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THE ENERGY OF DETONATION

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U. S. NAVAL ORDNANCE LABORATORY

WHITE OAK, MARYLAND

THE ENERGY OF DETONATION

By:

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ABSTRACT: In this paper the energy of detonation is calcu-
lated for a "gamma law" gas using two simple models for the
hydrodynamic problem. In the first a Taylor wave expansion
follows the detonation. In the second a piston follows the
detonated gas to maintain a constant pressure in it. The
energy distribution in the Taylor wave is found for the case
gamma equal to 3. It is shown that the average energy
release by the chemical reaction per gram is given by:
$e_o = p_1/2(\gamma - 1)\rho_o$ where p_1 is the C-J pressure and ρ_o is
the initial loading density to produce that pressure. The
value of gamma, taken as constant, can be evaluated from
detonation pressure data. These approximate results should
be of use in gaining an understanding of the disposition of
energy in a detonating charge of finite dimensions.

Approved by: _J. E. ABLARD, Chief_
Explosives Research Department

The report presented herein is based on a paper that was
given at a symposium which was held in May 1956 at the
Ballistic Research Laboratories. This paper is now pub-
lished as an unclassified report to make the information
accessible to a larger group of people who may be inter-
ested in the contents. The results obtained and the
conclusions represent the opinions of the author. While
the results are considered valid and informative, they
may not represent the final judgment of the Laboratory.
The work was done under Task Assignment NOL 260 in the
Detonation Division of the Explosives Research Department.

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                        Captain, USN
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                        By direction

                              ii

CONTENTS

ILLUSTRATIONS

TABLES

THE ENERGY OF DETONATION

I. Introduction

A perennial question concerning explosives is "how much work can the explosive perform upon its environment when it is detonated?" Though the answer is bound up in the theory of detonations and rarefactions following detonations, it has never been clearly brought out. This is probably due to the complexity of the thermodynamic hydrodynamic problem which is usually brought to mind when the question is posed. In this paper an attempt is made to answer the question by semi-quantitative solution of a typical detonation problem using simplifying assumptions. Details of the energy distribution and a summation of the total energy released by a given quantity of explosive are brought out. Two models are chosen: a) a one-dimensional detonation in a closed cylinder, and b) a one-dimensional detonation in a cylinder in which a piston does work on the explosive at a rate given by the particle velocity in the steady detonation. It is found that the energy released per gram can be easily accounted for in both the nonsteady process, a), and the steady process, b). This energy is just the energy of explosion at constant volume as will be shown by a comparison with the Hugoniot relation.

The result is probably not new and might have been anticipated but the method should lead to a better understanding of the energy of detonation. It is believed that a better understanding of the detonation energy can assist us in improving the efficiency of energy transfer, one of the major goals of ordnance research.

