various aliphatic amine nitrates. The very substantial promise shown by these propellants has recently been discussed,¹⁻³ and test fixtures have been successfully fired. At least partially because pure HAN is difficult to prepare and handle, there has been little fundamental research on its thermodynamic properties. This fundamental knowledge, however, can reasonably be expected to become of greater importance as development of these propellants proceeds. This report will discuss the state of the current knowledge of the properties of HAN solutions and some related compounds and the possibility of computer simulation of them by modeling them as molten salts. The work that has been completed on the development of computer codes for this purpose will be summarized, and recommendations made concerning possible further work, both theoretical and experimental, on these substances.

II. THE MONTE CARLO AND MOLECULAR DYNAMICS METHODS

Simple monatomic liquids, which can be adequately characterized by a known or assumed intermolecular potential (usually central), have been extensively studied in recent years. The most thoroughly understood substance is surely argon, and the detailed knowledge of the intermolecular interaction^{4,5} which is available for this simple substance is sufficient that it appears that all of its thermodynamic properties in the liquid, gas and solid phases can be computed even to megabar pressures, i.e. close to the metallic transition. A comparable degree of knowledge exists for the other rare gases, but there are many substances, especially more complex ones, for which the interactions are quite poorly characterized.

When a substance with a known intermolecular potential is studied, the question of the method of calculation of its thermodynamic properties arises. In a dilute gas, the low density means that the virial expansion, which is a power series in the density, is rapidly convergent and so all the equilibrium thermodynamic properties can be reasonably simply calculated; the transport properties of a dilute gas can also be obtained from the Chapman-

¹W. P. Morrison, "The Application of Liquid Propellant Gun Technology to Field Artillery," presented at the 1982 JANNAF Propulsion Meeting.

²E. Freedman, ed., "An Outline of Liquid Propellants," to be published.

³W. O. Seals, "Vulnerability Studies for a Liquid Propellant System," presented at the JANNAF Propulsion Systems Subcommittee Meeting (1983).

⁴J. A. Barker, R. A. Fisher, and R. O. Watts, *Mol. Phys.*, 21, 657 (1971).

⁵J. Barker and D. Henderson, *Revs. Mod. Phys.* 48, 587 (1976).

Enskog and other solutions to the Boltzmann equation. In the other limit, a solid, although its density is high, has a fixed structure, and simple lattice summations and harmonic-approximation lattice dynamics (and its generalizations) are usually satisfactory. But there are difficult intermediate cases: Liquids, dense gases and highly anharmonic solids (e.g., quantum solids and those near melting), where the above simpler techniques fail. In these cases, although some simpler techniques such as perturbation theory are sufficiently accurate to be of use, only machine simulation techniques will yield exact results.

The two principal machine simulation techniques, each of which has some variants, are the Monte Carlo (MC) and molecular dynamics (MD) methods. Because they have been discussed in detail in many places,⁶ only a brief overview of the usual procedures will be given here. In each method, a system of a few hundred particles is set up on a computer, with the particles being confined to a cubical box whose side L is chosen to reproduce the density of the physical system one wishes to simulate. In order to minimize surface effects, the nearest-image periodic boundary condition convention is used. In the MC method as formulated by Metropolis *et al.*,⁷ particles make random moves, which are accepted or rejected with a probability proportional to the Boltzmann factor $\exp(-U/kT)$, where U is the known or assumed potential energy, k is the Boltzmann constant, and T is the Kelvin temperature. This procedure is a Markov process, and the average of such equilibrium thermodynamic properties as the energy, pressure, heat capacity, bulk modulus and radial distribution function over the configurations generated with the above probability is a presumably exact calculation of these properties of the actual physical system. The Monte Carlo method thus used can provide all the equilibrium thermodynamic properties of the system, although it may be necessary to perform a number of these simulations over a range of temperatures and/or densities and integrate the results with respect to temperature or density in order to obtain certain properties, especially the entropy.

