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CONFERENCE

Notes and Comments on the Round-Table Conference on Detonations

Colorado Springs, June 20-21, 1972

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scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

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Compiled by

W. C. Davis

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ABSTRACT

Notes, comments, questions, and abstracts furnished by attendees at the informal Round-Table Discussion on Detonation are presented to provide a substitute for the usual Proceedings.

I. INTRODUCTION - W. C. Davis (LASL)

The "Round-Table Conference on Detonations" was organized by M. J. Kamlet of Naval Ordnance Laboratory and R. R. McGuire of the Air Force Academy. Two paragraphs from their letter of invitation defining their conception of it follow:

> "2. Subjects to be discussed at the conference will include (but will not necessarily be limited to):
>
> a) Mechanisms of shock initiation to detonation and deflagration to detonation transition.
> b) The C-J hypothesis, true or false?
> c) The nature of the detonation state (steady state?).
> d) Ideal vs non-ideal detonations.
> e) The "slow reactors": aluminum, inorganic nitrates, inorganic perchlorates.
> f) Equations of state for detonations.
> g) The chemistry of detonations.
> h) Detonation calculations.
>
> Emphasis is to be on theory and mechanism rather than on hardware and detailed design of experiments (except, however, where differing interpretations of the experiment have led to important differences in theoretical conclusions).
>
> 3. The conference will have neither a fixed agenda nor formal presentation of papers. Each of the above subjects is characterized by the fact that unresolved differences of opinion on basic questions exist among knowledgeable and well-respected researchers in the field. Conference participants with a variety of viewpoints and backgrounds will be encouraged to engage in free cross-discussion, so that these differences may be fully aired and, hopefully, some progress made toward their resolution."

Since there were no formal papers, there could be no issuance of Proceedings. It seemed to me a waste to let the memory of the valuable discussions be stored only in a few brain cells, so I have collected here some notes made by the participants. These have not been edited or altered in any way, except that I have rephrased some of the brief questions, and abstracted from some of the rough notes which were sent to me. I have tried not to inject my own ideas. The compilation is somewhat repetitive, but perhaps the more valuable for that, because it shows the differences in points of view of the various writers.

II. NOTES, COMMENTS, QUESTIONS AND ABSTRACTS

J. HERSHKOWITZ (PICATINNY)

These are notes in connection with a round-table conference on detonations which was held at the Frank J. Seiler Research Laboratory (AFSC), U.S. Air Force Academy in Colorado on the 20th and 21st of June 1972.

1. Dr. Kamlet of NOL indicated that gamma is a strong function of the chemistry, that is, of the composition of the explosive products. His derivation of a value of gamma was based upon his previously published approach to the calculation of the Chapman-Jouguet properties of explosives. The participants recognized that gamma is not a constant but a complex function of volume related to the intermolecular potentials. Its behavior, for example, in coupling to loads is reflected in the JWL equation of state used by Livermore. Gamma changes even when the BKW equation of state is used along the isentrope. However, it is recognized that for approximate calculations one can use a gamma law equation of state. All participants have done this on occasion when the desired results are sufficiently approximated by this method. I do not see the advantages of Kamlet's shortcut techniques over the use of the TIGER, RUBY, or BKW computer programs. To the extent that the assumptions or input data are incorrect as fed into the computer programs, they should be corrected. It is not necessary to use a hand-type calculation. On the other hand the work of Kamlet with the shortcut method does give some insight into the differences between explosives.

2. A discussion took place with respect to the experimental measures of the peak pressure in the detonation wave. Los Alamos uses the technique of measuring the velocity of the free surface of an aluminum plate in contact with the explosive as a function of the thickness of plate which is reduced in thickness and finally asymptotically one has a free surface velocity for zero thickness. From this one deduces the peak pressure that existed at the interface between the explosive and the aluminum. Livermore observes the shock velocity generated in Lucite by using a stack of Lucite plates and deducing by extrapolation the particle velocity at the interface. In general, one recognizes that the peak pressure depends upon the length of the explosive, the overdrive of the explosive, and the effect of the reaction zone interior. This last is in the sense that the pressure is a function of the degree of completion of the reaction and as you approach the Chapman-Jouguet pressure to get the last increment (the last delta p toward the Chapman-Jouguet pressure) the degree of reaction must go, let us say, from 99.5% to 99.9%. The point is that one never gets complete reaction. It would be interesting to study the peak pressure for an explosive in which the detonation zone had been lengthened by the addition of inerts for the condensed phase or by diluents in the liquid phase in such a way that we had a rate dependent content. Sternberg of NOL referred to a paper he had published having to do with the relationship between the possibility of steady state existing and the order of the reaction. His presentation may be found in Astronautica Acta of 1970 Volume 15, pages 359 to 369 under the title "On the Mathematical Theory of the Chapman-Jouguet State".

3. A discussion ensued about the proper way of treating the coupling of explosives to loads in so far as the equation of state is concerned. My own viewpoint of this long discussion is that one must use the JWL equation of state in the problems where the lower part of the isentrope (as determined by cylinder and sphere tests) is a proper description of the explosive action in the coupling. On the other hand when one has problems in which the upper half of the isentrope is concerned, as in the case of small detonators or shaped charges, it is very important to know the peak pressure and the shape of the isentrope from this peak pressure.

