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LAWRENCE LIVERMORE LABORATORY

University of California/Livermore, California

PARTICIPATION OF LLL IN JSEXP

PART A: PERFORMANCE OF NON-IDEAL HE

PART B: CHARACTERIZATION OF ECX FOR CONVENTIONAL MUNITIONS

(Unclassified)

30 June 1974

F. E. Walker

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TECHNICAL REPORT

LAWRENCE LIVERMORE LABORATORY

Livermore, California 94550

Phone: (415) 447-1100

LLL PROPOSAL OMD-72-7

"PARTICIPATION OF LLL IN JSEXP"

ARPA Order No. 2502

Program Code No. 3G10

Effective Date of Contract: 13 April 1973

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Principal Investigators:	M. Finger	Ext. 7856	(Task A)
	K. Scribner	Ext. 7366	(Task B)
	H. Hornig	Ext. 3717	(Task C)

Project Scientist:	F. Walker	Ext. 7856
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TECHNICAL REPORT

PARTICIPATION OF LLL IN JSEXP

REPORT SUMMARY

- PART A: Performance of Non-Ideal HE
- PART B: Characterization of ECX for Conventional Munitions
- PART C: Optimization of Active Warhead Designs for Appropriate Targets (Classified; Forwarded Separately)

30 June 1974

This research was supported by the Advanced Research Projects Agency of the Department of Defense and was monitored by Dr. Charles Church and Mr. Charles Ravitsky under ARPA Order No. 2502.

TECHNICAL REPORT SUMMARY

Introduction

The research program reported on in this summary was developed as a cooperative effort between the Advanced Research Projects Agency (ARPA), the Office of the Director of Defense Research and Engineering (DDR and E), and the Joint Services Explosives Program (JSEXP). Funding for the projects, which are the subject of this report, was provided by ARPA, Picatinny Arsenal, and Eglin AFB. These projects are an integral part of the JSEXP Research Agenda. Picatinny Arsenal provided \$30K for additional work on composite explosives and \$30K for the development of a less-expensive ECX. Eglin AFB provided \$100K in FY 73 for active-warhead studies.

Program Purposes

Three distinct purposes were established for this program, and they have been designated as Tasks A, B and C.

Task A:

Complete experiments and code calculations to determine a hydrodynamic model for the initiation and detonation of composite explosives. This information is important to the success of the Alternate Fills Program.

Task B:

Complete formulation studies and experiments with extrusion cast explosives (ECX) for application to the improvement of shaped charge performance at acceptable costs.

Task C:

Complete parametric and fundamental studies of the "active warhead" concept for application to the design of specific munition systems.

Discussion

A short discussion of the technical problems, general methodology, technical results, and the implications of the research for each task follows:

Task A: Performance of Non-Ideal HE

1. Several technical problems are being addressed in Task A. The fundamental problem is that of understanding and then being able to calculate the kinetics and, thus, the performance of composite explosives (those formulated from two or more oxidizer and fuel ingredients). In order to solve this fundamental problem, hydrodynamic data from experiments with specified geometries (cylinders and spheres) of explosive samples must be collected and compared with hydrodynamic code calculations based on the assumed kinetic model. In this way the model is adjusted and refined until the kinetics and performance are understood.
2. This work involves some literature study, theoretical calculations and modeling, precise instrumentation and firing of explosive samples, and analysis of the data obtained.
3. A model has been formulated for the kinetics and the hydrodynamic effects. A series of cylindrical charges of the composite explosive selected (ammonium perchlorate and gelled nitromethane) has been instrumented and fired. A series of hemispherical charges has been fired in specially-designed and fabricated containers. Data from the cylindrical charges in which the particle size of the NH_4ClO_4 (oxidizer) was varied are reasonably consistent with the first model selected. (See Part A.) We need to complete the series of hemispherical charges before we can correlate the new data with the model.

A series of computer calculations was made using our proposed kinetics-hydrodynamics model to compare with the results of the cylinder shots fired at our Site 300. It was found in the calculations that by varying the rate of release of part of the chemical energy in the composite explosives it was possible to increase or decrease the peak pressure at the detonation front. As predicted by this result, the change in pressure is reflected in a change of reaction-transit-time, which was measured experimentally across a series of plastic witness plates.

In order to properly evaluate the role of transport phenomena (primarily diffusion) in the burning of composite high explosives, it is important to know the reaction temperature as well as pressure. A series of experiments was completed in which the thermal radiation from the detonation front in nitromethane was measured and the temperature was calculated.

A study was completed of the application of kinetic theories for the prediction of diffusion coefficients at the high temperatures and pressures encountered in the burning of composite explosives. Additionally, we developed an experimental method for studying the profile of the pressure wave in reacting composite explosives.

4. The implications of further research are that since we now have developed a basic calculational model for the understanding of the reaction of composite explosives, have obtained some of the data needed to expand and refine that model, have developed experimental methods for temperature and pressure determinations in the ranges

important to the model, and have found a satisfactory theoretical method for estimating diffusion coefficients at high temperatures and pressures, we are in an excellent position to gain a good understanding of the explosive reaction of composite explosives. This should lead us to the satisfactory development of a refined calculational model that should have wide application and accelerate the effective use of composites as military explosives.

Task B: ECX for Conventional Munitions

1. The technical problems in the ECX study are not too difficult. The ECX must be formulated and extruded into the shaped charge to leave no voids and to provide a smooth and homogeneous explosive layer next to the shaped charge liner. We have had considerable experience in the formulation and processing of ECX materials.
2. This work involves some formulation and processing, but it is mainly an experimental program to compare the effectiveness in penetration of shaped charges loaded with conventional explosives to those loaded with our ECX.
3. The data obtained in our experimental program show significant improvement in the performance of shaped charges loaded with our ECX (RX-08-BA) over charges loaded with either RDX or Comp B, between 4 and 12 cone-diameter standoffs. High quality, homogeneous charges were obtained with simple, straightforward loading techniques.
4. The implication of further research is that we now have data that give us clues to the understanding of improved and more reproducible shaped charge performance, and additional experimentation and 2-D

computer analysis with the ECX system can elucidate what has been a disturbing problem. Additional improvement in performance seems feasible, and a reduction in the cost of the ECX explosive may be obtained.

Task C: Active Warhead Designs for Appropriate Targets

1. The most important technical problem in the "active warhead" study is obtaining an understanding of the effects of changing the parameters in the "active warhead" system. We are also looking for improvements by changing the basic design geometries, since this is a relatively new technology.
2. The general methodology for this project involves some literature study, but it is primarily a parametric experimental program with computer analyses and modeling.
3. Some of the parametric experiments have been completed, and we have observed significant enhancement of the explosive properties involved. (See Part C, Classified, for a complete summary of the experimental results.)
4. The principal implication of further research is that a significant advance in weapon technology in many specific applications of explosive devices appears to be feasible, and the research completed to date has shown the concept can provide some unique weapon effects. We now have a data base on which to build some specific weapon designs.
5. The "active warhead" concepts are classified as Secret, NSI. Please see Part C, Classified, for specific information on this task.

Equipment Purchased or Developed

No important equipment has been purchased or built under the terms of this contract.

Conclusions

Task A

The kinetic and hydrodynamic model we have proposed appears to be a good basic model for understanding the performance of composite explosives. The experimental and theoretical studies are progressing well, and they have provided the information and methods that can lead to a successful conclusion of this task.

Task B

The shaped charges loaded with ECX which have been tested in this project show improved performance between 4 and 12 cone diameters. The work indicates we can obtain further understanding of the important factors which determine shaped charge performance through the experiments we are conducting and through the use of 2-D hydrodynamic code calculations.

Task C

We have observed significant enhancement of explosive effects in the parametric experiments completed. We are confident that important advances in weapon technology can be achieved and unique weapon effects can be demonstrated, for we now have a data base for application to specific weapon designs.

PART A

PARTICIPATION OF LLL IN JSEXP

TASK A: PERFORMANCE OF NON-IDEAL HE

M. Finger
E. Lee
F. Helm
H. Cheung
D. Miller
E. Chambers

PERFORMANCE OF NON-IDEAL EXPLOSIVES

EXPERIMENTAL

The development of a model for the performance of non-ideal explosives is heavily dependent on the data obtained from carefully conducted hydrodynamic tests. In particular, detonation performance parameters must be obtained from scaled hydrodynamic experiments in which the explosive composition and particle sizes have been carefully controlled.

Experimental Plan

In the last progress report we presented our experimental plan for obtaining the necessary data. Table 1 is an up-date of that plan. All the X's surrounded by a square are data completed since the last progress report.

Explosive Formulations

Rather than conduct our basic studies on the fairly complex AMATEX (RDX/TNT/AN) family of high explosives, we chose instead to concentrate on simple, easily-characterized-and-controlled explosive systems. The formulations we are testing are based on gelled nitromethane (NM) which is a homogeneous detonable fuel.^(1,2) Oxidizers of varying particle sizes and excess oxygen content are uniformly suspended in the gelled NM. Porosity can also be easily introduced in the form of microballoons. The oxidizers selected for investigation are ammonium nitrate, ammonium perchlorate, and potassium perchlorate, having 1, 2, and 4 excess oxygen atoms, respectively, for participation in the diffusion-controlled fuel-oxidizer reactions.

TABLE 1. ARPA PROGRAM
PERFORMANCE TESTS/DATA

<u>NO. OF FREE [O]</u>	<u>MATERIAL</u>	<u>RT</u>	<u>PD</u>	<u>PS</u>	<u>S-8</u>	<u>S-16</u>	<u>C-1</u>	<u>C-2</u>	<u>C-4</u>	<u>CW-1</u>	<u>ASM</u>	<u>DEE</u>	<u>W</u>	<u>CDV</u>
1 - [O]	<u>NH₄NO₃</u>													
Particle Size	2000 μ	X	X	X										
Particle Size	200 μ	X	X	X			X	X						
Particle Size	20 μ		X	X										
Particle Size	2-5 μ	X	X	X			X	X						
2 - [O]	<u>NH₄ClO₄</u>													
Particle Size	2000 μ	X	X	X										
Particle Size	200 μ	X		X	X	X	X	X	X	X	X	X	X	X
Particle Size	20 μ		X	X										
Particle Size	2-5 μ	X	X	X	X	X	X	X			X	X	X	
4 - [O]	<u>KClO₄</u>													
	2000 μ			X										
	200 μ	X	X	X			X	X						
	20 μ		X	X										
	2-5 μ	X	X	X			X	X						

 Previously completed
 Completed this reporting period
 Attempted but unsuccessful

NOTES FOR TABLE 1.

1. All compositions CO_2 balanced, or CO if CO_2 not obtainable.
2. RT Ruby-Tiger code prediction for full, partial and incomplete reaction.
3. PD 1" diam. plate dent in standard configuration.
4. PS Particle size analysis.
5. S Sphere test, -8 and -16, 8-in. and 16-in. diam.
6. C Cylinder test, -1, -2, -4; 1, 2, and 4-in. diam scaled wall.
7. CW Cylinder test conducted in H_2O , -1, 1-in. diam.
8. ASM Axially symmetric probe for u_p and reaction zone length.
9. DEE Detonation electric effect, for detonation pressure.
10. W Wedge expts.
11. CDV Continuous detonation velocity.

We have completed all the cylinder and sphere shots using 200 micron ammonium perchlorate (AP). We have been hindered in obtaining experimental results with other oxidizers because of the difficulty of obtaining discrete particle size fractions and the aging and agglomeration problem with AN, AP, and KP. We expect to obtain shortly 5 and 2,000 μ AP, 5 and 20 μ AN, and 5 and 200 μ KP. We have sufficient quantities of 20 and 200 μ AP to complete our planned experiments.