II. The Equation of State

The ideal polytropic gas assumption has made it possible to develop a considerable amount of knowledge concerning real gases at moderate pressures even though it is known that real gases do not have constant specific heats. For a similar reason, the use of the polytropic gas equation for the very non-ideal gases resulting from the detonation of solid explosives is very attractive. Considerable background has been built up to give us confidence in the use of this approximation which may be expressed by the isentropic equation:
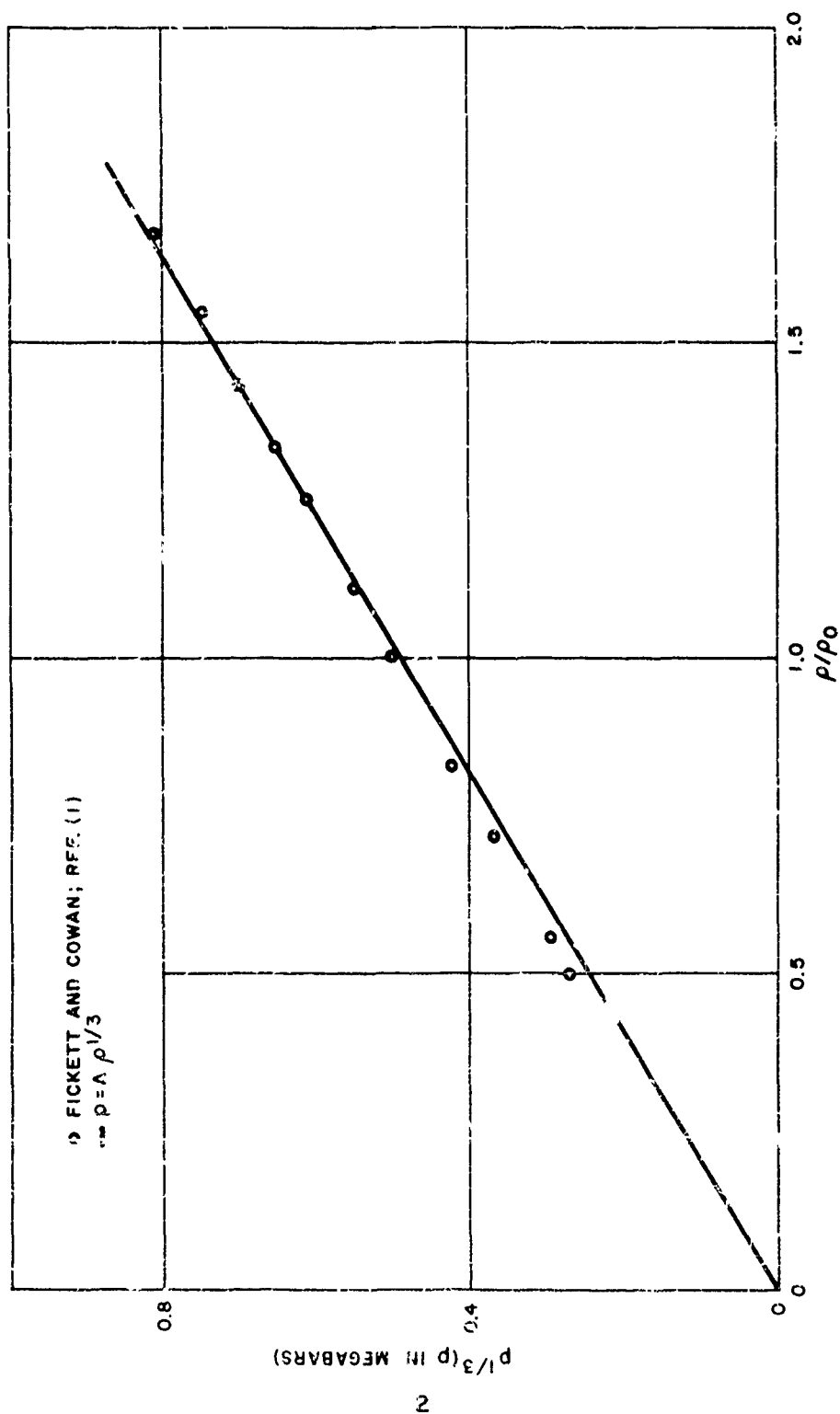
$$p = A \rho^{\kappa} \qquad 1)$$

1

FIG. I PRESSURE VS DENSITY FOR 65/35 CYCLOTOL

In equation 1), "A" is a function of entropy. γ is a constant which may be as large as 3 or more. This equation has the virtue of simplifying both thermodynamic and hydrodynamic calculations. Hydrodynamic calculations, particularly for the case $\gamma = 3$, have shown satisfactory agreement with experiment over wide ranges of pressure. The fit to isentropic expansion curves derived from more detailed calculation with equations of state believed to be more acceptable is quite good, as can be seen in Figure 1. Here, the pressure computed by Fickett and Cowan[1] for a modified Kistiakowsky-Wilson equation of state for 65/35 cyclotol is seen to vary almost as the cube of the density. The measured pressure of detonation, e.g., Deal[2], Duff and Houston[3], Mallory[4] permit us to compute γ and A at the C-J state when equation 1) is used. An extension of equation 1) which becomes a more general equation of state will be adopted, namely:

$$e = p/(\gamma - 1)\rho \qquad 2)$$

where e is the internal energy per gram. Equation 2) is true for ideal polytropic gases where γ is defined as the ratio of specific heats. Equation 1) for entropy, s, constant follows from equation 2) because of the thermodynamic relation

$$de = T\,ds - pdv \qquad 3)$$

Certainly equation 2) holds to the extent that 1) is true for the single isentrope through the C-J state provided we set e = 0 when $\rho = 0$, a most reasonable choice. In the discussion to follow the energy defined by equation 2) is computed only along the curve s = s(C-J) except where noted.