4. Dr. Jacobs of NOL presented the equation of state which he has recently developed. This will be called the JCZ equation for Jacobs, Cowperthwaite, and Zwisler and will be published shortly. A presentation is available in the report submitted on the explosive fill program. There followed a discussion on what could be done to improve the equation of state and some of the troubles that existed. Wildon Fickett of Los Alamos suggested some basic experiments. For example, he wished to work with liquid oxygen and liquid ozone and to obtain shock Hugoniots under these conditions. He would use a calibration obtained from the liquid oxygen for the liquid ozone to prove the nature of the potential that he had assumed. I raised the possibility of doing static compression of gases to approach the pressures found in the Chapman-Jouguet state and particularly those along the isentrope. Dr. Jacobs

of NOL stated that if one does just static compression one will not be able to reach the repulsive state region and it is the description of the repulsive state region which is critical for a proper equation of state. Others concurred. Dr. Lee of LLL pointed out that shock work on individual gases is available and he made reference to the Van Thiel (LLL) compilation. Drs. Cowperthwaite and Shaw of SRI pointed out that they have developed an empirical way to fit Hugoniot data for liquids which provides curvature at low pressures and makes the limit correspond with the sound speed. This is otherwise not reached when the ordinary straightline fits are used. Dr. Finger of LLL described the series of experimental results which are being obtained on explosives. This includes not only detonation velocity but pressures and other properties. The data will serve as a base from which it will be possible to deduce the efficiency of the description of the explosives. I raised the question of the use in the computer programs of carbon in the form of graphite. The general feeling at first was that this was indeed a problem; however, as the discussion continued the point of view was achieved that it is quite possible that graphite could be formed in the time allowed to reach the Chapman-Jouguet state. This does not correspond to my own viewpoint.

5. Dr. Milton Finger described the work with blasting agents underway at Livermore. They have been using a special aluminum provided by Alcoa which has a high surface area, 14,000 centimeter square per gram. It is 99.5% aluminum and one-tenth percent stearate and is called Aluminate. The objective in the addition of this material is to act as a trigger to get non-detonable diameters to detonate, that is, to reduce the failure diameter. Dr. Watson of the Bureau of Mines commented that this approach in his experience does not do any good except in the case of slurries. At Livermore they have also been pursuing a computational approach for non-ideal explosives in relation to coupling to loads. They use two JWL equations, one representing a material which has undergone 25% reaction and the other which has undergone a 100% burn. They then use a ramp which represents a linear combination between the two equations and adjusts the time during which this linear combination goes between the two extremes. They have found that their ability to accurately predict the coupling of the explosive to the load, that is the load behavior, is very sensitive to the ramp time chosen. Their hope is that a unique ramp time for a particular explosive will be applicable to many different cases. To date they have had a measure of success with this approach. The work at Livermore is being done by Dr. Henry Chung in cooperation with Dr. Ed Lee.

6. In a discussion of low velocity detonation Dr. Shaw of SRI pointed out that in the case of two organic explosives of supposedly similar structure low velocity detonation was obtained for the first 1-1 dinitroethane whereas it could not be obtained for the second which was 1-1 dinitropropane.

7. The next topic was Transverse Waves. Dr. Frey of BRL presented the results obtained by Dr. Phil Howe. Dr. Davis of Los Alamos felt that these results were not evidence of transverse waves in the condensed explosives but represented an edge effect. In the discussion it was suggested that one could generate disturbances and observe the effect of these disturbances, that is, whether they would grow or die out by inserting a mesh into the explosive. This had been done by Dr. Davis and he referred to different meshes that he had used in the past. Dr. Fickett of Los Alamos suggested that the work done by White in the case of gases was most precise and effort should be made to emulate it in the area of liquids.

8. Dr. Fickett referred to his work and that of Wood and Erpenbeck with respect to the possible modes of propagation which can exist. He showed a plot with ordinate the fraction achieved of one reaction and the abscissa representing the fraction achieved of another reaction. The starting point would be the origin where neither reaction (considered possible) had started and he pointed out that there was a Chapman-Jouguet point which could be approached from many final directions, all from the general direction of the starting point. But there also existed a saddle point in the vicinity which was kinetically dependent and one could not indicate in advance which solution would be obtained. He stated further that the same type of plot would exist in which the diameter of the charge takes the role described as one of the reactions. The same

type of plot could be made with one reaction as ordinate and a diameter say as the abscissa. Further he showed a plot of the detonation velocity as a function of diameter which was double-valued in detonation velocity. His presentation refers back to published work and can be read in full in a series of papers published from Los Alamos. Dr. Kamlet of NOL indicated that such theories could be checked by the use of explosives which were similar in thermodynamic respects but vastly different with respect to kinetics and that he could provide the names of such explosives to anyone who was interested.

9. Dr. Cowperthwaite of SRI presented calculations which he has made and published as an SRI report. However, he assumes that the particle velocity gradient is a function of the shock velocity (or of any other shock parameter) and then proceeds to consider a reactive step shock under the assumed conditions.