We made some initial attempts at loading 8 and 16 inch diameter hemispheres with AP/NM gel formulations. The effort was unsuccessful primarily because of plugging of an orifice plate in our loader-deaerator. The guar gum gelling agent apparently promoted bridging of solids in the 1/16 inch diameter holes of the orifice plate. We have since modified the orifice plate by enlarging the holes to 1/8" diameter. However, while modifications were taking place we attempted to load the hemispheres by hand. This method led to the inclusion of unacceptable amounts of air. The two 8-inch hemispheres were fired. The AP/NM gel containing 200 μ AP was fluid enough to allow most of the entrapped air to rise out of the shot by gravity prior to the test. The results of this shot were satisfactory, and the results are tabulated under the section on sphere shots (noted in parentheses). The AP/NM gel containing 5 μ AP held the air bubbles in suspension, which caused early jetting through the aluminum wall. The streaking camera records were of no value. In Figures 1 and 2 a few selected frames from the framing camera records show the difference between the premature breakup caused by air and the uniform expansion of a well-loaded air-bubble-free system.

0 μ s

4 μ s

12 μ s

Figure 1: Sphere Expansion - Premature Breakup Because of Entrapped Air

0 μ s

24 μ s

51 μ s

Figure 2: Sphere Expansion - Uniform Expansion with Void Free Explosive

EXPLOSIVES PERFORMANCE

Cylinder Test

In addition to the standard one- and two-inch-diameter cylinder test, we tested the 200 μ particle size AP/NM-CO₂ balanced system in a 4-inch diameter cylinder.⁽⁴⁾ In the last progress report we showed that 5 μ AP in the same stoichiometric composition behaved almost as an ideal explosive in the one- and two-inch diameter tests. Whereas, the 200 μ AP showed distinct non-ideal behavior in one- and two-inch cylinders similar to that observed in other systems.⁽⁵⁾ We fired a 4-inch test to see if we could find some geometry limits to the non-ideal performance of the 200 μ AP. The cylinder test shot set-up is shown in Fig. 3. In Fig. 4 the 4-inch cylinder test expansion streaking camera record is shown. Table 2 reviews the one- and two-inch results for 5 and 200 μ AP and gives the 4-inch results for 200 μ AP. Table 3 gives an incremental comparison of the expansion of 1, 2, and 4-inch diameter cylinder tests on 200 μ AP.

Sphere Shots

All of the hardware necessary for a series of up to 20 sphere experiments has been built. A typical sphere test shot assembly is shown in Fig. 5. Initial attempts at loading the hemispheres met with mixed results. Difficulty in loading, as described above, resulted in unuseable data from the 8-inch spheres loaded with the 5 μ AP. The data from the 8-inch sphere containing 200 μ AP was fair, but we were reluctant to trust these data because of the poor experience with the 5 μ AP sphere shot. We repeated the 8-inch using an improved loading technique and also fired a 16-inch hemisphere. The results are tabulated in Table 4 and shown graphically in Fig. 6. The results are very good. The spheres expanded uniformly to a large volume, as can be seen from framing camera records. (See fig. 2 as an example.) The

Figure 3: Cylinder Test Set-up

Figure 4: 4-inch Diameter Cylinder Test
Streaking Camera Record

TABLE 2. SUMMARY OF CYLINDER TEST RESULTS

Composition:	Wt. % <u>Ammonium Perchlorate</u>	<u>Nitromethane + 3% Guar</u>		
RX-30-AA	61.8 (5 μ)	38.2		
RX-30-AB	59.3 (200 μ)	40.7		
Nominal	59.1	40.9		
Performance:	<u>1" cylinder</u>	<u>2" cylinder</u>	<u>4" cylinder</u>	
RX-30-AA				
Density, g/cc	1.517	1.528		
Det. Vel., mm/s	6.940	7.150		
Wall Vel. at 6 mm, mm/ μ sec	1.30	1.28		
Wall Vel. at 19 mm, mm/ μ sec	1.50	1.50		
RX-30-AB				
Density, g/cc	1.515	1.513		1.513
Det. Vel., mm/s	5.380	5.490		5.68
Wall Vel. at 6 mm, mm/ μ sec	0.98	1.07		1.18
Wall Vel. at 15 mm, mm/ μ sec	1.14	1.27		1.37
Wall Vel. at 19 mm, mm/ μ sec	-	1.32		1.41

TABLE 3. CYLINDER TEST SCALED WALL VELOCITIES,
mm/ μ sec FOR 200 μ AP.

R-R ₀ , mm	RX-30-AB* 200 μ AP, 1"	RX-30-AB 200 μ AP, 2"	RX-30-AB 200 μ AP, 4"
6	.981	1.068	1.18
7	1.010	1.104	1.21
8	1.028	1.138	1.24
9	1.047	1.168	1.26
10	1.071	1.191	1.29
11	1.096	1.209	1.31
12	1.115	1.224	1.32
13	1.126	1.238	1.34
14	1.133	1.253	1.36
15	1.146	1.268	1.37
16	1.165	1.283	1.39
17	1.172	1.298	1.40
18		1.310	1.41
19		1.319	1.41
20		1.326	1.42
21		1.332	1.43
22		1.339	1.43
23		1.347	1.44
24		1.356	1.45
25		1.364	1.46
26		1.369	1.46
27		1.371	1.47
28			1.48
29			1.49
30			1.50

* Nominal composition RX-30
 Nitromethane with 3 wt.% }
 GM-512 Guar Gum } 40.9 wt%
 Ammonium perchlorate } 59.1 wt%

Figure 5: Sphere Test Assembly

TABLE 4. SPHERE WALL VELOCITIES FOR 200 μ AP*

	8 in. Sphere [‡]		16 in. Sphere	
Density, g/cc	1.513		1.513	
Det. Vel. mm/μsec	4.98		5.02	
Wall Motion:				
<u>R-R₀</u>	<u>Time, μ sec</u>	<u>Vel, mm/μsec</u>	<u>Time, μsec</u>	<u>Vel, mm/μsec</u>
5	3.20 (2.76)	1.85 (1.75)	2.82	1.90
10	5.69 (5.37)	2.14 (2.11)	5.22	2.26
15	7.92 (7.59)	2.34 (2.37)	7.32	2.50
20	10.00 (9.66)	2.45 (2.45)	9.26	2.62
25	12.01 (11.67)	2.51 (2.53)	11.15	2.69
30	13.98 (13.61)	2.57 (2.63)	12.98	2.75
35	15.91 (15.48)	2.62 (2.70)	14.78	2.82
40	17.80 (17.32)	2.67 (2.73)	16.53	2.88
45	19.65 (19.14)	2.73 (2.78)	18.25	2.92
50	21.46 (20.90)	2.79 (2.86)	19.96	2.95
55	23.24 (22.65)	2.84 (2.87)	21.64	2.99
60	24.99	2.88	23.30	3.04
65	26.72	2.90	24.92	3.11
70	28.43	2.92	26.52	3.13
75	30.14	2.93		
80	31.85	2.94		
85	33.55	2.95		
90	35.24	2.97		
95	36.92	3.00		
100	38.57	3.04		
105	40.20	3.10		
110	41.80	3.16		
115	43.36	3.23		
120	44.89	3.29		
125	46.40	3.35		
130	47.88	3.38		

‡ Data in () is for first sphere shot loaded by hand.

* Nominal composition

Nitromethane with 3 wt% GM-512 Guar Gum	40.9 wt.%
Ammonium Perchlorate	59.1 wt.%

data again show a non-ideal behavior. Since the mass-of-HE-to-wall thickness is scaled to be constant, the wall velocities should be identical if the HE were performing as an ideal explosive. However, we do not see scaling in the wall motion.

Detonation Pressure

Because of the relatively low detonation pressures in these composite explosives, the signal level in shocked materials has been marginal for unequivocal measurements. We are pursuing several approaches. We are looking at ways to enhance the signal obtained in the Detonation Electric Effect^(6,7) as reported in another section. We are also attempting to implement the axially-symmetric magnetic probe (ASMP).⁽⁸⁾ This technique would give a direct measurement of the particle velocity of the detonation products. We could then obtain detonation pressure and reaction zone dimensions.

Continuous Detonation Velocity

In a non-ideal explosive we believe that the detonation parameters are changing as a function of run distance through the charge. A method of monitoring this would be to use a continuous detonation velocity probe (CDV). We attempted to do this using the method of Ribovich and Watson.⁽⁹⁾ We placed the CDV in our 4-inch cylinder test in an area that would not disturb the wall expansion measurement. The CDV assembly is shown in Fig. 7. We obtained no record; probably because the detonation pressure was too low to cause shorting of the coaxial wire sensors.

FIG. 6 SPHERE SHOT RESULTS
200 μ AP

CONTINUOUS DETONATION VELOCITY PROBE
FIG. 7

REFERENCES

1. Participation of LLL in JSEXP, Part A, Performance of Non-Ideal HE, APPA Order No. 2502, UCID-16424, 30 December, 1973.
2. F. Helm, M. Finger, R. Boat, and D. Wooster, "The Development and Manufacture of a Gelled Nitromethane Explosive for Project Essex," UCRL-51536, May, 1974.
3. E. L. Lee, H. C. Hornig, J. W. Kury, "Adiabatic Expansion of High Explosive Detonation Products," UCRL-50422, May 2, 1966.
4. J. W. Kury, H. C. Hornig, E. L. Lee, J. L. McDonnell, D. L. Ornellas, M. Finger, F. M. Strange, M. L. Wilkins, "Metal Acceleration by Chemical Explosives," Fourth Symposium on Detonation, p. 3, Office of Naval Research (1965).
5. M. Finger, H. C. Hornig, E. L. Lee, J. W. Kury, "Metal Acceleration by Composite Explosives," Fifth Symposium on Detonation, p. 137, Office of Naval Research (1970).
6. B. Hayes, "The Detonation Electric Effect," J. Appl. Phys. 38, 507 (1967)
7. B. Hayes, "Electric Signals Generated by Shock and Detonation Waves," presented at the Western States Section of the Combustion Institute, October 28, 1968.
8. B. Hayes and J. N. Fritz, "Measurement of Mass Motion in Detonation Products by an Axially-Symmetric Electromagnetic Technique," Fifth Symposium on Detonation, p. 447, Office of Naval Research (1970).
9. J. Ribovich, R. W. Watson, and F. C. Gibson, American Institute of Aeronautics and Astronautics Journal 6, (7), 1260 (1968).

CHEMICAL KINETICS AND
THE DETONATION OF HETEROGENEOUS HE

INTRODUCTION

During detonation of an ideal high explosive (HE) the chemical energy is released within a fraction of a microsecond, i.e., the reaction zone is thin by comparison with other physical dimensions of the detonating system. In hydrodynamic calculations of detonation only a single equation of state expressing the behavior of the combustion products suffices to describe the flow. On the other hand, during the detonation of a heterogeneous explosive, defined as one containing two or more reactants which are physically admixed, only a portion of the chemical energy is released immediately, as in the case of an ideal HE. The remaining portion of the energy is released behind the detonation front during periods which may last many microseconds, and the reaction zone is correspondingly more extensive. Because the composition is changing and energy is being added continuously, it is no longer adequate to represent the behavior of the partially-burned material behind the front by a single invariant equation of state. Instead, it is postulated in the present work that a time-and-composition-dependent equation would be required. In the following, such an equation of state was used to calculate the hypothetical effect of such a description of chemical kinetics upon the experimentally observed parameters of an ideal HE in order to determine the possible application of the procedure to the more complicated case of a heterogeneous HE.

EXPERIMENT

A piece of LX-04 HE 4 in. in diameter and 4 in. long was initiated at one end with a P-40 plane wave lens. At the far end of the piece were placed five disks of Lucite, each having the same diameter and nominally 0.2 in. thick.

The transit times of the detonating shock across the sheets of Lucite were determined as was the detonation velocity. The C-J pressures were derived from these measurements. These data, given in Table 1, are obtained from Ref. 1.

CALCULATION PROCEDURE

The one-dimension computer code, KO,⁽²⁾ was modified to incorporate an equation of state which is both time- and composition-dependent. In the original version of KO, the propagation of a detonation wave is simulated by the so-called "C-J" burn model. The constant,

$$\beta = \gamma_{CJ} + 1 = \frac{1}{1 - V_{CJ}}$$

is a property of the HE equation of state, where the subscript CJ denotes the Chapman-Jouget condition. The burn fraction in each zone is defined as

$$F(J) = \beta(1 - V(J))$$

Thus, when the zone is compressed, it is caused to burn by some fraction which gives rise to a pressure of

$$P(J) = P_{eos}(V, E)F(J).$$

The foregoing formulation reproduces steady state detonations only, and is unrelated to the physics of the initiation of HE burn or the rate of energy release behind the detonation front.