In the MD method due originally to Alder and Wainwright,⁸ the particles move, not at random, but in accordance with the known or assumed force law (the force is the negative gradient of the potential energy U). In other words, one simply integrates Newton's equations of motion for the system. Rather than the canonical ensemble average used in the Monte Carlo method, thermodynamic properties are evaluated as time averages in the microcanonical ensemble, with the agreement of the results of the two approaches following from the ergodic theorem of statistical mechanics.

In comparing the two techniques, it must be stated that both yield all

⁶J. P. Hansen and J. R. McDonald, *Theory of Simple Liquids*, Academic Press, NY (1976).

⁷N. Metropolis, A. W. Rosenbluth, N. W. Rosenbluth, A. H. Teller, and E. Teller, *J. Chem. Phys.* 21, 1087 (1953).

⁸B. J. Alder and T. E. Wainwright, *J. Chem. Phys.* 27, 1208 (1957).

the equilibrium thermodynamic properties of a system, including the radial distribution function (also called the "pair correlation function"), $g(r)$. For purposes of comparison with experiment, the Fourier transform of $g(r)$, usually called the "liquid structure factor" and denoted by $S(k)$, is directly proportional to the differential scattering cross-section for elastic X-ray or neutron scattering. The constant of proportionality is, however, different in the two cases because X-rays are scattered by atomic electrons (Thompson scattering), whereas neutrons are scattered by nuclei. Molecular dynamics yields also the dynamic structure factor $S(k, \omega)$ which is directly proportional to the doubly-differentiated (with respect to angle and energy) cross-section for inelastic neutron scattering. In addition, the molecular dynamics method can yield some transport properties, especially the diffusion coefficient, without much difficulty. Unfortunately for the current application, in which the viscosity is of considerable interest, this is a notoriously difficult property to calculate because it is a many-body effect rather than a single-particle property. To illustrate the difficulty of the viscosity calculation, we quote Erpenbeck and Wood⁹ in discussing MD work on a system of hard spheres (the simplest imaginable potential) which had consumed thirty-four hours on a Cray computer: "...it is quite possible that at high density the asymptotic behavior is not established until times substantially longer than those attainable in the present work" and "To obtain a better estimate of (the viscosity), then, would appear to require both a theory for the decay of the cross and potential terms and much more extensive molecular dynamics calculations for the 4000-particle system. The latter would appear to be at the limit of practicality with current computer speeds."

The MC and MD methods have been applied to more complex liquid systems, e.g., those with noncentral intermolecular interactions and systems with two or more different types of molecules. A system composed of two types of molecules is characterized by three different intermolecular interactions and three different pair-correlated functions, the Fourier transforms of which are called "partial structure factors." In the current effort, only the MC method has been undertaken to date, primarily because it is easier to use. Until the basic mechanisms governing the behavior of the liquid have been identified and the intermolecular interactions well enough determined that equilibrium properties can be reasonably accurately calculated, there seems to be little point in attempting the more difficult calculation of transport properties.

III. EXPERIMENTAL DATA ON STRUCTURE AND THERMODYNAMIC PROPERTIES

The machine simulation techniques require as input the intermolecular potentials and the accuracy of the output calculations of thermodynamic properties depends on the accuracy of the potentials. It has become quite plain that in the case of HAN there are virtually no experimental data on the pure substance beyond a report by Ross¹⁰ that its melting point is 48°C. There is more information available about other hydroxylammonium salts. The

⁹J. J. Erpenbeck and W. W. Wood, *J. Stat. Phys.* 24, 455 (1981).