10. Dr. M. Fulk of Livermore talked about the changes in activation energy of explosives which could be achieved by the use of electric fields and mechanical history. He referred to striking an explosive in advance at low levels actually changing the activation energy. The general feeling was one of disbelief. I used this occasion to make the group aware of the work under way at the Explosives Division of FRL in the area of altering properties, that is, initiation properties of explosives by consideration of the Solid State properties and attempts to alter these. I was asked later by Dr. Fickett of Los Alamos about this subject and referred him to Dr. Fair and extended an invitation for him to visit and discuss this with Dr. Fair and Dr. Gora in greater detail. I also mentioned that we were doing molecular orbital calculations with an eye to using this type of calculation for a better understanding of the initiation properties of explosives and the co-volume of the product species.

11. The meeting was most valuable for the interchange of viewpoints, for the leads presented, and additional meetings of this type should occur.

* * *

M. FINGER (LLL)

Rule for Gamma - M. Kamlet: Kamlet presented a correlation of gamma as a function of density. As expected for all CHNO HE's, there appeared to be a good correlation. Exceptions were Nitroguanidine, Hydrazine nitrate (HNO), benzo trifuroxane (CNO), and trinitro triazido benzene (CNO). He presented the data with the assumptions that C-J theory must apply and charge geometry was relatively unimportant. CHNO HE's within a narrow grouping of oxygen balance and density all appear to behave normally. CHNO HE's with oxygen balances well below CO or above CO_2, HNO, CNO, HNF, CHNOF explosives, etc., all behave significantly differently suggesting that our thermo hydro-codes or their input require fixing. Although it is helpful at times to take things apart and examine them, the whole relationship of Γ vs. ρ seemed like a circular argument.

Later on Finger presented data on the series of explosives of varying elemental compositions. This is being done to provide better experimental data for refining thermo-hydro codes such as BKW, RUBY, TIGER.

What Do We Mean By C-J State - Sternberg: Sternberg presented an argument that U+C depends on lengths of charge. The details are given in his paper presented in Astronautica Acta, Vol. 15, pp. 359-369, 1970, Pergamon Press.

General Discussion on Detonation Pressure Measurements - LLL, LASL: Craig presented more u_{fs} vs. X plots for varying thickness metal plates. LLL presented its Plexiglas shock velocity data. The usual discussion of scaling problems, treatment of data, significance of a few % which could indicate buildup, etc., ensued. No new light shed on this old argument.

Finger presented data on solid and liquid TNT at the same density. Once the enthalpy correction for temperature was made the solid and liquid behaved identically in detonation velocity and cylinder test expansion.

Carbon in Explosives - Hershkowitz: Hershkowitz wondered about the state of free carbon in the detonation. Was there sufficient time for carbon to condense? to what physical state?; and what ΔH_f^o should be assigned to C as a detonation product. The general opinion was that C_n (i.e., disordered graphite) does form with a ΔH_f^o of ∿ 10 - 15 kcal/mole.

EOS - Jacobs: Jacobs presented his status report on an attempt to establish an EOS for the detonation products from first principles. This has led to the JCZ (Jacobs, Cowperthwaite, Zwisler) EOS.

EOS - Fickett: Fickett did not believe that the EOS was the main thing that's wrong in the description of a detonation. At present, we do not understand in detail what goes on in a detonation. He discussed Phermex experiments with foils that measure X,t in order to learn about flow conditions. He proposed Shock Hugoniot measurements on liquid O_2, and then suggested performance measurements on liquid O_3. Hopefully this simple chemical system would shed light on the state of a detonation.

EOS - Lee: Lee pointed out that Burnham's static data (Penn-State) to 9 kbar does show structure on the isentrope as shown in Fig. 1. He also pointed out that Van Thiel's Compendium had some shock data that may be of use. A discussion followed about the nature of the potential function. Would data on van der Waal's materials, that is, Hugoniot data, show curvature in the u_s-u_p relationship, especially for u_p near zero. Materials such as N_2, Argon, CH_2, H_2O, and CO_2 are all in this class.

EOS - Cowperthwaite, Shaw: Cowperthwaite presented data on the sound velocity in H_2O. They had developed an empirical, Universal Hugoniot and tested it with CCl_4, glycerol, etc., in order to obtain a calibrated EOS. Their treatment includes curvature and constrains $u_s \rightarrow C_0$ as $u_p \rightarrow 0$. In a progress report on TIGER, he mentioned that they were putting various EOS (including JCZ) into TIGER.

Initiation - F. Walker: Walker presented some data that indicated some small decomposition in nitromethane when shocked below its initiation threshold. He reported seeing changes in the transmitted shock velocity, which implied 1-3% decomposition. He thought this indicated some reaction in the shock front.

Aluminized HE's - Non-Ideal HE: Finger presented data on various aluminized HE's. A composition containing TATB, Al, and TNM was fired in a cylinder test and the resultant cylinder wall velocity indicated nearly all the theoretical energy had been produced. Additional work on commercial slurry blasting agents was reviewed. Watson of the Bureau of Mines puzzled over the aluminum behavior. In slurry blasting agents it acts as both a sensitizer and a source of energy.