To describe the effect of chemical kinetics upon the equation of state, it is postulated that the pressure may be expressed as

$$p = (1 - f)p_1(V, E) + f p_2(V, E)$$

where $p_1(V, E)$ is an equation of state describing the behavior of the partially-burned product resulting from propagation of a detonation front, as described

in the C-J burn model above. f is the fraction of that portion of the chemical energy which has not been released immediately by the propagation of the C-J burn. Thus, immediately following passage of the detonation front, f is zero, so that the partially-burned material is described by p_1 . Upon completion of burning, $f = 1$, and p_2 applies. In this work p_1 and p_2 are JWL equations of state for LX-04 HE as given in Ref. 3.

It remains to express f as a function of time. As a first approximation, it has been assumed that the rate of energy release behind the detonation front is constant, so that

$$f = \frac{1}{E_d} \int_{t_0}^t \frac{dE}{dt} dt = \frac{kt}{E_d}$$

where E_d is the total energy resulting from afterburning. t_0 may be taken as the time when the C-J burn was complete, or a subsequent induction period may be added if desired.

RESULTS OF CALCULATIONS

It was anticipated that the rate of energy release behind the front would influence the detonation velocity and the pressure profile at the detonation front. As a result, the transit time across the Lucite plates depends upon the rate of energy release. A series of calculations was made to determine the effects of releasing 50% of the chemical energy of the HE over durations ranging from 0.02 to 10 μ sec. The induction time was taken to be zero.

EFFECT ON PRESSURE

The rate of energy release affects both the peak pressure at the detonation front and the pressure profile, as shown graphically in Fig. 1. When the rate

of energy release is rapid, under 0.1 μ sec, a sharp, narrow, high peak is created at the front. At intermediate rates, 0.5 to 2 μ sec, a pressure pulse of substantial width and height is produced. For the slower rates, the influence of the second portion of the energy is not manifested because of the limited dimension of the system.

EFFECT ON DETONATION VELOCITY

The effect of the rate of energy release upon the detonation velocity is shown in Fig. 2. When the energy is released under 0.1 μ sec, there is no appreciable effect on the detonation velocity. For longer durations, it can be seen that a certain distance must be traversed before the detonation velocity corresponding to immediate release of the total chemical energy is attained. At 0.5 μ sec, this distance is nearly the full length of the charge under consideration.

TRANSIT TIME ACROSS LUCITE PLATES

The variation of calculated transit time as a function of rate of energy release is depicted in Fig. 3, whereon the ordinate is the difference between calculated and experimental values; i.e., exact agreement between the two sets is expressed by the null horizontal line. Positive value means that the calculated transit time is shorter than the experimental time. The curve marked zero delay duration corresponds to the C-J burn model. It can be seen that the calculated transit time for this case differs by as much as 46 nanoseconds at the 10 cm station. This difference is believed to be due to slight inaccuracies of the equation of state used.

The transit time is determined by the pressure profile existing when the detonation front arrives at the end of the HE. Figs. 1 and 3 show that for the short durations of 0.1 μ sec or less, the transit time is nearly independent of the rate of energy release, in spite of the appearance of a high pressure spike at the front. As the width of the high pressure pulse at the front increases, however, as in the cases of 0.5 and 1 μ sec, the calculated transit times become progressively shorter. For very long durations, $>10 \mu$ sec, the delayed portion of the energy has no influence on the transit time because of the limited length of the HE.

CONCLUSIONS

By varying the rate of release of a part of the chemical energy, it is possible to increase or decrease the peak pressure at the detonation front and to decrease or increase the transit time across a set of Lucite witness plates in the experiment under consideration. In heterogeneous explosives, which contain more than one reactant, it has been observed experimentally that not all of the chemical energy is released immediately at the passage of the detonation wave. Instead, a portion of the energy is released during a period of many microseconds later. It appears that a kinetic model such as described here should be applicable to reaction in heterogeneous explosives.

Table 1

Transit Time in PMMA

P-40 initiated LX-04, 10 cm diameter 10 cm long

<u>Distance,</u> <u>cm</u>	<u>Time,</u> <u>μsec</u>
0.5	0.712
1.0	1.448
1.5	2.208
2.0	2.968
2.5	3.752

REFERENCES

1. Private communication, J. Kurrle, Burlington AEC Plant.
2. Mark L. Wilkins, Calculation of Elastic-Plastic Flow, Lawrence Livermore Laboratory, Livermore, Rept. UCRL-7322, Rev. I (1969).
3. E. L. Lee, H. C. Hornig, J. W. Kury, Adiabatic Expansion of High Explosive Detonation Products, Lawrence Livermore Laboratory, Livermore, Rept. UCRL-50422 (1968).

Figure 1: Effect of Burning Time on Pressure

Figure 2: Effect of Burning Time on Detonation Velocity

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Figure 3: Effect of Burning Time on PMMA Transit Time

Brightness Temperature of the Detonation Wave in Some Liquid Explosives

In order to evaluate the role of the transport phenomena (primarily diffusion) in the burning of a composite high explosive, it is important to know both the pressure and the temperature. As pointed out in the preceding section, the diffusion coefficient can exhibit significant dependence on both quantities. The temperature may have an even greater effect on the initiation behavior of the high explosive. For that reason we undertook the task to measure the temperature in the detonation front of nitromethane, which is our standard high explosive, and also in the detonation front of hydrazine-hydrazine nitrate mixtures which contain no carbon. The latter mixtures are of interest for high explosives systems that produce little or no carbon - for instance, slurries with high ammonium nitrate loading.

An optical technique is being used which measures the amount of thermal radiation that is emitted by the detonation front as it propagates through the explosive medium. The system is illustrated in Fig. 1. It consists of a stainless steel test chamber 15 cm long which contains the explosive liquid. The detonation wave is initiated by a conventional HE lens and booster combination, and radiation emitted from the detonation front is collected by a photodetector at the opposite end of the tube. Proper size aperture and interference filter limit the amount of radiation entering the detector and thereby provide geometrical and spectral control on the incident light. The intensity of the incoming light is recorded on the oscilloscope.

A typical result from such an experiment is illustrated in Fig. 2. The cutoff view of the upper portion of the test chamber shows the path of the detonation wave and provides the spatial coordinate to the time-space plane above it.

The actual intensity record is shown on the right along the corresponding time coordinate. Also shown is the trace of the brightness temperature as deduced from the intensity record.

The brightness temperature of the detonation wave in nitromethane was measured at several wavelenths, and the results are shown in Fig. 3. Judging from the results of other investigators^(1,2) who looked into the emissivity of the detonation front in nitromethane, the most reliable data come from the near infrared part of the spectrum where radiation was found to be very close to that of a black body. Therefore, one can even conclude that at these wavelengths the brightness temperature is also very close to the true temperature, and for nitromethane the detonation temperature then comes out to be 3300 ± 50 K. In the 70/30 and 21/79 hydrazine/hydrazine nitrate solutions, the brightness temperatures were found to be 2200 K and 2860 K, respectively. No emissivity data for the latter solutions are available.

Having a relatively simple technique to measure the temperature of the detonation wave, further investigations are planned with other explosive liquids such as tetranitromethane and its various mixtures with nitromethane and water.

Figure 1

Figure 2

Figure 3

REFERENCES

1. J. T. A. Burton and J. A. Hicks, "Detonation Emissivities and Temperatures in Some Liquid Explosives," Nature 202, 758 (1964).
2. A. N. Dremine and S. D. Savrov, "Emission Spectrum of a Detonation Wave in Nitromethane," Zh. PMTF 1, 103 (1965).

THE ESTIMATION OF DIFFUSION COEFFICIENTS AT HIGH TEMPERATURES AND PRESSURES

Abstract

Energy release in heterogeneous explosives appears to be diffusion controlled. There are, unfortunately, no diffusion data of any kind in the region of 1500-3000 K and 50-200 kbar. This report summarizes an examination of how well kinetic theories might predict diffusion coefficients in this region. Estimation procedures and comparisons with molecular dynamics calculations were reviewed.

It appears that the Lennard-Jones potential with a temperature correction determined in this study and the Enskog correction using the Carnahan-Starling hard-sphere equation of state give fair estimates (within 50% at moderate pressures and 100% at higher pressures). These estimates should be adequate for energy release calculations.

The procedure described leads to an analytical equation that can be used in computer programs.

I. Introduction

The overall rate of energy release of a detonating heterogeneous explosive depends on the rates of energy release of each of the individual phases. Each phase may react chemically, and the reaction products of each phase may in turn react. The secondary reaction appears to be diffusion controlled, and is the rate determining step.¹

Whether or not diffusion controls the rate depends on the value of the diffusion coefficients of the gaseous materials. In the detonation region (1500-3000 K and 50-200 kbar), there are, unfortunately, no experimental data. Consequently, it was deemed desirable to examine how well kinetic theories might predict diffusion coefficients in this high temperature, high pressure region.

A review of estimation procedures (described in part in Reid and Sherwood's text²) and comparisons with molecular dynamics calculations lead to the following conclusions:

- Low pressure diffusion coefficients calculated from tabulated Lennard-Jones 6-12 parameters are satisfactory at low temperatures but become increasingly poor with increasing temperature. We have found a crude temperature correction factor that reduces errors to the 5 to 15% level. Calculations must be based on viscosity (i. e., transport) Lennard-Jones parameters because the PVT parameters yield grossly inaccurate results.

- To calculate high pressure, high temperature diffusion coefficients from the low pressure, high temperature Lennard-Jones approximation, we have used the

Enskog hard sphere equation with the Carnahan-Starling equation of state. This leads to errors of perhaps 15 to 35% compared to molecular dynamics hard sphere calculations. Molecular dynamics values are in reasonable agreement with existing moderate pressure data, particularly if the hard core size is determined from PVT data.

Overall errors from the above described estimation procedure are of the order of 50% for moderate pressures and perhaps 100% at higher pressures. These estimates should be adequate for energy release calculations.

The estimation procedure is in the form of an analytical equation that can be used in computer codes. This equation is compared with some of the scant diffusion data available and gives good results in most cases. Also presented are the D's along the water Hugoniot and some high pressure calculations for H₂O and CO₂ to indicate the general trends. Tables of Lennard-Jones parameters and methods for estimating those not included are provided.

II. Kinetic Theory Description of Low-Pressure Diffusion Coefficients

A. GENERAL FORMULA

The value of the low pressure mutual diffusion coefficient D_{12}^0 is given for a binary system in Refs. 2 and 3 as

$$D_{12}^0 = \frac{0.001858 T^{3/2} \left[\frac{M_1 + M_2}{M_1 M_2} \right]^{1/2}}{P \sigma_{12}^2 \Omega_D}, \quad (1)$$

where D_{12}^0 is in cm²/s, P is the pressure in atm, T is the temperature in K, and M_i is molecular weight. The collision diameter σ_{12} is one of the force constants for the mixture in Å. The reduced cross section Ω_D is a function only of kT/ϵ_{12} , where the interaction energy ϵ_{12} is the other force constant in K, and k is Boltzmann's constant. The choice of intermolecular potential determines the values of ϵ_{12} and σ_{12} and also the functional form of Ω_D .

Equation (1) is a first approximation. The higher approximations contain a complicated factor that includes the concentration dependence. Since the factor varies only from 1.00 to 1.03, it can be neglected.

The self-diffusion coefficient, obtained by setting $M_1 = M_2$ in Eq. (1), is

$$D^0 = \frac{0.002628 T^{3/2}}{P \sigma^2 \Omega_D M^{1/2}}. \quad (2)$$

B. INTERMOLECULAR POTENTIALS

The definition of Ω_D is such that $\Omega_D = 1$ for rigid spheres (Ref. 3, p. 544). However, rigid spheres give a poor fit to self-diffusion data, and other potentials such as the Lennard-Jones or square-well are better (Ref. 3, pp. 594-596). The choice of potential is determined by the polarity of the gases.