¹⁰W. H. Ross, *Proc. Trans. Nova Scotia Inst. of Science*, 11, 95 (1906).

structure of hydroxylamine¹¹ itself, as well as those of hydroxylammonium chloride,¹² hydroxylammonium bromide,¹¹ and hydroxylammonium perchlorate (HAP) are known. The case of HAP illustrates nicely the interplay between X-ray and neutron diffraction. Dickens,¹³ using X-ray techniques alone, was able to make only a partial structure determination because X-rays, since they are scattered by atomic electrons, do not see protons; neutrons, which are scattered by nuclei, can detect the position of protons (or, more easily, deuterons), and the structure of HAP was completely determined in a later paper¹⁴ by neutron diffraction. The structures of the solid phase of a number of nitrate salts with simpler cations are well known; for example, the structures of the nitrates of potassium, rubidium, silver and lithium were reported in 1913 by Ewald and Hermann.¹⁵

There is no structure information available on the liquid phase of HAN or on aqueous solutions of HAN. There are both theoretical and experimental determinations of the structure and properties of some anhydrous molten salts, especially the alkali halides.¹⁶ There are also neutron diffraction structure determinations¹⁷ of a number of concentrated aqueous solutions, including alkali halides and calcium and nickel chloride. There is no structure information on the pure liquid phases of other hydroxylammonium salts, but neutron measurements of the structure factor of the molten nitrates of lithium, silver, sodium, potassium, rubidium and cesium have been reported in the literature.¹⁸

IV. PRESENT STATE OF MONTE CARLO WORK

The work done this summer has provided a substantial start on the computational capability that will be required for a fundamental understanding of the equilibrium properties of HAN. The specific accomplishments are threefold. First, a formula not previously found in the literature has been derived in order to permit evaluation of the heat capacity at constant pressure of a system at a given temperature and density by means of a single MC or MD run. Because of its complexity, this formula will be put into the MC code at a later date. Second, an existing MC code, which due to its

¹¹E. A. Meyers and W. N. Lipscomb, *Acta Cryst.* 8, 583 (1955).

¹²B. Jerslev, *Acta Cryst.* 1, 21 (1947).

¹³B. Dickens, *Acta Cryst.* B25, 1875 (1969).

¹⁴E. Prince, B. Dickens, and J. Rush, *Acta Cryst.* B30, 1167 (1974).

¹⁵P. P. Ewald and C. Hermann, *Z. Fuer Krist.* 1, 3 (1913).

¹⁶See, for example, D. L. Price and J. R. Copley, *Phys. Rev.* A11, 2124 (1978).

¹⁷J. E. Enderby, in *Ionic Liquids*, D. Inman and D. G. Loevring, eds., Plenum Press, New York (1981).

¹⁸K. Susuhi and Y. Fukushima, *Z. Naturforsch.* 32A, 1438 (1977).

flexibility has been applied by the author to a wide variety of one-component systems, has been generalized to calculate the properties of a two-component system with arbitrary short-range central interactions. Third, the MC code has also been generalized to study a molten salt using a suggestion of Ceperley and Chester.¹⁹ It will now avoid the cumbersome Ewald summation that is usually required in the case of the Coulomb potential; the code will now do (at least in debugging runs) only that portion which must be done by MC, the remainder to be treated as a perturbation.

V. RECOMMENDATIONS FOR FURTHER STUDIES

Further progress on understanding the fundamental properties of these systems will require additional theoretical calculations and experimental data, since there has been practically no work done on them to date. If it is possible in spite of the difficulty of working with pure HAN, it would be highly desirable to have structure information on both pure anhydrous HAN and its aqueous solutions as a function of concentration from both X-ray and neutron diffraction experiments. Any equation of state and latent heat data available would be similarly helpful.

Some knowledge of the three interionic interactions (those between pairs of hydroxylammonium ions, between nitrate ions, and between a nitrate and a hydroxylammonium ion) is essential. The above structure data will be a testing ground for these potentials. The most likely source of initial information about these interionic potentials is *ab initio* quantum chemistry calculations. Although the first step must of necessity be to obtain and use effective (spherically averaged) central potentials, these potentials cannot be expected to reproduce the finer details of these complex systems. As more information becomes available, a generalization of the MC code to deal with non-central interactions will be justified. In addition, electrical conductivity, nuclear magnetic resonance, and Raman scattering measurements will provide more knowledge of the basic mechanisms that determine the behavior of the system. By shedding light on such questions as the structure of molecules within the liquids, solvation, hydration and hydrogen bonding, these experiments will help to determine the validity of modeling these systems as molten salts and suggest how to do more detailed (presumably MD) calculations. As this information about the basic physical processes in the liquids becomes available and as the interactions are refined, the use of the MD code to calculate such transport properties as diffusivity and electrical conductivity (and the viscosity, provided there is some advance in computational techniques) will make sense.