Sternberg reviewed the problem of calculating aluminized explosives. He stated that: (1) The first point of view - (presented by LLL) is that Al does not react in the shock front or reaction zone, but feeds in energy later. (2) The second point of view (Cook & Mader) - Al does react in the front and because its (product) EOS is very different, therefore its energy comes out later.

Sternberg pointed out that there was time for Al to react and to affect the results in shocked air at the 3-bar level.

Coleburn discussed the treatment of aluminized explosives that he and Roslund had published. He emphasized the charge size effect.

Some of Mader's comments on the treatment of aluminized HE's were discussed. Reference was made to Alex 20 described in LA-2900. Some discussion of a buffering temperature concerning time for Al to liquify and time for Al_2O_3 to condense took place in an effort to get at when the Al reacts.

Lee discussed the two-part EOS and "burntime" that he and Cheung had developed for calculating non-ideal HE behavior.

Watson reported on some BM work that showed how the Al surface area affected the cap sensitivity of NH_4NO_3,$NaNO_3$,H_2O slurries. The studies

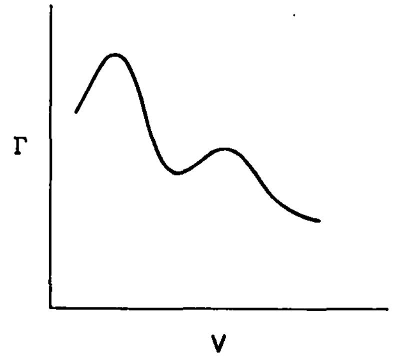


Fig. 1. Variation of Γ with v.

Finger, continued

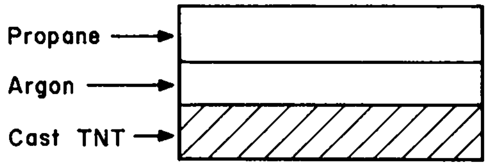


Fig. 2. Frey's experimental arrangements.

encompassed materials of 0.2 - 8 m^2/g surface area. Surface area of $\geq 2\ m^2/g$ - produced cap sensitive materials.

LVD - Watson: Watson reported a new Dutch Sensitivity Test (Will get reference). The Dutch observed LVD in nitromethane. They use PETN/KCl pellets of varying composition, heavily confined, to vary input shock pressures.

Shaw pointed out the difference in sensitivity of a family of dinitro alkanes. In some observations that Woolfolk had made it was noted that once perturbations were established in the liquids, they were not damped quickly. 0.3 mil optical flats were floated on liq. HE, H_2O, $PbClO_4$ solution, NM to make these observations. (Also some of a stainless steel wire mesh, why?)

Transverse Waves - Frey: A method for observing transverse waves was described by Frey. It consists of an open shutter high-speed camera with the arrangement shown in Fig. 2.

There was some discussion concerning the geometry of the test and the validity of surface observations.

Fickett: Fickett suggested doing an expanding TNT sphere using the BRL technique.

Kinetics Overview - Fickett:

Ideal and Non-Ideal Behaviors

(1) Transverse Waves, indicated cellular front structure
   (a) Should make observation on a liquid that doesn't have a cell structure like solid. Fickett suggested work like that of White's, on gases, be done with liquids because we can't see in solids. The C-J state is in error by 10-15%; could be because of difficulty of establishing exact points of tangency on rapidly changing function as shown in Fig. 3.

Finger, continued

(2) C-J theory; is it a problem of thermodynamics or kinetics? Fickett suggested doing experiments on a pair of HE's with equal thermodynamic properties but different kinetics. Example: 1,1-dinitropropane & 2,2-dinitropropane.

(3) Composite Explosives - Time Scale & Energy magnitude of various effects: entrainment, diffusion, time scales, guess on kinetics. The problem of describing the steady state.

Kamlet suggested a list of materials with different structures but which were of the same composition as test vehicles.

Decomposition/Sensitivity - Shaw: Shaw reported that 1,1-dinitropropane does not undergo LVD, but that 1,1-dinitroethane does. It was suggested that the limiting value for LVD is the detonation velocity in the gas phase; however, all detonation velocities calculate less than LVD. (??Do They? Gas velocities should be 2,000 m/sec for most HE's)

Shaw reported on static high pressure, high temperature decomposition studies [which they (De Carli, Lee, Stromberg) reported at Western States Combustion Meeting]. They conducted decomposition studies at 1,10, and 50 kbars on a series of compounds of

$$R - C(NO_2)_2\ CH_2CH_3;\ \text{where } R = H,F\ .$$

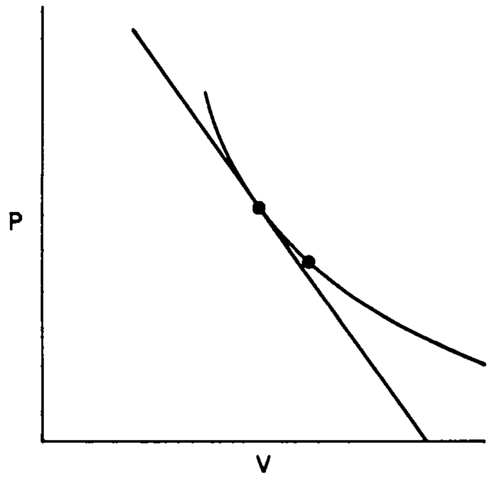
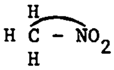
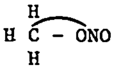


Fig. 3. Large variation of p with small departure from tangency.