1. Nonpolar Mixtures

For nonpolar mixtures, the Lennard-Jones 6-12 potential is a reasonable choice, and Table 1 contains the values of Ω_D as a function of kT/ϵ . To obtain values of ϵ_{12} and

Table 1. Values of the collision integral Ω_D based on the Lennard-Jones potential.^a

kT/ϵ	Ω_D	kT/ϵ	Ω_D	kT/ϵ	Ω_D
0.30	2.662	1.65	1.153	4.0	0.8836
0.35	2.476	1.70	1.140	4.1	0.8788
0.40	2.318	1.75	1.128	4.2	0.8740
0.45	2.184	1.80	1.116	4.3	0.8694
0.50	2.066	1.85	1.105	4.4	0.8652
0.55	1.966	1.90	1.094	4.5	0.8610
0.60	1.877	1.95	1.084	4.6	0.8568
0.65	1.798	2.00	1.075	4.7	0.8530
0.70	1.729	2.1	1.057	4.8	0.8492
0.75	1.667	2.2	1.041	4.9	0.8456
0.80	1.612	2.3	1.026	5.0	0.8422
0.85	1.562	2.4	1.012	6	0.8124
0.90	1.517	2.5	0.9996	7	0.7896
0.95	1.476	2.6	0.9878	8	0.7712
1.00	1.439	2.7	0.9770	9	0.7556
1.05	1.406	2.8	0.9672	10	0.7424
1.10	1.375	2.9	0.9576	20	0.6640
1.15	1.346	3.0	0.9490	30	0.6232
1.20	1.320	3.1	0.9406	40	0.5960
1.25	1.296	3.2	0.9328	50	0.5756
1.30	1.273	3.3	0.9256	60	0.5596
1.35	1.253	3.4	0.9186	70	0.5464
1.40	1.233	3.5	0.9120	80	0.5352
1.45	1.215	3.6	0.9058	90	0.5256
1.50	1.198	3.7	0.8998	100	0.5130
1.55	1.182	3.8	0.8942	200	0.4644
				300	0.4360
1.60	1.167	3.9	0.8888	400	0.4170

^aData from Ref. 3.

σ_{12} from the values of ϵ and σ of the pure components, it is customary to use the Lorentz-Berthelot combining rules (Ref. 2, p. 523; Ref. 3, p. 567; and Ref. 4),

$$\epsilon_{12} = \sqrt{\epsilon_1 \epsilon_2} \quad (3)$$

and

$$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2} \quad (4)$$

Values of Lennard-Jones ϵ_i/k and σ_i for pure gases are given in Table 2 (Ref. 2, Appendix G). If the compound is not in Table 2, estimates that are reasonably consistent with Table 2 are given by the following equations (Ref. 2, pp. 40 and 525):

$$\epsilon/k = 0.75 T_c = 1.21 T_b; \quad (5)$$

$$\sigma = 2.393 \left(\frac{T_c}{P_c} \right) = 1.18 V_b^{1/3}. \quad (6)$$

Here, c and b refer to the critical and boiling points, respectively, and V is the molal volume in cm^3/mol .

2. Polar-Nonpolar Mixtures

Estimated diffusion coefficients for polar-nonpolar mixtures are not as good as those for nonpolar mixtures. They can be improved by using the Lennard-Jones parameters ϵ_n , σ_n for the nonpolar constituent, and Stockmayer parameters ϵ_p , σ_p for the polar constituent. Reference 3 (p. 600) suggests calculating the mixture parameters ϵ_{np} and σ_{np} as follows:

$$\sigma_{np} = \left[\frac{\sigma_n + \sigma_p}{2} \right] \xi^{1/6} \quad (7)$$

$$\epsilon_{np} = (\epsilon_n \epsilon_p)^{1/2} \xi^2 \quad (8)$$

$$\xi = \left[1 + \frac{\sqrt{2}}{2} \alpha_n^* t_p^* \left(\frac{\epsilon_p}{\epsilon_n} \right)^{1/2} \right]. \quad (9)$$

Table 2. Lennard-Jones potentials as determined from viscosity data.^a

Molecule	Compound	σ (Å)	ϵ/k (K)
A	Argon	3.542	93.3
He	Helium	2.551	10.22
Kr	Krypton	3.655	178.9
Ne	Neon	2.820	32.8
Xe	Xenon	4.047	231.0
Air	Air	3.711	78.6
AsH ₂	Arsine	4.145	259.8
BCl ₂	Boron chloride	5.127	337.7
BF ₂	Boron fluoride	4.198	186.3
B(OCH ₃) ₃	Methyl borate	5.503	396.7
Br ₂	Bromine	4.296	507.9
CCl ₄	Carbon tetrachloride	5.947	322.7
CF ₄	Carbon tetrafluoride	4.662	134.0
CHCl ₃	Chloroform	5.389	340.2
CH ₂ Cl ₂	Methylene chloride	4.898	356.3
CH ₃ Br	Methyl bromide	4.118	449.2
CH ₃ Cl	Methyl chloride	4.182	350
CH ₃ OH	Methanol	3.626	481.8
CH ₄	Methane	3.758	148.6
CO	Carbon monoxide	3.690	91.7
COS	Carbonyl sulfide	4.130	336.0
CO ₂	Carbon dioxide	3.941	195.2
CS ₂	Carbon disulfide	4.483	467
C ₂ H ₂	Acetylene	4.033	231.8
C ₂ H ₄	Ethylene	4.163	224.7
C ₂ H ₆	Ethane	4.443	215.7
C ₂ H ₅ Cl	Ethyl chloride	4.898	300
C ₂ H ₅ OH	Ethanol	4.530	362.6
C ₂ N ₂	Cyanogen	4.361	348.6
CH ₃ OCH ₃	Methyl ether	4.307	395.0
CH ₂ CHCH ₃	Propylene	4.678	298.9
CH ₃ CCH	Methylacetylene	4.761	251.8
C ₃ H ₆	Cyclopropane	4.807	248.9
C ₃ H ₈	Propane	5.118	237.1
n-C ₃ H ₇ OH	n-Propyl alcohol	4.549	576.7
CH ₃ COCH ₃	Acetone	4.600	560.2
CH ₃ COOCH ₃	Methyl acetate	4.936	469.8
n-C ₄ H ₁₀	n-Butane	4.687	531.4

Table 2. (continued)

Molecule	Compound	σ (Å)	ϵ/k (K)
iso-C ₄ H ₁₀	Isobutane	5.278	330.1
C ₂ H ₅ OC ₂ H ₅	Ethyl ether	5.678	313.8
CH ₃ COOC ₂ H ₅	Ethyl acetate	5.205	521.3
n-C ₅ H ₁₂	n-Pentane	5.784	341.1
C(CH ₃) ₄	2,2-Dimethylpropane	6.464	193.4
C ₆ H ₆	Benzene	5.349	412.3
C ₆ H ₁₂	Cyclohexane	6.182	297.1
n-C ₆ H ₁₄	n-Hexane	5.949	399.3
Cl ₂	Chlorine	4.217	316.0
F ₂	Fluorine	3.357	112.6
HBr	Hydrogen bromide	3.353	449
HCN	Hydrogen cyanide	3.630	569.1
HCl	Hydrogen chloride	3.339	344.7
HF	Hydrogen fluoride	3.148	330
HI	Hydrogen iodide	4.211	288.7
H ₂	Hydrogen	2.827	59.7
H ₂ O	Water	2.641	809.1
H ₂ O ₂	Hydrogen peroxide	4.196	289.3
H ₂ S	Hydrogen sulfide	3.623	301.1
Hg	Mercury	2.969	750
HgBr ₂	Mercuric bromide	5.080	686.2
HgCl ₂	Mercuric chloride	4.550	750
HgI ₂	Mercuric iodide	5.625	695.6
I ₂	Iodine	5.160	474.2
NH ₃	Ammonia	2.900	558.3
NO	Nitric oxide	3.492	116.7
NOCl	Nitrosyl chloride	4.112	395.3
N ₂	Nitrogen	3.798	71.4
N ₂ O	Nitrous oxide	3.828	232.4
O ₂	Oxygen	3.467	106.7
PH ₃	Phosphine	3.981	251.5
SF ₆	Sulfur hexafluoride	5.128	222.1
SO ₂	Sulfur dioxide	4.112	335.4
SiF ₄	Silicon tetrafluoride	4.880	171.9
SiH ₄	Silicon hydride	4.084	207.6
SnBr ₄	Stannic bromide	6.388	563.7
UF ₆	Uranium hexafluoride	5.967	236.8

^aData from Ref. 2., pp. 632-633.

The quantities ϵ_n and σ_n are given in Table 2; ϵ_p , σ_p , and t^* are given in Table 3 (Ref. 2, p. 72). The reduced polarizability α_n^* is calculated from

$$\alpha_n^* = \frac{\alpha_n}{\sigma_n^3}, \quad (10)$$

and the polarizabilities α_n are given in Table 4 (Ref. 2, p. 529). The Stockmayer parameters are discrepant among different tabulations; our table of parameters is quite different from the one in Ref. 3 (p. 214). For nonresonating compounds, the α_n

Table 3. Stockmayer-potential parameters.^a

	Dipole moment μ , debyes	σ (Å)	ϵ_0/k (K)	t^*
H ₂ O	1.85	2.52	775	0.7
NH ₂	1.47	3.15	358	0.5
HCl	1.08	3.36	328	0.24
HBr	0.80	3.41	417	0.10
HI	0.42	4.13	313	0.20
SO ₂	1.63	4.04	347	0.30
H ₂ S	0.92	3.49	343	0.15
NOCl	1.83	3.53	690	0.3
CHCl ₃	1.013	5.31	355	0.05
CH ₂ Cl ₂	1.57	4.52	483	0.14
CH ₃ Cl	1.87	3.94	414	0.35
CH ₃ Br	1.80	4.25	382	0.3
C ₂ H ₅ Cl	2.03	4.45	423	0.3
CH ₃ OH	1.70	3.69	417	0.35
C ₂ H ₅ OH	1.69	4.31	431	0.2
n-C ₃ H ₇ OH	1.69	4.71	495	0.14
i-C ₃ H ₇ OH	1.69	4.64	518	0.14
(CH ₃) ₂ O	1.30	4.21	432	0.13
(C ₂ H ₅) ₂ O	1.15	5.49	362	0.06
(CH ₃) ₂ CO	1.20	3.82	428	0.9
CH ₃ COOCH ₃	1.72	5.04	418	0.14
CH ₃ COOC ₂ H ₅	1.78	5.24	499	0.11
CH ₃ NO ₂	2.15	4.16	290	1.6

NOTE

$$t^* = \mu^2 / 2 \sqrt{2} \epsilon_0 \sigma^2$$

^aData from Ref. 2, p. 72.

Table 4. Polarizability of molecules.^a

Compound	$10^{25} \alpha_n$ (cm ³)	Compound	$10^{25} \alpha_n$ (cm ³)
H ₂	7.9	C ₆ H ₅ CH ₃	122.6
N ₂	17.6	p-C ₆ H ₄ (CH ₃) ₂	142
O ₂	16.0	m-C ₆ H ₄ (CH ₃) ₂	141.8
Cl ₂	46.1	o-C ₆ H ₄ (CH ₃) ₂	141
HF	24.6	CH ₃ Cl	45.6
HCl	26.3	CH ₃ Br	55.5
HBr	36.1	CH ₂ Cl ₂	64.8
HI	54.5	CHCl ₃	82.3
N ₂ O	30.0	CCl ₄	105
CO	19.5	C ₂ H ₅ Cl	64
CO ₂	26.5	C ₆ H ₅ Cl	122.5
SO ₂	37.2	p-C ₆ H ₄ Cl ₂	144.7
H ₂ S	37.8	m-C ₆ H ₄ Cl ₂	142.3
CS ₂	87.4	o-C ₆ H ₄ Cl ₂	141.7
NH ₃	22.6	CH ₃ OH	32.3
(CN) ₂	50.1	CH ₃ OCH ₃	51.6
HCN	25.9	C ₂ H ₅ OC ₂ H ₅	87.3
SnCl ₄	137.7	C ₃ H ₇ OC ₃ H ₇	125
CH ₄	26.0	C ₄ H ₈ O ₂	94.4
C ₂ H ₆	44.7	CH ₃ COCH ₃	63.3
C ₂ H ₄	42.6	CH ₃ COC ₂ H ₅	81.3
C ₂ H ₂	33.3	C ₂ H ₅ COC ₂ H ₅	99.3
C ₃ H ₈	62.9	CH ₃ COC ₃ H ₇	99.3
C ₆ H ₁₂	108.7	C ₆ H ₅ NO ₂	129.2
C ₆ H ₆	103.2	C ₆ H ₅ N	95

^aData from Ref. 2, p. 529.

can be estimated using the additive bond polarizabilities described in Ref. 3 (pp. 947-951).