¹⁹D. M. Ceperley and G. V. Chester, *Phys. Rev.* A15, 755 (1977).

VI. ACKNOWLEDGEMENTS

I would like to express my sincere thanks to the U. S. Army Research Office for the summer appointment during which this work was done and to the Ballistic Research Laboratory and to Dr. Ingo May and the Advanced Ballistic Concepts Branch for their hospitality. Useful conversations with Dr. Walter F. Morrison, Jr., Dr. Nathan Klein, and Dr. George Adams and the members of his group contributed greatly to this work. Finally, it is a pleasure to acknowledge the great debt I owe to Dr. Eli Freedman for his assistance and counsel on occasions too numerous to enumerate.

REFERENCES

1. W. F. Morrison, "The Application of Liquid Propellant Gun Technology to Field Artillery," presented at the 1982 JANNAF Propulsion Meeting.
2. E. Freedman, ed., "An Outline of Liquid Propellants," to be published
3. W. O. Seals, "Vulnerability Studies for a Liquid Propellant System," presented at the JANNAF Propulsion Systems Subcommittee Meeting (1983).
4. J. A. Barker, R. A. Fisher, and R. O. Watts, Mol. Phys., 21, 657 (1971).
5. J. A. Barker and D. Henderson, Revs. Mod. Phys. 48, 587 (1976).
6. J. P. Hansen and J. R. McDonald, Theory of Simple Liquids, Academic Press, NY (1976).
7. N. Metropolis, A. W. Rosenbluth, N. W. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. 21, 1087 (1953).
8. B. J. Alder and T. E. Wainwright, J. Chem. Phys. 27, 1208 (1957).
9. J. J. Erpenbeck and W. W. Wood, J. Stat. Phys. 24, 455 (1981).
10. W. H. Ross, Proc. Trans. Nova Scotia Inst. of Science 11, 95 (1906).
11. E. A. Meyers and W. N. Lipscomb, Acta Cryst. 8, 583 (1955).
12. B. Jerslev, Acta Cryst. 1, 21 (1947).
13. B. Dickens, Acta Cryst. B25, 1875 (1969).
14. E. Prince, B. Dickens, and J. Rush, Acta Cryst. B30, 1167 (1974).
15. P. P. Ewald and C. Hermann, Z. Fuer Krist. 1, 3 (1913).
16. See, for example, D. L. Price and J. R. Copley, Phys. Rev. A11, 2124 (1978).
17. J. E. Enderby, in Ionic Liquids, D. Inman and D. G. Loevring, eds., Plenum Press, New York (1981).
18. K. Suzuhi and Y. Fukushima, Z. Naturforsch. 32A, 1438 (1977).
19. D. M. Ceperley and G. V. Chester, Phys. Rev. A15, 755 (1977).