They observed an increased rate of decomposition going from 1,10, and 50 kbar (using Zinn data at 1 kbar need a 127 kcal/mole activation energy?).

Attempting to correlate decomposition data with shock initiation.

Reported on Nitromethane  $H\overset{H}{\underset{H}{C}}-NO_2$ ← 60 kcal

and Methyl Nitrite  $H\overset{H}{\underset{H}{C}}-ONO$ ← 40 kcal

experiments done at -40°F, 10 atms for methylnitrite, and room temp. for NM as shown in Table I.

Table I

	D mm/μsec	ρ g/cm^3
NM	6.3	1.14
MN	5.6	0.99

Planning to do at 60°C, where liquids are

$H\,C(NO_2)_2\,CH_2CH_3$

& $H_3CC(NO_2)_2\,CH_3$.

<u>Altering Detonation - M. Fulk</u>: Fulk discussed the possibility of magnetic/electrical fields to reduce activation energies and thereby change the detonation behavior of HE's.

W. FICKETT (LASL)

Empirical Correlation of Explosive Properties - Kamlet, NOL: The empirical correlation

$$p_J \propto \rho_o^2\phi \; ; \; D \propto (a + b\rho_o)\phi \; ; \; \phi = NM^{\frac{1}{2}}Q^{\frac{1}{2}},$$

where N is number of moles of gas, M = mol. wt. of gas, Q = heat release, reproduces much of the experimental data within ± 10%. A new result for γ_J is

$$\gamma_J = 0.656/\rho_o + 0.703 + 1.105\rho_o .$$

Kamlet's comment that measurements of p_J appear to be converging with time is disputed by LASL, citing recent published work by Venable and Davis showing a large range of values for Comp. B. (268 to 312 kb.).

Cylinder Test and Explosive Performance - Kury, Lee, Finger, LLL: The standard cylinder test consists of a copper cylinder with 0.1" thick walls 12" long (L) and 1" internal diameter (D) loaded with the explosive to be studied and initiated at one end by a plane-wave lens. The wall motion is measured at the station L/D = 9 out to a radius about twice the initial value and compared with the results of a HEMP 2-dimensional calculation (both experiment and calculation show steady 2-dimensional flow at this point). TNT, 9404, and Comp. B. give the same (scaled) results in 1", 2", and 4" diameter. The HEMP calculation agrees well with a steady 2-dimensional calculation by the method of characteristics (assuming a plane front with instantaneous reaction) made at AWRE; this comparison has been published by Wilkins. The wall motion is reasonably sensitive to changes in the isentrope, particularly at lower pressures. The equation of state is obtained by matching to cylinder test results plus measured C-J pressure p_J. The LLL prescription for HE is that the equation of state so obtained (the JWL equation of state) be used together with simple C-J theory (instantaneous initiation to C-J velocity). Kury states unequivocally that this recipe is used with no fudging in all design calculations at LLL and that they have a number of satisfied customers. LASL is conspicuously absent from this list, and LASL people questioned whether AWRE should have been included.

A systematic study of a well-chosen set of "ideal" (quick-reacting) explosives covering extremes of composition is in progress. For each, the measurement consists of a standard cylinder test with a Hayes Lucite stack on the end to get p_J. This is, in my opinion, a valuable set of data against which to test future equations of state and theories of detonation. My principal reservation is that what we may eventually learn later about the troubles with measurement of p_J could suggest a better experimental design, but this is not a good enough reason for suspending the work. Some comments under Fundamentals below relate to this work.

Many "non-ideal" (slow-reacting) explosives show strong diameter effects in the cylinder test. HEMP calculations for these are being performed with a simple reaction law for the slow component as shown in Fig. 4. In some cases reasonably good

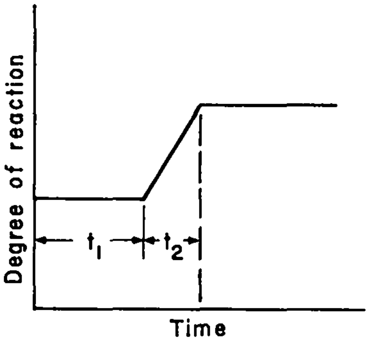


Fig. 4. Reaction law for calculations of slow-reacting explosives.

agreement with the cylinder test results is obtained by proper choice of the two time constants.

Fundamentals - Craig, Davis, Fickett, LASL; Frey, BRL; Shaw, SRI: Free-surface (u_{fs}) versus plate thickness results for nitromethane scale approximately as x/L in plane geometry and as $(x/D)^{1/2}$ in long cylinders, where x is plate thickness, L is charge length, and D is charge diameter. Most of the standard measurements for solid explosives are made with $L/D = 1$ and analyzed as one-dimensional (e.g., Deal's classic measurements on several standard explosives). However, for this L/D the calculated rate of decrease of u_{fs} with thickness is too large by a factor of 2. Kury questions the interpretation of Deal's data on the grounds that calculations show an appreciable deceleration of the free-surface as it traverses his flash gap and that this effect is not taken into account in analyzing the data. He is apparently unaware of or unconvinced by our experimental result that the free surface is observed to move at a nearly constant velocity as though a thin layer is spalling off and is thus unaffected by the following tension wave. We pointed out that other more recent measurements of u_{fs} vs plate thickness published by Davis and Venable agree with Deal but are essentially not subject to this criticism. The question remained unresolved for lack of time.