III. The Available Work in a Detonation (Model I)

$$\rho_o, \; p_o = 0, \; u_o = 0$$

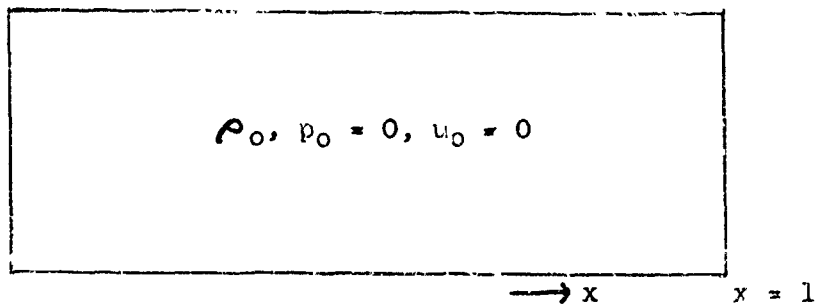$\longrightarrow x \qquad x = 1$

Figure 2

Let us consider a model in which explosive is loaded into
a rigid (non-expanding) cylinder of unit cross-section and of
unit length. The density of loading is ρ_0. The initial
pressure is taken as zero. Let the explosive column be con-
fined at each end by rigid closures. This gives us a closed
bomb of constant unit volume, Figure 1. Let us assure that a
detonation with negligible reaction zone is started at $x = 0$,
and proceeds to the right. There will be a sudden rise to the
detonation pressure, as the wave progresses, followed by a
spreading rarefaction. At a time $t = 1/D$, the detonation
front will reach the right boundary at $x = 1$. At this instant
all of the explosive is detonated. Because the confining walls
and closures have not moved, the external work done by the
products of explosion is zero. Inside the container the pres-
sure, density and particle velocity will be distributed, as
shown by Taylor[5] in a simple (or progressive) rarefaction
wave. As shown by Cole[6] the particle velocity will be zero
in the region $0 < x \leq 1/2$. In the region $1/2 < x < 1$ the particle
velocity will be a linearly function of distance. It will
have the value $u = u_1$, at $x = 1$. For the detonation front the
following well known conditions express the conservation of
mass, momentum and energy, respectively:

$$\rho_1/\rho_0 = D/(D - u) \qquad 4)$$

$$p_1 = D u_1 \rho_0 \qquad 5)$$

$$e_1 - e_0 = \frac{1}{2} p_1 \left[1/\rho_0 - 1/\rho_1 \right] \qquad 6)$$

The C-J hypotesis imposes the further limitation:

$$D - u_1 = c_1 \qquad 7)$$

c_1 is the sound speed immediately behind the detonation front.
The polytropic gas assumption (Eq. 1) leads to the result:

$$D/u_1 = \gamma + 1 \qquad 8)$$

This follows from equations 1), 4), 5) and 7) and the defi-
nition of sound speeds $c^2 = (dp/d\rho)_s$.
From 4) and 5)

$$p_1 = (D - u_1) \rho_1 u_1$$

With equation 7) this gives:

$$p_1 = c_1 \rho_1 u_1 \qquad 9)$$

By definition of c and equation 1)

$$c^2 = \gamma A \rho^{\gamma-1} = \gamma p/\rho \qquad 10)$$

By equating pressures in state 1):

$$c_1^2 \rho_1/\gamma = c_1 \rho_1 u_1 \qquad 11)$$

Therefore:

$$c_1/u_1 = \gamma \qquad 12)$$

and

$$D/u_1 = \gamma + 1; \quad D/c_1 = (\gamma + 1)/\gamma \qquad 13)$$

The Taylor expansion is characterized by a centered rarefaction as shown in Figure 3.
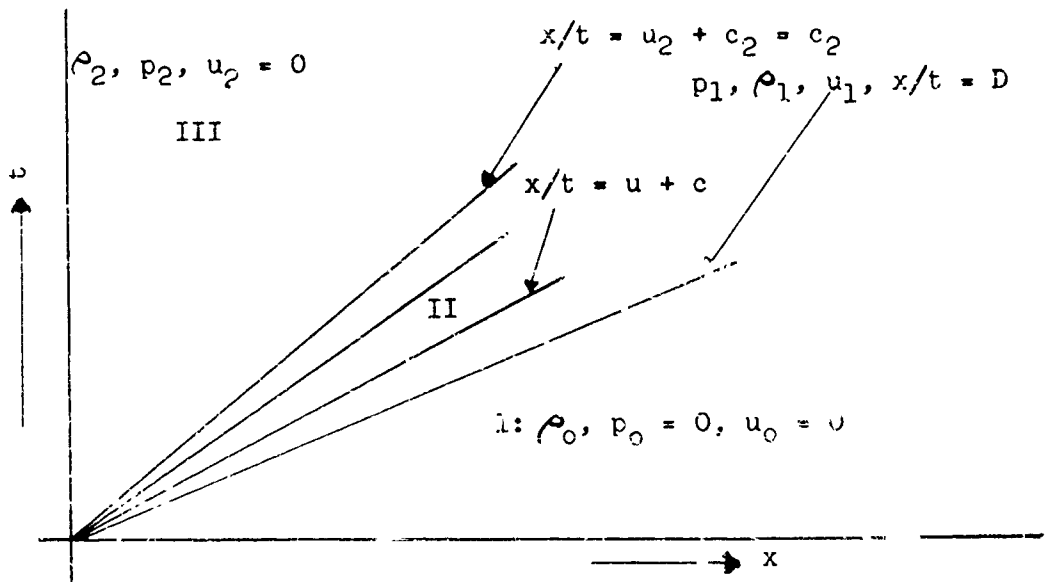