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
12	Commander Defense Technical Info Center ATTN: DTIC-DDA Cameron Station Alexandria, VA 22314	1	Commander US Army Armament M Chemical Command ATTN: AMSMC -LEP-L Rock Island, IL 61
1	Director Defense Advanced Research Projects Agency ATTN: H. Fair 1400 Wilson Boulevard Arlington, VA 22209	1	Commander US Army Aviation Re and Development C ATTN: AMSAV-E 4300 Goodfellow Blv St. Louis, MO 6312
1	HQDA (DAMA, C. Church) Washington, DC 20310	1	Director US Army Air Mobilit and Development C
1	Commander US Army Materiel Command ATTN: AMCDRA-ST 5001 Eisenhower Avenue Alexandria, VA 22333	1	Ames Research Cente Moffett Field, CA
2	Commander US Army Armament R & D Center ATTN: SMCAR-TSS SMCAR-SCA, M. Devine Dover, NJ 07801	1	Commander US Army Communicati Rsch and Developm ATTN: AMSEL-ATDD Fort Monmouth, NJ
5	Commander US Army Armament R & D Center ATTN: SMCAR-LCA, D. Downs A. Beardell SMCAR-LCE, N. Slagg SMCAR-LCS, W. Quine SMCAR-TDC, D. Gyorog Dover, NJ 07801	1	Commander US Army Harry Diam ATTN; DELHD-TA-L 2800 Powder Mill R Adelphi, MD 20783
2	Commander US Army Armament Munitions and Chemical Command Benet Weapons Laboratory ATTN: SMCAR-LCB-TL P. Votis Watervliet, NY 12189	1	Commander US Army Missile Co ATTN: AMSMI--R Redstone Arsenal,
		1	Commander US Army Missile Co ATTN: AMSMI-YDL Redstone Arsenal,

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
2	Commander US Army Mobility Equipment Rsch and Development Cmd ATTN: AMDME-WC AMSME-RZT Fort Belvoir, VA 22060	2	Commander Naval Weapons Center ATTN: C. Mallory S. Wood China Lake, CA 93555
1	Commander US Army Tank Automotive Command ATTN: AMSTA-TSL Warren, MI 48090	2	Commander Naval Ordnance Station ATTN: K. Mueller G. Poudrier Indian Head, MD 20640
1	US Army Research Office Durham ATTN: R. Singleton P.O. Box 12211 Research Triangle Park, NC 27709	1	Superintendent Naval Postgraduate School Monterey, CA 93940
1	Director US Army TRADOC Systems Analysis Activity ATTN: ATAA-SL White Sands Missile Range NM 88002	2	AFATL/ATWG, O. Heiney DLD, D. Davis Eglin, AFB, FL 32542
1	Office of the Chief of Naval Operations ATTN: Code NOP-351G Washington, DC 20350	1	AFOSR/NA (L. Caveny) Bldg. 410 Bolling AFB, DC 20332
1	Commander Naval Sea Systems Command ATTN: J.W. Murrin (SEA-62R2) National Center Building 2, Room 6E08 Washington, DC 20360	1	AFWL/SUL Kirtland AFB, NM 87117
1	Commander Naval Surface Weapons Center ATTN: W.C. Wieland Dahlgren, VA 22448	1	HQDA DAMA-ART-M Washington, DC 20310
2	Commander Naval Surface Weapons Center ATTN: O. Dengel K. Thorsted Silver Spring, MD 20910	1	Commandant US Army Infantry School ATTN: ATSH-CD-CSO-OR Fort Benning, GA 31905
		1	Commander US Army Development & Employment Agency ATTN: MODE-TED-SAB Fort Lewis, WA 98433
		1	Director Jet Propulsion Lab ATTN: Tech Lab 4800 Oak Grove Drive Pasadena, CA 91109