Craig presented some of the evidence on the question of the free-surface motion.

Craig reviewed some of the evidence that perturbations on the detonation front appear to survive "forever".

I urged that tests of equation of state and detonation theory (including the standard LLL tests described above) be pursued with the simplest systems, the prime candidate being liquid ozone. The consensus was that, even though its detonation velocity has been measured, this is a nasty and dangerous material to work with. Finger (LLL) suggested liquid N_2O_4 as a compromise substitute.

Frey has calculated one-dimensional pulsating detonations in ideal gases. He finds that instability is increased by lowering γ or putting in an induction zone so that the time of maximum energy release rate is delayed. He also reported on apparent front structure in solid explosives as evidenced by luminous tracks in argon at the edge of the charge. There is some question of how much of the apparent structure may be due to edge effects but the patterns are quite similar to those observed in gases. The cell sizes are relatively large, on the order of 1 cm for cast TNT.

Shaw reported that in low pressure shock initiation experiments, methyl nitrite, an isomer of nitromethane, shows a significantly different reaction rate from nitromethane. I see that this material is the perfect complement to our "Acenina" isomer (nitric acid, acetonitrile, water). Acenina has nearly the same density as nitromethane but significantly lower energy; methyl nitrite has nearly the same energy but significantly lower density. A disadvantage is that it is a gas at STP, requiring about 10 atm pressure to liquefy. Synthesis and handling descriptions suggest that perhaps remote handling might not be required.

Equation of State - Lee, LLL; Cowperthwaite, SRI; Jacobs, NOL: Work on the TIGER code continues with the JCZ (Jacobs, Cowperthwaite, Zwisler) equation of state being installed, and partial freezing of equilibrium and determination of sonic point capability being added.

Lee is impressed by the performance of a simple form of the Barnes equation of state which he is studying.

Non-Ideal Explosives - Lee, LLL; Fickett, LASL; Sternberg, NOL; Hershkowitz, Picatinny: The rate of reaction of aluminum particles in aluminized

Fickett, continued

explosives is controversial. A recent analysis of plane-wave p-u data by Sternberg supports Mader's well-documented contention that instantaneous reaction is a good model. Hershkowitz claims that any reasonable calculation of heat conduction will give a relatively slow reaction. Lee says that LLL believes that at least part of the reaction is slow but did not present the detailed evidence for this. There is little doubt that slow reactions are important in some explosives, such as those loaded with ammonium perchlorate. This whole subject received less attention than I had anticipated. I am disappointed to find that no one seems to have considered in any systematic way the magnitudes of the effects of the other rate processes such as entrainment and heat conduction. I urged that this be done and that the various magnitudes be calculated and displayed in some simple situation such as steady flow. I also pointed out the possibility of the kinetically determined eigenvalue detonation instead of the thermodynamically determined C-J detonation.

Initiation - Fulk, LLL; Kennedy, Sandia; Cowperthwaite, SRI: Kennedy is continuing his studies of initiating PBX-9404 using a gas gun as the driver and quartz pressure gauges on both faces of the 9404 target. This work, together with that extending to higher pressure already published by Craig, constitutes an extensive study. Cowperthwaite presented a simple analytic "growing square wave" model of the process. Mader has published computations reproducing most of Craig's results, but the computational model incorporates an assumed x-t path for the shock. The next step is to come up with a more conventional computational model based solely on assumed constitutive relations. It would seem that the time is ripe for this.

Fulk discussed experiments on internal electrical effects in solids, claiming that they are of great importance to the reaction kinetics in the initiation regime. I was unable to understand much of what he said, but if his claims are true, study of this subject would be well repaid.

Acronyms and Terms:

C-J - Chapman Jouguet
sub J - Chapman-Jouguet

Fickett, continued

AWRE - Atomic Weapons Research Establishment, Aldermaston, UK
Hayes stack - a stack of Lucite plates. Electrical signals generated by the passage of the shock across each interface are picked up by an antenna to give a distance-time history of the shock.
PBX - Plastic-bonded explosive

W.C. DAVIS (LASL)

A Round-Table Conference on Detonations, organized by M. J. Kamlet, USNOL, and R. R. McGuire, USAF, was held at the Air Force Academy at Colorado Springs, on June 20-21, 1972. It was held to (in Kamlet's words) "discuss and perhaps settle the unresolved problems and disagreements in the field of detonations".

There were no prepared papers for this meeting, and the discussion was free and continuous, with several conversations often going on at once. It is difficult to give a complete review of all that went on. Instead, I will try to divide the discussions according to topics, although the meeting itself was not so divided, and to list some of the items discussed.