For non-hydrogen-bonded materials, estimates of σ_p and ϵ_p can be obtained from the following equations (Ref. 2, pp. 28, 73):

$$\epsilon_p/k = 0.897 T_c; \quad (11)$$

$$\sigma_p = 0.785 V_c^{1/3} = 3.41 \left(\frac{Z_c T_c}{P_c} \right)^{1/3}. \quad (12)$$

For hydrogen-bonded substances, a rough approximate rule (Ref. 2, p. 73) is

$$\epsilon_p/k = \frac{0.00331 T_c}{Z_c^4} \quad (13)$$

and

$$\sigma_p = 36.9 V_c^{1/3} Z_c^{2.75} = 160.3 \left(\frac{T_c}{P_c} \right)^{1/3} Z_c^{3.08} \quad (14)$$

Finally, for mixtures of water with a nonpolar gas, a rough estimate is obtained by multiplying the Lennard-Jones D_{12} value by 1.09 (Ref. 2, pp. 533, 540).

C. ANALYTICAL FORM FOR THE LENNARD-JONES Ω_D

For computer use, an analytical form for $\Omega_D(kT/\epsilon)$ would be much more convenient than Table 1. Consequently, we considered the fits of a large number of three, four, and five-constant equations to y as a function of x , $z (= x^{1/2})$ or $u (= 1/x)$. If s stands for any of x , z , or u , and r stands for any of y , $1/y$, or $\ln y$, then the equations tried can be written for the five-constant form as

$$r = a + bs + cs^2 + ds^3 + es^4 \quad (15a)$$

$$r = a + (b/x) + cx + dx^2 + ex^3 \quad (15b)$$

$$r = a + (b/u) + cu + du^2 + eu^3 \quad (15c)$$

$$r = a \ln s + bs + cs^2 + ds^3 + es^4 \quad (15d)$$

$$r = a \ln s + b + cs + ds^2 + es^3 \quad (15e)$$

A large general purpose least squares program was prepared for these equations using OMNITAB, a National Bureau of Standards data handling code. The program is in two parts; one for Eqs. (15a)-(15c) and one for Eqs. (15d) and (15e).

Applying this program to $y = \Omega_D$ and $x = kT/\epsilon$, we obtained an equation of the form of Eq. (15e) as the simplest best equation with $r = \ln y$ and $s = 1/x$. The result can be written in exponential form as

$$\Omega_D = \mu^{0.13921} \left[\exp(-0.031692 + 0.44932 \mu - 0.059144 \mu^2) \right] \quad (16)$$

where

$$\mu = \epsilon/kT \quad (17)$$

and the maximum error is within 1.5% for all of Table 1. A more complex five-term equation fits to 1%, but the difference of 0.5% is small compared to the other errors in the overall estimation procedure.

D. THE LOW PRESSURE KINETIC THEORY RESULTS FOR D_{12} AND D

After calculating ϵ_{12} and σ_{12} for Eqs. (3) and (4) or (7) and (8) together with the tables or the estimation equations noted in Section IIB above, we obtain D_{12}° and D° from the following formulas:

$$D_{12}^\circ = \frac{0.001858 T^{3/2} \left[\frac{M_1 + M_2}{M_1 M_2} \right]^{1/2}}{P \sigma_{12}^2 \mu^{0.13921} \exp(-0.031692 + 0.44932 \mu - 0.059144 \mu^2)} \quad (18)$$

and

$$D^\circ = \frac{0.002628 T^{3/2}}{P \sigma^2 M^{1/2} \mu^{0.13921} \exp(-0.031692 + 0.44932 \mu - 0.059144 \mu^2)}, \quad (19)$$

where

$$\mu = \epsilon_{12}/kT. \quad (20)$$

E. ERRORS AND COMPARISON WITH EXPERIMENT

The general consensus of those doing high temperature measurements of low pressure diffusion coefficients is that the low pressure Lennard-Jones parameters calculated from experimental virial coefficients and viscosity do not give accurate predictions of D° . The virial parameters are useless. The results using viscosity parameters are increasingly low, up to about 10%, for such pairs as N_2 - CO_2 , He- N_2 , CO_2 -Ar, CO_2 - N_2 , CO-CO, and CO- N_2 . For more polar mixtures such as CO_2 - CO_2 and NH_3 - H_2 , the errors are still larger at high temperatures.

In general, the simple, spherically-symmetric potential functions (such as the Lennard-Jones and exponential-6) do not yield self-consistent parameters for viscosity, diffusion, and PVT. One of the many reasons, is that few molecules are spherical. It has been shown for argon that both equilibrium and transport properties can be fit with a single potential, but this potential is complicated and has 13 parameters instead of just two.⁵

Although Lennard-Jones type potentials are not universally valid, an adequate set of parameters for interpolation can be found for each property of a substance. Moreover, there seems to be a correlation between D based on viscosity parameters and D based on experimental values. As noted earlier, D based on L-J viscosity parameters is generally low.

Amdur⁶ compared best values from molecular beam experiments with those calculated from viscosity-based L-J parameters at 1000, 5000, and 15 000 K for Ar-Ar

and N_2-N_2 systems. The errors increase to nearly 40% at 15 000 K. If Amdur's results are plotted against T, a very approximate straight line can be drawn through the scattered points. The equation for the line is

$$g = 1 + 3.4 \times 10^{-5} T = (\text{best value})/(\text{L-J value}). \quad (21)$$

The factor g should reduce the errors at the higher temperatures to the 5 to 15% level. Consequently, if we denote the D's calculated by Eqs. (18) and (19) by D_{LJ} , then the best estimate of the low-pressure, high-temperature diffusion coefficients is

$$D_{\text{low p}} = D_{LJ} [1 + 3.4 \times 10^{-5} T]. \quad (22)$$

III. Diffusion Coefficients at Higher Pressures

A. GENERAL CONSIDERATIONS

Enskog showed that the diffusion coefficient of a high pressure gas of rigid spheres could be related to its low pressure value at the same temperature by the following equation (Ref. 2, p. 540; Ref. 3, pp 646, 647; and Ref. 7, pp 311, 312):

$$\frac{D_{12\rho}}{(D_{12\rho})^0} = \left(\frac{D_{12}P}{Z} \right) / \left(\frac{D_{12}P}{Z} \right)^0 = \frac{1}{Y_{12}}, \quad (23)$$

where the superscript zero refers to the low pressure values from Eq. (22) at the same temperature, ρ is the density, and Y_{12} is an equation-of-state factor. The Z in Eq. (23) is the compressibility factor, which is defined by

$$Z = \frac{PV}{n\hat{R}T}, \quad (24)$$

where V is the volume, n is the number of moles, and $\hat{R}$ is the gas constant.

B. PURE RIGID SPHERE GAS

For a pure gas of rigid spheres with diameter σ ,

$$Z = 1 + \frac{nb}{V} Y = 1 + y, \quad (25)$$

where

$$y = \frac{nb}{V} Y \quad (26)$$

and

$$b = \frac{2}{3} N_A \bar{\sigma}^3. \quad (27)$$

Here, N_A is Avogadro's number (Ref. 3, pp. 634-636), and $\bar{\sigma}$ is the high pressure σ , which is different in general from the low pressure value. It can also be shown that

$$Y = 1 + 0.625 \frac{nb}{V} + 0.2869 \left(\frac{nb}{V}\right)^2 + 0.110 \left(\frac{nb}{V}\right)^3 + \dots, \quad (28)$$

where the coefficient 0.110 is a more recent value than the 0.115 given in Ref. 3.

Let us define x as

$$x = \frac{nb}{4V} = \frac{1}{6} \frac{n}{V} \pi N_A \bar{\sigma}^3. \quad (29)$$

Then, by Eqs. (25), (26), and (27),

$$Y = \frac{y}{4x} = \frac{Z - 1}{4x}. \quad (30)$$

Carnahan and Starling⁸ have presented the following approximation to the equation of state of fluid-phase rigid spheres (which is good to within 1%)*:

$$Z = \frac{1 + x + x^2 - x^3}{(1 - x)^3} \quad (31)$$

or

$$y = Z - 1 = \frac{2x(2 - x)}{(1 - x)^3}. \quad (32)$$

In terms of this approximation, we may thus write Y as

$$Y = \frac{2 - x}{2(1 - x)^3}. \quad (33)$$

C. SELF-DIFFUSION

If we evaluate the low pressure diffusion coefficient $D_{\text{low } p}$ of Eq. (23) at 1 atm, then $P^\circ = 1$ and $Z^\circ \approx 1$. Consequently, we obtain by means of Eq. (30)

$$D = \frac{D_{\text{low } p} Z}{PY} = \frac{D_{\text{low } p}}{P} \left(\frac{Z}{Z - 1} \right) (4x). \quad (34)$$

*There are a number of other such approximations mentioned in Ref. 8 that are less accurate.

Using the Carnahan-Starling approximation given in Eqs. (31) and (33), we can transform Eq. (34) to

$$D = \frac{D_{\text{low } p}}{P} R(x), \quad (35)$$

where the pressure "correction factor" $R(x)$ is given by

$$R(x) = \frac{1 + x + x^2 - x^3}{\left(1 - \frac{x}{2}\right)}. \quad (36)$$

We can also write $R(x)$ as a series:

$$R(x) = 1 + \frac{3}{2}x + \frac{7}{4}x^2 - \frac{x^3}{8} - \sum_{j=4}^{\infty} \left(\frac{x}{2}\right)^j, \quad (37)$$

where the series to x^3 terms is good to 1% for $x \leq 0.7$ ($Z \leq 70$).

For the purpose of writing computer programs to examine diffusion effects, a more convenient variable than x is often the density ρ . This is because the equation-of-state codes now in use employ the density as a variable. Since

$$\rho = \frac{\text{weight}}{\text{volume}} = \frac{nM}{V}, \quad (38)$$

we find that x is proportional to ρ as follows:

$$x = \frac{nb}{4} = \frac{b\rho}{4M} = \frac{\pi N_A \sigma^3}{6M} \rho = \text{constant} \cdot \rho. \quad (39)$$

Alternatively, $R(x)$ can be put in terms of Z because x is an implicit function of Z by Eq. (31). Thus, a table of R and Z as parametric functions can be formed. Examination of various plots of functions of R and Z showed that $R(x)$ vs $\ln Z(x)$ is nearly a straight line for Z between 1 and 70. The equation of that line was determined to be

$$R = 1 + 0.445 \ln Z, \quad (40)$$

for

$$1 \leq Z \leq 70.$$

Hence, D can be written in terms of Z as

$$D = \frac{D_{\text{low } p}}{P} (1 + 0.445 \ln Z). \quad (41)$$

Although, $R(x)$ can be written in terms of the density or volume alone without a need to know the temperature explicitly, $\bar{\sigma}$ is pressure dependent. Furthermore, a knowledge of T is required to calculate $D_{\text{low } p}$, and P is required in Eq. (35). Consequently PVT data are required to calculate a high pressure diffusion coefficient. Since Z is also given in terms of these data by Eq. (24), it is ultimately more convenient to determine R from Eq. (40).

Since a hard sphere gas cannot have a negative x , Z must always be greater than or equal to 1. But we can always consider the empirical utility of assuming that Eq. (4) is also valid when Z is less than 1. As will be seen below, this assumption does bring calculated and experimental results closer together.