Figure 3

In the absence of the left boundary restraint the expansion
would be a continuous fan of straight lines terminating at a
particle velocity consistant with $c = 0$. The left boundary
condition, $u = 0$ at $x = 0$, causes the wave to cease expanding
when $u = 0$. This creates a steady region, III. The straight
lines x/t = constant are, by Riemann's theory, (see, e.g.,
Courant & Friedricks[7] of slope equal to $u + c$ which remains
constant on each of the lines. At the detonation front
$u + c = u_1 + c_1 = D$, the detonation velocity. In the region
of expansion u is a monatonic function of c. The value of u
is derived from the Riemann condition

$$du = d\sigma = cd\rho/\rho \qquad 14)$$

For isentropic expansion based on equation 1)

$$u - u_1 = 2(c - c_1)/(\gamma - 1) \qquad 15)$$

Therefore:

$$x/t = u + c = u_1 + c + 2(c - c_1)/(\gamma - 1) \qquad 16)$$

When $t = 1/D$

$$x = (u + c)/D; \quad u \gtreqless 0 \qquad 17)$$

Substitutions and simplification of the result leads to the
equation:

$$x = \left[\gamma/(\gamma - 1)\right] (c/c_1 - 1/\gamma) \qquad 18)$$

or

$$c/c_1 = \left[(\gamma - 1) x + 1\right] /\gamma \qquad 19)$$

p and ρ are related to c by equations 10) and 1) so we may
write:

$$p/p_1 = (c/c_1)^{2\gamma/(\gamma - 1)} \qquad 20)$$

$$\rho/\rho_1 = (c/c_1)^{2/(\gamma - 1)} \qquad 21)$$

This gives us p and ρ as functions of x by using equation
19). To solve the problem at hand we also need u as a func-
tion of x. This is given, using equation 17) by:

$$u/D = x - c/D$$

or:

$$u/c_1 = (\gamma + 1) \, x / \gamma - c/c_1$$

which simplifies by equation 19) to:

$$u/c_1 = (2x - 1)/\gamma \qquad\qquad 22)$$

The energy in the cylinder available to do work at the time the detonation reaches the point $x = 1$ is distributed as kinetic and potential and can be expressed as follows:

Kinetic Energy:

$$K.E. = \int_{1/2}^{1} \frac{1}{2} \, u_x^2 \, \rho_x \, dx \qquad\qquad 23)$$

Potential Energy $(1/2 < x < 1)$:

$$(P.E.)_{II} = \int_{1/2}^{1} \frac{1}{\gamma-1} \left(\frac{p_x}{\rho_x}\right) \rho_x \, dx \qquad\qquad 24)$$

Potential Energy $(0 < x < 1/2)$; the steady region:

$$(P.E.)_{III} = \frac{1}{\gamma-1} \left(\frac{p_2}{\rho_2}\right) \rho_2 \cdot \frac{1}{2} \qquad\qquad 25)$$

The sum of these three terms express the total energy in the system. Integrals can be evaluated by substitution of p, ρ and u as functions of x. The integration is quite simple for $\gamma = 3$ and only this solution will be given here.

Solution for $\gamma = 3$:

c, p, ρ and u become functions of x only by equations 19), 20), 21) and 22). These functions are (for $\gamma = 3$):