DISTRIBUTION LIST

<u>No. of Copies</u>	<u>Organization</u>	<u>No. of Copies</u>	<u>Organization</u>
1	Director National Aeronautics and Space Administration Manned Spacecraft Center Houston, TX 77058	1	Science Applications, Inc. ATTN: R. Edelman 23146 Cumorah Crest Woodland Hills, CA 91364
1	The BDM Corporation ATTN: Dr. T.P. Goddard P.O. Box 2019 2600 Cearden Rd Monterey, CA 93940	1	AFELM, The Rand Corporation ATTN: Library-D 1700 Main Street Santa Monica, CA 90406
1	Calspan Corporation ATTN: E. Fisher P.O. Box 235 Buffalo, NY 14221	1	TRW Systems ATTN: RI-1032, E. Fishman One Space Park Redondo Beach, CA 90278
1	Food & Machinery Corporation Northern Ordnance Division ATTN: J. Oberg Columbia Heights Post Office Minneapolis, MN 55421	1	Director Applied Physics Laboratory The Johns Hopkins University Johns Hopkins Road Laurel, Md 20707
3	General Electric Ordnance Dpt ATTN: J. Mandzy R.E. Mayer H. West 100 Plastics Avenue Pittsfield, MA 01201	2	Director Chemical Propulsion Info Agency The Johns Hopkins University ATTN: T. Christian Tech Lib Johns Hopkins Road Laurel, MD 20707
2	General Electric Company Armanent Systems Department ATTN: E. Ashley M. Bulman Burlington, VT 05401	1	Pennsylvania State University Dept. of Mechanical Eng ATTN: K. Kuo University Park, PA 16802
1	Director US Bureau of Mines ATTN: R.A. Watson 4800 Forbes Street Pittsburgh, PA 15213	2	Princeton Combustion Rsch Laboratories, Inc. ATTN: N.A. Messina M. Summerfield 475 US Highway One Monmouth Junction, NJ 08852
1	Director Los Alamos Scientific Lab ATTN: D. Butler PO Box 1663 Los Alamos, NM 87544	2	Director National Aeronautics and Space Administration ATTN: MS-603, Tech Lib MS-86, Dr. Povinelli 21000 Brookpark Road Lewis Research Center Cleveland, OH 44135

DISTRIBUTION LIST

No. of
Copies Organization

1 SRI International
 ATTN: Code L3106, G.A. Branch
 333 Ravenswood Avenue
 Menlo Park, CA 94025

1 University of Arkansas
 Department of Chemical
 Engineering
 227 Engineering Building
 Fayetteville, AR 72701

Aberdeen Proving Ground

Dir, USAMSAA
 ATTN: AMXS-D
 AMXS-MP, H. Cohen

Cdr, USATECOM
 ATTN: AMSTE -TO-F

Cdr, CRDC, AMCCOM
 ATTN: SMCCR-RSP-A
 SMCCR-MU
 SMCCR-SPS-IL

USER EVALUATION SHEET/CHANGE OF ADDRESS

This Laboratory undertakes a continuing effort to improve the quality of the reports it publishes. Your comments/answers to the items/questions below will aid us in our efforts.

1. BRL Report Number _____ Date of Report _____

2. Date Report Received _____

3. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which the report will be used.) _____

4. How specifically, is the report being used? (Information source, design data, procedure, source of ideas, etc.) _____

5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided or efficiencies achieved, etc? If so, please elaborate. _____

6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.) _____

CURRENT ADDRESS

Name

Organization

Address

City, State, Zip

7. If indicating a Change of Address or Address Correction, please provide the New or Correct Address in Block 6 above and the Old or Incorrect address below.

OLD ADDRESS

Name

Organization

Address

City, State, Zip

(Remove this sheet along the perforation, fold as indicated, staple or tape closed, and mail.)

FOLD HERE

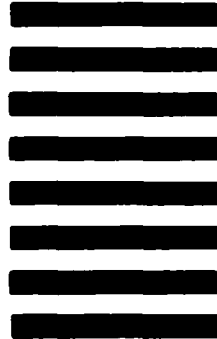
Director
US Army Ballistic Research Laboratory
ATTN: AMXBR-OD-ST
Aberdeen Proving Ground, MD 21005-5066



NO POSTAGE
NECESSARY
IF MAILED
IN THE
UNITED STATES

OFFICIAL BUSINESS
PENALTY FOR PRIVATE USE, \$300

BUSINESS REPLY MAIL
FIRST CLASS PERMIT NO 12062 WASHINGTON, DC
POSTAGE WILL BE PAID BY DEPARTMENT OF THE ARMY



Director
US Army Ballistic Research Laboratory
ATTN: AMXBR-OD-ST
Aberdeen Proving Ground, MD 21005-9989

FOLD HERE