D. MUTUAL DIFFUSION

The theoretical Enskog corrections are much more complicated for mutual diffusion than for self-diffusion.^{3,7} However, if the mixture is considered to be a single gas with a Z corresponding to the mixture, Eq. (40) can be used to obtain the correction factor R . The best way to obtain R is to use an experimental value of Z from PVT data for the composition at the appropriate temperature and pressure. Alternatively, generalized compressibility charts can be used to obtain Z from a knowledge of T_r and P_r , where

$$T_r = \frac{T}{T_c} \quad (42)$$

and

$$P_r = \frac{P}{P_c} \quad (43)$$

Such charts, e.g., the Nelson-Obert charts (Ref. 2, pp. 50-52; Ref. 9), provide reasonably good values of Z for $0 \leq T_r \leq 15$ and $0 \leq P_r \leq 40$ (i.e., for pressures to about 2 kbar). For mixtures, the values of T_c and P_c to be used are the "pseudo-critical" values calculated from

$$T_c = N_1 T_{c1} + N_2 T_{c2} \quad (44)$$

and

$$P_c = N_1 P_{c1} + N_2 P_{c2} \quad (45)$$

where N_i , P_{ci} , and T_{ci} are the mole fraction, critical pressure, and critical temperature of component i . These equations give a composition dependent Z and, thus, a slightly composition dependent D at pressures above a few atmospheres.

E. ERROR ESTIMATES

Enskog's high pressure correction is based on rigid sphere collisions. Our previous formulas come from a consideration of uncorrelated binary collisions. It is possible to calculate a more exact hard sphere result using molecular dynamics, and taking into account the correlation between successive collisions.¹⁰ The ratio of the exact hard sphere result to the approximate Enskog calculation increases as a function of increasing density from 1.0 to 1.34 at $\rho/\rho_{cp} = 0.333$, and then declines to 0.84 at $\rho/\rho_{cp} = 0.625$, where ρ_{cp} is the close packed density. Thus, the Enskog correction compared to hard spheres has errors of $\pm 35\%$.

Besides this error, there is also the question of whether hard spheres is a good approximation at higher densities. Comparison with data at moderate pressures shows that hard spheres is reasonably satisfactory if the hard sphere core size is determined from PVT data.¹⁰⁻¹² (This justifies using Z or determining x from Z as noted previously.) Thus, using the simpler Enskog correction leads to errors of the order of 35 to 50% at higher pressures.

IV. Final Equations

For computer calculations, it is useful to put Eqs. (18), (22), (35) and (41) together into one formula. Thus, the final result is

$$D_{12} = \frac{0.001858 T^{3/2} \left(\frac{M_1 + M_2}{M_1 M_2} \right)^{1/2} [1 + 3.4 \times 10^{-5} T] [1 + 0.445 \ln Z]}{P \sigma_{12}^2 \left[\mu^{0.13921} \exp(-0.031692 + 0.44932 \mu - 0.059144 \mu^2) \right]} \quad (46)$$

where Z must be obtained from PVT data, σ_{12} from Eqs. (3) or (8), μ from Eq. (20), and the ϵ_{12} of Eq. (20) from Eqs. (4) or (7). It is important to have PVT data because Z may reach values of 50 to 60 at lower temperatures and several hundred kilobars. In these cases $R(Z)$ is close to 3.

Equation (46) and the equations to get ϵ_{12}/k and σ_{12} from tabulated data (Tables 2-4) are all in analytical form. Consequently, they can be easily incorporated into explosives calculations as long as PVT are either input or can be calculated from an equation of state. The self-diffusion result is obtained by setting $M_1 = M_2$, $\sigma_1 = \sigma_2$, and $\epsilon_1 = \epsilon_2$.

V. Comparison with Experiment

Although no high pressure, high temperature data exist, there are some data at high temperatures and low pressure; and some at low temperatures and moderate pressures ranging up to nearly 2 kbar. Some of these data are compared with calculated values from Eq. (46) in Tables 5 and 6. In all cases, the σ_{12} and ϵ_{12} are calculated from Eqs. (3) and (4) using the σ_i and ϵ_i from Table 2.

Table 5A. Comparison of D in cm^2/s at 1 atm and various temperatures with Eq. (46).

T (K)	$\text{N}_2 - \text{N}_2$ (Ref. 13)			$\text{Ne} - \text{Ne}$ (Ref. 13)			$\text{Ar} - \text{Ar}$ (Ref. 13)		
	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)
300	—	—	—	—	—	—	—	—	—
500	—	—	—	—	—	—	—	—	—
1 000	1.56	1.62	+4	3.93	3.94	0	1.51	1.50	0
3 000	10.4	10.7	+3	25.2	25.7	+2	10.4	9.97	-4
10 000	95.5	94.4	-1	207	225.3	+9	93.2	88.1	-5
T (K)	$\text{Kr} - \text{Kr}$ (Ref. 13)			$\text{Xe} - \text{Xe}$ (Ref. 13)			$\text{CO} - \text{O}_2$ (Ref. 14) ^a		
	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)
300	—	—	—	—	—	—	0.211	0.206	-2
500	—	—	—	—	—	—	0.508	0.506	0
1 000	0.853	0.853	0	0.502	0.529	+5	1.68	1.67	0
3 000	5.67	5.79	+2	3.32	3.65	+10	11.2	11.1	0
10 000	49.6	51.6	+4	27.2	32.7	+20	88.9	98.3	+11
T (K)	$\text{N}_2 - \text{Ar}$ (Ref. 14) ^a			$\text{N}_2 - \text{H}_2$ (Ref. 14)			$\text{Ar} - \text{H}_2$ (Ref. 14)		
	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)
300	0.198	0.196	-1	0.784	0.752	-4	0.828	0.781	-6
500	0.484	0.478	-1	1.90	1.82	-4	2.07	1.89	-9
1 000	1.63	1.57	-4	6.33	5.92	-6	6.99	6.20	-11
3 000	11.2	10.4	-7	43.3	38.9	-10	47.2	40.9	-13
10 000	92.1	91.5	-1	369	343	-7	386	360	-7

^aCalculated from equations given in Ref. 14; all are at $N_1 = N_2 = 0.5$.

In Table 5A are the low pressure, very high temperature values based on molecular beam scattering potentials. Equation (46) agrees with the reported values to within about $\pm 10\%$ up to 10 000 K, except for Xe-Xe, which is within 20%.

In Table 5B are low pressure, moderately high temperature data for CO_2 - $^{14}\text{CO}_2$ and CO_2 -Ar. These systems are under consideration for high pressure diffusion measurements at LLL. Below 500 K, the calculated and experimental values are in good agreement. Between 1000 and 2000 K, the calculated values are systematically lower than the reported experimental results, about 25% for CO_2 - CO_2 and 10-12% for both compositions of CO_2 -Ar. These data are from Pakurar and Ferron.^{16,18} It has been noted before that CO_2 does not give as good results for D_{12} with the viscosity values of σ and ϵ as do nonpolar mixtures. Alternatively, there could be systematic errors in the Pakurar and Ferron measurements. If Pakurar and Ferron's data are correct, good estimated values of D_{12} can be obtained from a knowledge of one datum point. This datum point is used to calculate an adjustment factor, which works because the errors are systematic.

Tables 6A-E list the higher pressure data. In all cases, Z was obtained from the Nelson-Obert charts.^{2,9} For mixtures, the reduced temperatures and pressures were obtained from pseudo-critical constants calculated using Eqs. (44) and (45). Generally, the chart Z 's compare with experimental values to a few percent²⁰ and the error in Eq. (40) is about one-third less.

Table 5B. Comparison of D in cm^2/s at 1 atm and various temperatures with Eq. (46) for $\text{CO}_2 - {}^{14}\text{CO}_2$ and $\text{CO}_2 - \text{Ar}$.

$\text{CO}_2 - {}^{14}\text{CO}_2$				
T (K)	D_{expt}	$D_{12 \text{ calc}}$	Error (%)	Reference
315.8	0.129	0.124	-4	15
423.4	0.226	0.213	-6	15
500.1	0.310	0.289	-7	15
1103	1.63	1.18	-28	16
1302	2.26	1.57	-31	16
1498	2.49	2.01	-19	16
1703	3.33	2.51	-25	16
1944	4.30	3.17	-26	16
$\text{CO}_2 - \text{Ar}$				
276.2	0.1326	0.125	-6	17
317.2	0.1652	0.161	-3	17
$N_{\text{Ar}} = 0.1$				
1146	1.77	1.54	-13	18
1366	2.27	2.09	-8	18
1545	2.96	2.58	-13	18
1761	3.50	3.24	-7	18
$N_{\text{Ar}} = 0.5$				
1181	1.88	1.63	-13	18
1388	2.43	2.13	-12	18
1495	3.17	2.75	-13	18
1633	3.21	2.98	-7	18

Table 6A. D in cm²/s at various pressures of N₂ - H₂.

T = 313.15 K (Ref. 19)				
P _(atm)	Z ^{a,b}	10 ³ D _{expt}	10 ³ D _{12 calc}	Error (%)
1	1	—	811	—
68.05	1.05	11.5	12.2	+6
170.1	1.13	4.62	5.02	+9
340.2	1.28	2.40	2.64	+10
510.3	1.44	1.66	1.85	+11
680.5	1.63	1.32	1.45	+10

T = 298 K (Ref. 12)				
1	1	—	744	—
272	1.12	2.20	2.87	+30
681	1.61	0.87	1.32	+52
1090	2.13	0.63	0.91	+44
1360	2.41	0.59	0.76	+29

^aThe compressibility factor was read off the Nelson-Obert generalized compressibility charts (Ref. 2, pp. 50-52 and Ref. 9), using the pseudo-critical constants to calculate T_r and P_r. The pseudo-critical constants were calculated using Eqs. (44) and (45).

^bThe data of Ref. 12 are for H₂ as a trace, so that T_c and P_c are essentially those of N₂.

Table 6B. D in cm²/s at various pressures of Ar - H₂.

T = 298 K (Ref. 12)				
P _(atm)	Z ^{a,b}	10 ³ D _{expt}	10 ³ D _{12 calc}	Error (%)
1	1	—	771	—
272	1.00	1.83	2.84	+55
681	1.38	0.76	1.29	+70
1090	1.80	0.52	0.89	+71
1360	2.08	0.45	0.75	+67

^aThe compressibility factor was read off the Nelson-Obert generalized compressibility charts (Ref. 2, pp. 50-52 and Ref. 9), using the pseudo-critical constants to calculate T_r and P_r. The pseudo-critical constants were calculated using Eqs. (44) and (45).

^bThese data are for H₂ as a trace, so that T_c and P_c are essentially those of Ar.

Table 6C. D in cm^2/s at various pressures of CH_4 - $^{14}\text{CH}_4$.

T = 297 K (Ref. 20)					T = 353.8 K (Ref. 20)				
P (atm)	Z ^{a,b}	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)	P (atm)	Z ^{a,b}	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)
1	1	—	221	—	1	1	—	296	—
52.46	0.95	3.84	4.01	+4	67.57	0.96	4.26	4.31	+1
94.31	0.87	2.05	2.14	+4	114.3	0.94	2.39	2.52	+5
161.3	0.82	1.12	1.22	+9	179.6	0.93	1.54	1.60	+4
205.5	0.85	0.881	0.971	+10	238.0	0.96	1.17	1.22	+4
283.1	0.91	0.658	0.728	+11	319.7	1.02	0.876	0.935	+7
408	1.09	0.502	0.547	+9	410.0	1.12	0.722	0.759	+5
T = 273 K (Ref. 21)					T = 298 K (Ref. 21)				
1	1	—	184	—	1	1	—	217	—
45	0.90	4.04	3.90	-3	125	0.84	1.51	1.59	+5
82	0.82	2.00	2.05	+2.5	314	0.96	0.637	0.677	+6
151	0.76	0.965	1.07	+11	513	1.23	0.448	0.461	+3
249	0.83	0.583	0.678	+16	748	1.59	0.360	0.349	-3
500	1.25	0.380	0.405	+7	1005	1.98	0.316	0.281	-11
1000	2.00	0.244	0.241	-1	1258	2.30	0.265	0.236	-11
1840	3.20	0.165	0.152	-8	1470	2.59	0.238	0.210	-12
					1846	3.08	0.211	0.176	-17

^aThe compressibility factor was read off the Nelson-Obert generalized compressibility charts (Ref. 2, pp. 50-52 and Ref. 9), using the pseudo-critical constants to calculate T and P . The pseudo-critical constants were calculated using Eqs. (44) and (45).