Ideal Detonations: The discussion of high-order detonation in "ideal" explosives divided into two parts. The first was devoted to the use of "recipes" for calculating the behavior of systems employing explosives, and the best of these seemed to be the JWL equation of state used at LLL and the BKW equation of state with build-up used at LASL by Mader. There seemed to be general agreement that these were calibrated calculational methods which gave good results over some region, but which were not really detailed equations of state which describe real materials. It was not clear how the equation of state interacts with the C-J model which is always used, and with the details of the computing scheme. Apparently a careful comparison of the accuracy and useful domain of the LLL and LASL methods has never been made.

The second part of the discussion of detonation was devoted to trying to understand in detail all the physics involved in a detonation. This discussion involved evaluations of the measurement techniques that have been used, and so became deeply involved with the first part of the discussion, because the interpretation of the experiments depends upon the results of the calculations. All participants seemed to agree that the C-J model worked as well as most simple physical theories, and that the departures were fairly small. Beyond that, it was obvious that new advances in theory, experiment, model making, and calculations are badly needed.

Everyone seems to have money troubles now, and there were no volunteers for costly programs. Many participants agreed, however, that

1. Someone ought to make a careful comparison of the various recipes used for calculating explosives behavior, trying to compare them with experiment, using two-dimensional codes since the results are more sensitive to the recipe.
2. Someone ought to make time-dependent calculations about the behavior of detonations with kinetics chosen to give pathological reaction zones, and with kinetics chosen to mock up those of real explosives.
3. Someone ought to make a theoretical effort to understand decay zones and other rapid pressure falls behind detonation fronts.
4. Someone ought to make measurements of simple systems at high pressure for comparison with Jacob's new intermolecular-potential equation of state which he is putting into TIGER. Liquid oxygen and liquid ozone were suggested as experimental materials.
5. Someone ought to make measurements of the structure of the shock or detonation front in materials which have reaction or phase changes. Hayes' magnetic technique would be an ideal approach.
6. Someone ought to see whether changing the parameters in a BKW-like equation of state code would improve the calculations. LLL people are doing experiments with CHON, HNO, CON, and other explosives to try to separate the effects of different molecular constants.
7. Someone ought to continue to do experiments measuring free-surface velocities, foil motions, metal plate front and rear surface positions, etc., to improve the methods of obtaining particle-velocity data.

Non-Ideal Detonations: Discussions about "non-ideal" detonations also divided into two parts, which were concerned with detonations which were non-ideal because the charge was small compared to the reaction zone, and detonations which were non-ideal because the inherent instabilities of the reaction zone caused significant deviation from the steady C-J detonation.

In the first group were discussions of carbon agglomeration in the reaction zone, presumably a slow diffusion controlled process, and its possible effects; aluminum loaded explosives in which the slow process is the burning of the relatively large aluminum particles; the LLL perchlorate explosives which have relatively large particle sizes; and blasting agents and other composites. The LLL group showed that they get good agreement between cylinder test experiments and their calculations by using a two-step reaction zone with the slow step lasting as long as 12 μsec, and that they can choose a single time to fit a range of experiments of various diameter. Sternberg of NOL discussed attempts to fit experiments using aluminized explosives over a wide range of conditions from small sticks to large underwater explosions. It seems that recipes are available which do an adequate job of reproducing experimental results. Questions about the actual physical processes and their relative times remain.

In the second group were discussions of front structure and how to measure it, and some discussion of the theory. Frey of APG showed some beautiful pictures of waves on a free surface of TNT charges, with structures very similar to those seen in gases. There is some evidence that these waves are oscillatory failure waves on the surface rather than waves really representative of the structure of the detonation wave itself. All attendees seemed agreed that more work was necessary, but just what to do and how to do it wasn't at all clear.

Initiation: Little time was devoted to initiation, and there seemed to be few new results. Kennedy of SLA described his experiments using pressure gauges to measure pressure changes in initiating solid explosives, and gave a good consistent picture of events. Shaw of SRI described experiments with methyl nitrite, which has the same atomic composition as nitromethane. These aroused interest not only because they showed that methyl nitrite is more easily initiated than nitromethane, indicating that the kinetics are different, but also stimulated suggestions for the use of methyl nitrite in additional experiments to vary the initial state as nitromethane and acinina were used previously. Fulk of LLL gave an interesting review of recent work he has done on the internal electrical fields produced in explosives when they are shocked. He believes that electrical effects may be extremely important, possibly controlling, in initiation. He answered the objection that fields of 10^8 v/cm would be necessary to change energy states in molecules by 1 v with arguments that the fields could be concentrated by various processes involving electron traps in the material. Watson from Bruceton described experiments in which a low-velocity detonation in nitromethane was produced when a confined booster charge was used. Cowperthwaite showed some special solutions to the equations which can be used to understand some of the behavior of build-up to detonation.

J.O. ERKMAN (NOL)

1. No one was very specific about Petrone's paper "Validity of the Classical Detonation Wave Structure for Condensed Explosives", Phys. Fluids 11, 1473 (1968). Davis stated that Petrone is wrong and that he should have used a 2-D code. Is it generally conceded that he is wrong? Has anyone published computations which are better?

2. Can the contrasting views of LASL and LLL be simply stated? Perhaps people were too polite at the meeting! Do explosive drivers for the experiments introduce something that is not reproducible? Or is it the recording methods?