^b P and Z found by iteration on the equation $P = ZT \rho_A / 273$ (Z , 1 atm, 273 K) using the Nelson-Obert charts and experimental densities in amagats ρ_A reported in Ref. 21.

Table 6D. D in cm^2/s at various pressures of CO_2 - $^{14}\text{CO}_2$.

T _r = 348 K (Ref. 22)					T = 373 K (Ref. 23)				
P (atm)	Z ^a	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)	P (atm)	Z ^a	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)
1	0.997	—	146.6	—	1	1	—	169	—
10	0.968	15.2	14.5	-5	21.61	0.942	7.68	7.61	-1
20	0.938	7.48	7.13	-5	41.29	0.896	3.90	3.89	0
30	0.907	4.81	4.68	-3	71.11	0.797	2.09	2.13	+2
40	0.867	3.51	3.44	-2	102.2	0.725	1.32	1.42	+8
50	0.835	2.71	2.70	-0.4	135.7	0.65	0.89	1.01	+13
					171.7	0.59	0.64	0.75	+17
					204.8	0.58	0.50	0.62	+24

^aThe compressibility factor was read off the Nelson-Obert generalized compressibility charts (Ref. 2, pp. 50-52 and Ref. 9), using the pseudo-critical constants to calculate T_r and P_r . The pseudo-critical constants were calculated using Eqs. (44) and (45).

Table 6E. D in cm^2/s at various pressures of CO_2 - Ar.

T = 298 K (Ref. 24)									
$N_{\text{Ar}} = 0.497$					$N_{\text{Ar}} = 0.719$				
P (atm)	Z^a	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)	P (atm)	Z^a	$10^3 D_{\text{expt}}$	$10^3 D_{12 \text{ calc}}$	Error (%)
1	1	—	143	—	1	1	—	143	—
14.48	0.962	8.77	9.74	+11	14.61	0.972	9.40	9.70	+3
20.3	0.950	6.09	6.91	+13	20.4	0.968	6.54	6.93	+6
61.9	0.85	1.84	2.15	+17	60.3	0.92	2.17	2.29	+6
102.7	0.75	1.00	1.22	+22	102.6	0.87	1.26	1.31	+4
146.1	0.68	0.65	0.81	+25	151.6	0.83	0.80	0.87	+9
199.7	0.67	0.45	0.59	+31	200.4	0.82	0.62	0.65	+5
					247.5	0.84	0.50	0.54	+8
T = 348 K (Ref. 24)									
1	1	—	190	—	1	1	—	190	—
14.44	0.980	11.7	13.1	+12	13.83	0.985	13.0	13.7	+5
52.1	0.923	3.14	3.52	+12	59.2	0.96	3.40	3.15	-7
101.0	0.88	1.57	1.77	+13	112.5	0.94	1.53	1.64	+7
153.3	0.84	0.98	1.14	+16	151.1	0.92	1.16	1.22	+5
200.4	0.82	0.74	0.86	+16	196.5	0.92	0.88	0.93	+10
					247.1	0.93	0.70	0.74	+6

^aThe compressibility factor was read off the Nelson-Obert generalized compressibility charts (Ref. 2, pp. 50-52 and Ref. 9), using the pseudo-critical constants to calculate T_r and P_r . The pseudo-critical constants were calculated using Eqs. (44) and (45).

The following examples were chosen:

$\text{N}_2\text{-H}_2$ and Ar-H_2 (Tables 6A and 6B), because the data for these systems were also available for high temperatures and low pressures.

$\text{CH}_4\text{-}^{14}\text{CH}_4$ (Table 6C), because this system has the highest pressures (1.8 kbar) for which D_{12} has been measured.

$\text{CO}_2\text{-}^{14}\text{CO}_2$ and $\text{CO}_2\text{-Ar}$ (Tables 6D and 6E), because they are of interest for the proposed LLL experiment.

With the exception of the data of Balenovic et al.¹² for $\text{N}_2\text{-H}_2$ and Ar-H_2 and the cases where $Z < 0.7$, all calculated values agree with experiment to $\pm 20\%$ or less.

The data of Balenovic et al.¹² are systematically low with respect to the calculated values, and the one overlap at 680 atm is equally low with respect to the experimental value of Berry and Koeller¹⁹ adjusted for the temperature difference of 15 K. The Balenovic data could be suspect on this ground, but were included because they go to the second highest pressure (1.4 kbar). If their data were correct, good estimated values would be obtained by adjusting Eq. (46) to one datum point because the errors are systematic.

The $\pm 20\%$ agreement is very encouraging, especially because it is valid for the $\text{CH}_4\text{-CH}_4$ system measured at the highest pressure (1.84 kbar). However, most of the results are at a few hundred bars and there is no real certainty as to how effective our approximations will be at 50 to 250 kbar. It is clear that experimental data are vitally needed at higher pressures (10 to 20 kbar seems possible) to test kinetic theory; molecular, dynamic and Monte Carlo calculations; and empirical estimation formulas such as Eq. (46).

VI. Sample Calculations

On the assumption that Eq. (46) gives at least plausible values of D_{12} at higher temperatures and pressures, we have calculated diffusion coefficients for some cases for which enough PVT data is available to compute Z .

Figure 1 is a semi-log plot of the diffusion coefficients of $\text{H}_2\text{O-H}_2\text{O}$ along the Hugoniot that starts at 298 K and 1 atm and ends at 3420 K and 450 kbar.²⁵ The D 's go through a minimum. The general shape of this curve is of interest in the energy release problem mentioned earlier.

Figure 2 is a log-log plot of D_{12} for $\text{H}_2\text{O-H}_2\text{O}$ along various isotherms from 293 to 1273 K (with three extrapolated points at 2273 K) and pressures to 250 kbar. The PVT data are from Refs. 25 and 26. Note the curvature in the isotherms. This is a direct result of the $R(Z)$ factor, which for example has the value 2.55 ($Z = 32$) at 773 K and 250 kbar.

Figure 3 contains isotherms for $\text{CO}_2\text{-CO}_2$ but at lower temperatures and pressures (up to 4 kbar) than Fig. 2. The PVT data are from Juza et al.²⁷ The higher pressure portion of this curve is at the lower end of the region in which the LLL high pressure diffusion experiment is proposed.

Fig. 1. A semi-log plot of the diffusion coefficients of $\text{H}_2\text{O} - \text{H}_2\text{O}$ vs the pressure; Z is from PVT and Hugoniot data given in Ref. 25.

Fig. 2. A log-log plot of the diffusion coefficients of $\text{H}_2\text{O} - \text{H}_2\text{O}$ along various isotherms and at various pressures; PVT data are from Refs. 25 and 26.

Fig. 3. A log-log plot of the diffusion coefficients of $\text{CO}_2 - \text{CO}_2$ along various isotherms and at various pressures.

References

1. H. Cheung, Kinetics of Energy Release of Heterogeneous High Explosives, Lawrence Livermore Laboratory, Rept. UCID-15962, (1971).
2. R. C. Reid and T. K. Sherwood, The Properties of Gases and Liquids (McGraw-Hill, New York, 1966), 2nd ed.
3. J. O. Herschfelder, C. F. Curtiss, and R. B. Bird, Molecular Theory of Gases and Liquids (John Wiley and Sons, New York, 1954).
4. J. S. Rowlinson, Liquids and Liquid Mixtures (Plenum Press, New York, 1969), 2nd ed., p. 243.
5. J. A. Barker, M. V. Bobetic, and A. Pompe, Molecular Physics **20**, 347 (1971).
6. I. Amdur, AIChEJ. **8**, 521 (1962).
7. S. Chapman and T. G. Cowling, The Mathematical Theory of Non-Uniform Gases (Cambridge University Press, Cambridge, 1970), 3rd ed.
8. N. F. Carnahan and K. E. Starling, J. Chem. Phys. **51**, 635 (1969).
9. L. C. Nelson and E. F. Obert, Chem. Eng. **61** (July), 203 (1954).
10. J. H. Dymond and B. J. Alder, J. Chem. Phys. **48**, 343 (1968).
11. J. H. Dymond and B. J. Alder, J. Chem. Phys. **52**, 923 (1970).
12. Z. Balenovic, M. N. Myers, and J. C. Giddings, J. Chem. Phys. **52**, 915 (1970).
13. I. Amdur and E. A. Mason, Phys. Fluids **1**, 370 (1958).
14. T. R. Marrero and E. A. Mason, J. Phys. Chem. Ref. Data **1**, 3 (1972).
15. F. L. Swinton in Diffusion Processes: Proceedings of the Thomas Graham Symposium (Gordon and Breach, London, 1971), vol. 1, p. 53.
16. T. A. Pakurar and J. R. Ferron, J. Chem. Phys. **43**, 2917 (1965).
17. O. N. Holsen and M. R. Strunk, Ind. Eng. Chem. Fundamentals **3**, 143 (1964).
18. T. A. Pakurar and J. R. Ferron, Ind. Eng. Chem. Fundamentals **5**, 553 (1966).
19. V. J. Berry and R. C. Koeller, AIChEJ. **6**, 274 (1960). Assumed $N_1 = N_2 = 0.5$.
20. R. Dawson, F. Khoury, and R. Kobayashi, AIChEJ. **16**, 725 (1970).
21. P. H. Oosting and N. J. Trappeniers, Physica **15**, 418 (1971).
22. S. Takahashi and H. Iwasaki, Rev. Phys. Chem. Japan **38**, 28 (1968).
23. H. A. O'Hern and J. J. Martin, Ind. Eng. Chem. **47**, 2081 (1955).
24. S. Takahashi and H. Iwasaki, Bull. Chem. Soc. Japan **41**, 1573 (1968).
25. M. H. Rice and J. M. Walsh, J. Chem. Phys. **26**, 824 (1957).
26. C. W. Burnham, J. R. Holloway, and N. F. Davis, Thermodynamic Properties of Water to 1000°C and 10000 Bars, Geol. Soc. Am., Boulder, Colo., Paper 132 (1969).
27. J. Juza, V. Kmonicek, and O. Sifner, Physica **31**, 1735 (1965).

SHOCK VELOCITY MEASUREMENTS,
DEVELOPMENT OF HAYES' TECHNIQUE

In the study of capacitor-type shock detectors, dielectrics were placed between metal electrodes. We looked for the piezoelectric effect in plastic sheets. If present, it is masked by the effect of a charged surface moving as the shock wave strikes it. The movement of the charge layer into an air gap gives much more signal than when this gap is filled, for instance, with oil. The moving charge changes internal capacitances and induces charges on the electrodes which are seen as transient voltage pulses. The capacitors, with plastic film dielectric, were tested by placing them between the halves of a Hopkinson split-bar apparatus. The surface of the film was charged in place by temporarily applying 300 V across the electrodes. The fast amplifier (line drive) was then connected. The bars were struck by an air-driven projectile. The resulting voltage pulse was recorded as shown in Figure 1. These results are explained by a model involving the movement of a charge sheet as discussed in Appendix 1.

To investigate the profile of the pressure pulse in composite HE's, we have adopted a technique developed by B. Hayes.^(1,2) It consists of a stack of plastic discs separated by air gaps. An electrode at the end serves as an "antenna." As the shock wave reaches the surface of each disc an electrical impulse transmitted to the "antenna" is recorded on an oscilloscope. We found that the magnitude of the pulse in the NM-AP composite is not large enough to give unambiguous signals using this method as first proposed. However, from experience with the capacitor shock detectors discussed above we believe the electrical impulse is caused by movement of a charge layer at the plastic-air

interface. (See Appendix.) If so, increasing the surface charge density of each disc should increase the magnitude of the output pulses and thus achieve a much more favorable signal-to-noise ratio.

Each disc was charged by exposure to positive ions in air from a 76 μm dia wire at 5 kV. Freshly charged, the surface charge density is $10.2 \mu\text{C}/\text{m}^2$, producing an electric field at the surface of 1.2 MV/m. This is 40% of the corona breakdown field (3 MV/m). After handling the discs in a manner similar to that to be used in the assembly of the final stack, the charge dropped to 20% of the original. This is still considerably higher than if the discs had been used without intentional charging.