3. Fickett says kinetics are a bigger problem than is the equation of state. Has any work been done on systems such as N_2O_4, as he suggested?

4. Is there any consensus on how aluminum reacts? Did anyone believe Sternberg's estimate of 0.2 μsec?

5. Are there any reports on Craig's work where he perturbed a detonation front and then observed roughness further down the explosive?

Erkman, continued

6. I'd rather not believe in transverse waves. Frey, Craig, and Mallory apparently do. But why is the front relatively smooth when viewed head-on? Does the excitement commence behind the detonation front?

7. Fulk brought up some fascinating ideas. Has he any experimental evidence to support his ideas?

R.W. WATSON (BUREAU OF MINES)

Sensitization of Water-Gel Explosives with Aluminum: The Bureau has been engaged in the development of water-gel explosives for a number of years as part of an overall program to improve the safety of permissible explosives used in underground coal mines. These explosives must be cap-sensitive and detonable in small diameters of the order of an inch. During the course of these investigations we have explored the effect of various types and grades of aluminum on the sensitivity of a typical water gel and found that the surface area/unit mass of aluminum plays an essential role in the sensitization process. Typical results are included in an attached table. It will be noted that if the aluminum has a surface area of approximately 2.0 m^2/g or greater, the resulting composition is sensitive to a No. 8 cap. This effect is probably associated with the generation of a "sufficient" number of hot spots for that particular level of sensitivity. The mechanism is apparently only operable in mixtures that contain water or other liquids that might react with the aluminum since other experiments with solid explosives, Minol 2 for example, show no significant effect of surface area on sensitivity. From the point of view of detonation chemistry, the sensitization effect is an interesting one since it implies extremely fast reaction rates in order that the energy released be available to support the growing initiation wave. Some results are shown in Table II.

Low Velocity Reactions in Nitromethane and TEGDN: During the Bureau's extensive research on the low-velocity detonation in liquid explosives, many attempts were made to observe stable low-velocity detonations in neat nitromethane using a wide range of conditions of confinement, initiation

Table II

EFFECT OF VARYING ALUMINUM SURFACE AREA ON THE CAP SENSITIVITY OF A WATER-GEL EXPLOSIVE

Aluminum Type	Surface Area (m^2/g)	No. 8 Cap Sensitivity
Alcoa #120	0.2	No
Alcoa #120 (special milling)	1.0	No
"	1.7	No
"	2.1	Yes
Alcoa #322 (flake)	2.5	Yes
Alcoa #120 (milled 4½ hours)	4.2	Yes
Alcoa #408 + #1660 (flake)	5.2	Yes
Reynolds 30-XD (flake)	7.4	Yes
Alcoa #120 (milled 8 hours)	8.3	Yes

strength, explosive temperature and charge diameter. None of these attempts were successful. However, in 1970, the OECD group presented some evidence of stable low-velocity detonation in NM using a shock sensitivity test which employs a PETN-KCL donor adjusted in composition to vary the shock strength delivered to the acceptor. Aside from the donor, the principal difference between this test and our card-gap test is that the donor is directly coupled to the acceptor and is inserted into the confinement tube so that there is heavy confinement at the donor-acceptor interface. Furthermore, the downstream end of the charge is also confined. The details of the arrangement are described in Report Technological Laboratory RVO, Ass. 8357 dated 24-9-1970, of the Netherlands National Defence Research Organization, Technological Laboratory RVO-TNO, Rijswik.

We repeated these tests using essentially the same arrangement and observed what appeared to be stable low-velocity detonations in both NM and TEGDN based on evidence of continuous velocity measurements and fragmentation of the confinement tube compared to fragmentation patterns using water control firings. The observed velocities are included in Table III, and are in essential agreement with the findings of the OECD group. However, it should be noted that in the case of firing #15,972 in the 60-inch long tube the velocity was considerably less than that observed in the 30-inch long tube (#15,940), indicating that the reaction is decelerating and thus unstable.

TABLE III

EXPERIMENTAL RESULTS (CLOSED-END BOMB)

(BOOSTER: 30% PETN/70% KCℓ, 200 TO 205 GRAMS)

Sample	Tube Length (inches)	Results (rate, mm/μsec)
Water (No. 15,939)	30	1.6 1/
Nitromethane (No. 15,940)	30	2.1 1/
Nitromethane (No. 15,972)	60 2/	1.6 1/
TEGDN (No. 15,948)	30	2.1 1/

1/ Rate at approximately one-half to two-thirds distance in charge when rate probe was knocked out by wall wave.

2/ 48-inch long rate probe in 60-inch long steel tube.

* * *

L.C. SMITH (LASL)

1. Mort Kamlet suggested that ammonium dinitroacetonitrile $NH_4C(NO_2)_2CN$ has the same atomic composition as RDX or HMX, but different heat of formation, and would be a useful substance for initial-state variation experiments. It has crystal density about 1.8 g/cc, and NOL might be persuaded to make some.

2. LLL and Air Force Academy are doing some experiments with tagged C or N in an explosive, say RDX, which is mixed at fairly large particle size with another explosive, say TNT, to see whether the chemical reaction mixes atoms from the two explosives in the products.

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