Figure 1. Voltage across capacitor resulting from projectile striking Hopkinson split-bar within which the capacitor was placed.

a. "Input" electrode charged to +300 V by applying battery to electrodes.

b. "Input" electrode charged to -300 V.

APPENDIX 1.

Model of charged dielectric, enclosed between sheet electrodes.

Consider a dielectric, with air gaps, enclosed between two sheet-metal electrodes. The charged surfaces of the dielectric may be the same (electret sheet) or different (and hence having a net charge). The two charge sheets will be considered separately and then added together (superposition principle). The pressure wave will close or partially close the 1st gap, then the 2nd gap.

As an example, take the 1st gap between positions 0 and 2, the dielectric between 2 and 4, and the 2nd gap between 4 and 6. The dielectric constant will be taken as 1 to simplify the calculation. V refers to the potential at the

charge sheet under consideration; Q is its charge. Each partial capacitor voltage is considered to be V . This holds as long as the voltage drop across electrodes 1 and 2 is small compared with V .

Before the pressure wave strikes, the potential of both electrodes is zero. Considering the negative sheet,

$$C_1 = \frac{\epsilon_0 A}{d} = \frac{\epsilon_0 A}{2}, \quad C_2 = \frac{\epsilon_0 A}{4},$$

and the compensating charge on electrode 1 is given by

$$Q_1 = C_1 V, \quad Q_2 = C_2 V, \quad Q = Q_1 + Q_2$$

$$V = \frac{Q_1}{C_1} = \frac{Q_2}{C_2} = \frac{Q - Q_1}{C_2}$$

$$Q_1 = \frac{C_1 Q}{C_1 + C_2} = \frac{d_2 Q}{d_1 + d_2}$$

Initially $d_1 = 2$, $d_2 = 4$.

$$\text{So } Q_1 = \frac{4Q}{2+4} = 0.667 Q, \quad Q_2 = Q - Q_1 = 0.333 Q.$$

Assume the 1st stage electrode 1 is moved from $x = 0$ to $x = 1$

$$\therefore d_1 = 1, \quad d_2 = 4$$

$$\text{So } Q_1 = \frac{4Q}{1+4} = 0.8 Q \text{ and } Q_2 = 0.2 Q.$$

Comparing with the initial state above:

$$\Delta Q_1 = (0.8 - 0.667)Q = 0.133 Q$$

$$\Delta Q_2 = (0.2 - 0.333)Q = -0.133 Q$$

Taking the difference gives $0.266 Q$ charge transferred. Electrode 2 becomes positive.

Assume the 2nd stage of compression moves the negative side of the dielectric from x-position 2 to x-position 3 then $d_1 = 1$, $d_2 = 3$ and

$$Q_1 = \frac{3Q}{1+3} = 0.75 Q, Q_2 = 0.25 Q.$$

Compared with the result of the 1st stage

$$\Delta Q_1 = (0.75 - 0.8)Q = -0.05Q$$

$$\Delta Q_2 = (0.25 - 0.2)Q = 0.05 Q$$

Taking the difference gives $-0.1 Q$ which reduces the charge transferred in the 1st stage to $(0.266 - 0.1)Q = 0.166 Q$.

The equal positive sheet will be symmetric but with the stages reversed (in the sense that the d magnitudes are reversed). Its charge contribution will also be $0.166 Q$. Thus the total charge transfer will be $0.332 Q$ in the direction to make electrode 2 positive. If the dielectric (electret) is reversed, electrode 2 will become negative.

REFERENCES

1. B. Hayes, "The Detonation Electric Effect," J. Appl. Phys., Vol. 38, pp. 507-511, Feb. 1967.
2. B. Hayes, "Electric Signals Generated by Shock and Detonation Waves," presented at the Western States Section of the Combustion Institute, Oct. 28, 1968.

PART B

PARTICIPATION OF LLL IN JSEXP

TASK B: CHARACTERIZATION OF ECX FOR CONVENTIONAL MUNITIONS

K. Scribner

J. Hallam

GLOSSARY

ECX	Extrusion Cast Explosive
DINOL	2,2,8,8-tetranitro-4,6-dioxa-1,9-nonane diol.
FEFO	<u>bis</u> (2-fluoro-2, 2-dinitroethyl)formal
HMX	1,3,5,7-tetranitro-1,3,5,7-tetrazacyclooctane
AFNOL	Polymerization product of DINOL and 4,4-dinitropimeloyl chloride
FEFO SOL	35 wt% FEFO in ethyl acetate solution
HMDI	Hexamethylene Diisocyanate
RX-08-BA	HMX/FEFO/AFNOL (78/18.6/3.4 wt.%)

SUMMARY

The objective of this program is to determine if improved homogeneity, increased energy and improved filling techniques will significantly upgrade the performance of shaped charges. The explosive used in the initial tests is an extrusion cast explosive designated RX-08-BA. The shaped charges are 2.2 in. diameter precision-made units, exactly the same as units made and tested with RDX and Composition-B by Firestone Tire and Rubber Co.⁽¹⁾

Test firings were made at 0.5, 1.5, 3, 6, 9, 12 and 20 charge diameter (CD) standoffs. The penetration vs. standoff curve developed from the test data shows that between 4 and 12 CD standoffs, the RX-08-BA produced significantly deeper penetrations than either RDX or Composition-B. At standoffs below 1.5 CD and greater than 15 CD, however, the penetrations from RX-08-BA were less than penetrations achieved with the other two explosives. It was determined from flash X-ray diagnosis that RX-08-BA charges developed higher jet tip velocities, but correspondingly faster jet breakup times than were achieved with either RDX or Composition-B.

INTRODUCTION

We have developed recently at LLL a new explosive technology to produce extrusion cast explosives (ECX's). We are studying the application of this technology to the development of improved shaped charge performance. Our work will include formulation studies of ECX's that can provide improved performance at acceptable costs and the firing of test models of shaped charges to obtain the performance data. ECX has some attractive features, including: ease of formulation, can be extruded like a paste, good energy, relatively good sensitivity, and superior mechanical properties in the cured state.

A detailed description of the preparation, loading and inspection of shaped charges containing RX-08-BA has been previously reported.⁽²⁾ This

report also presented a description of the experimental set-up for test firings, and data from tests up to 6 CD standoffs. Subsequent work has included tests at 9, 12, and 20 CD standoffs with flash X-ray diagnosis of the jets. Additionally, a single shot was fired at 20 CD standoff with a high speed framing camera record of the jet travel.

TEST FIRING

The basic target setup for test firing with flash X-ray diagnosis is shown in Figure 1. The overall setups for tests with two and three flash X-rays are shown in Figures 2 and 3, respectively. These tests were conducted at the Ravenna Army Ammunition Plant by personnel from the Firestone Tire & Rubber Co., Defense Research & Products Division.⁽³⁾

The total penetration from each shot was measured, and the hole volumes were determined by filling with water measured from a burette. In cases where the hole was partially plugged with the jet slug, the targets were X-rayed using two orthogonal views and the volume was calculated from the X-ray films. The results are summarized in Table I and plotted in Figure 4.

DISCUSSION:

Jet tip velocities were calculated from the flash X-ray films, and are summarized in Table II. These values are close to the detonation velocity of RX-08-BA which is 8.65 km/sec.⁽⁴⁾ Typical film records are shown in Figures 5 and 6. The jet tip velocity was also determined from a test at 9 CD standoff using foil switches for timing measurements. A high speed framing camera record of this particular shot recorded what appears to be an expanding hyperbolic shock front rather than the jet. By contrast, a similar test fired in vacuum (1 mm Hg, abs) (133 Pa), and at 20 CD standoff clearly showed the jet movement.

A model 189B framing camera was used in this test, and the jet tip velocity was determined by the plot shown in Figure 7.

Jet breakup times were determined by plotting the distance between the individual particles vs. time and extrapolating the zero distance. These plots fall in the general range of 80 to 100 μ sec. However, none of the radiographs showed a separation of the jet into finite particles up to 84 μ sec, although separation has obviously started. A value of 90 μ sec is considered to be as accurate a value for jet breakup time as can be determined from existing records.

CONCLUSIONS

It has been demonstrated that there is a significant improvement in the performance of shaped charges loaded with RX-08-BA over charges loaded with either RDX or Composition-B, between 4 and 12 CD standoffs. High quality, homogeneous charges are obtained with simple, straightforward loading techniques as previously reported.

Consideration should be given modifying the ECX formulation to produce a slower jet, resulting in a longer breakup time, and thereby improving the penetration performance at longer standoffs. An existing computer code (HEMP) could be useful in this study.

Fig. 1. Typical test setup.

Fig. 2. Schematic side view of open test site, 2 flash x-rays.

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TOP VIEW
Radiographic setup
on lower level

SIDE VIEW

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Fig. 3. Schematic side view of large test site, 3 flash x-rays.

Figure 4: Shaped Charge Performance
 2.2 inch diameter, 42° copper cone,
 1 cone diameter explosive head
 (Average values)

49.1 μ s

83.4 μ s

Figure 5: Radiographs of Shaped Charge Jet - Charge No. 13

Figure 6: Radiographs of Shaped Charge Jet - Charge No. 16

Figure 7: Distance of Jet Tip Travel in Vacuum vs. Time.

TABLE I

PENETRATION AND HOLE VOLUME VS. STANDOFF DATA

Standoff		Charge No.	Penetration		Volume, Cubic Inches
Charge Diameters	Inches		Charge Diameters	Inches	
0.5	1.1	1	3.52	7.74	3.11
		2	3.42	7.52	3.66
		<u>3</u>	<u>3.53</u>	<u>7.78</u>	<u>3.90</u>
		Ave.	3.48	7.68	3.54
1.5	3.3	4	5.34	11.76	4.02
		5	5.12	11.28	3.97
		<u>6</u>	<u>4.78</u>	<u>10.51</u>	<u>3.90</u>
		Ave.	5.09	11.18	3.97
3.0	6.6	7	5.91	13.00	3.54
		8	5.08	11.17	3.48
		<u>9</u>	<u>6.37</u>	<u>14.02</u>	<u>3.84</u>
		Ave.	5.78	12.73	3.60
6.0	13.2	10	7.00	15.40	3.17
		11	6.90	15.18	3.36
		12	6.96	15.32	3.36
		<u>18</u>	<u>6.97</u>	<u>15.35</u>	<u>3.23</u>
		Ave.	6.96	15.31	3.28
9.0	19.8	23	6.06	13.34	2.06
		19	5.76	12.67	2.87
		20	6.88	15.14	2.84
		<u>21</u>	<u>7.05</u>	<u>15.52</u>	<u>2.93</u>
		Ave.	6.44	14.16	2.68
12.0	26.4	22	5.79	12.74	2.58
		13	5.79	12.74	2.31
		<u>14</u>	<u>7.10</u>	<u>15.62</u>	<u>2.56</u>
		Ave.	6.22	13.71	2.48
20.0	44.0	15	3.40	7.48	2.32
		16	3.09	6.80	2.87
		<u>17</u>	<u>2.24</u>	<u>4.93</u>	<u>2.39</u>
		Ave.	2.91	6.40	2.52

TABLE II
JET TIP VELOCITIES

<u>Standoff</u> <u>CD</u>	<u>Charge</u> <u>No</u>	<u>Jet Tip Velocity</u> <u>km/sec</u>	<u>Medium</u>	<u>Diagnosis</u>
9	23	8.95	Air	Pins
12	13	8.76	Air	X-ray
12	14	8.52	Air	X-ray
20	15	8.89	Air	X-ray
20	16	8.85	Air	X-ray
20	17	8.71	Air	X-ray
20	26	8.94	Vacuum	Framing Camera

REFERENCES

1. Final Report, Shaped Charge Scaling Study, Contract No. 8AAA21-68-C-0124.
The Firestone Tire & Rubber Co., Defense Research Division, Akron Ohio,
March 1970.
2. Participation of LLL in JSEXP, Part B: Characterization of ECX for
Conventional Munitions, UCID-16424, Lawrence Livermore Laboratory,
Livermore, CA, 30 December, 1973.
3. Purchase Order No. 3771105, Lawrence Livermore Laboratory, 9 Oct. 1973.
4. ECX Detonation Velocities, Lawrence Livermore Laboratory Memorandum,
J. Hallam, 13 Feb. 1973.

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