$$c_x = c_1 \, (2x + 1)/3$$

$$p_x = p_1 \, (2x + 1)^3 /27$$

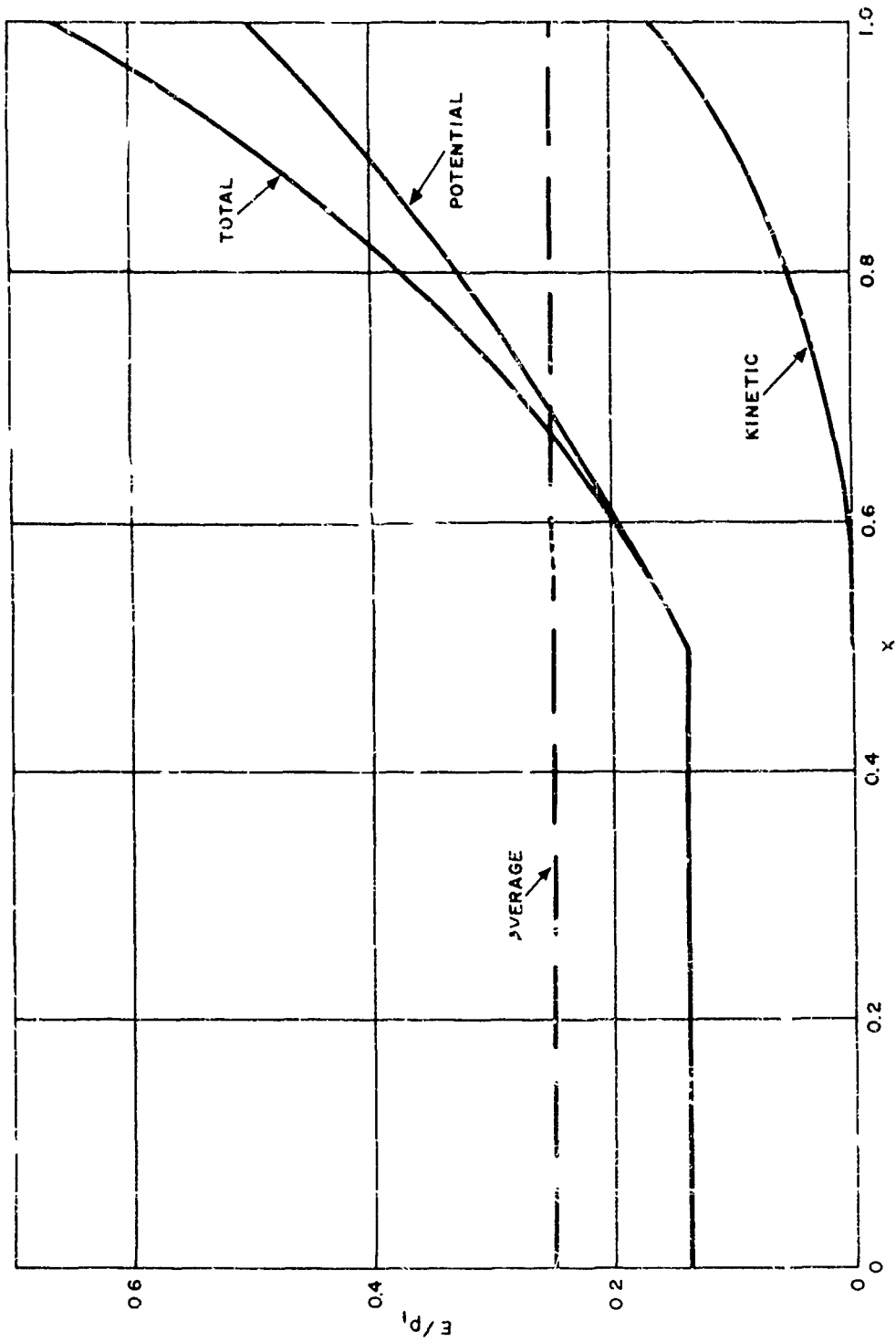$$\rho_x = \rho_1 \, (2x + 1)/3$$

$$u_x = c_1 \, (2x - 1)/3$$

FIG. 4 ENERGY DISTRIBUTION IN A TAYLOR WAVE ($\gamma = 3$)

When $x = 1/2$; $p_2 = 8 p_1/27$

The total energy in the system is therefore:

$$E = \frac{\rho_1 c_1^2}{54} \int_{1/2}^{1} (2x - 1)^2 (2x + 1)dx$$

$$+ \frac{p_1}{54} \int_{1/2}^{1} (2x + 1)^3 dx \qquad (26)$$

$$+ 2 p_1/27$$

The solution of the two integrals are easily found. The values after substitution of the limits are $11/24$ and $65/8$ respectively. The energy is therefore:

$$E = p_1 (11 + 65 + 32)/432 = p_1/4 \qquad (27)$$

In equation 27) we have substituted $3p_1$ for the term $\rho_1 c_1^2$ by using equations 9) and 12).

If we recall that this exercise was based on a cylinder of unit cross-section and unit length, we see that the energy is given per unit volume of explosive. Equation 27) therefore says that the energy per unit volume of explosive which is available to do work is p_1, the detonation pressure, divided by 4. We shall soon show that when γ differs from 3, the energy is $p_1/2(\gamma - 1)$. The energy per gram is therefore $e = p_1/4 \rho_0$ for $\gamma = 3$ and $p_1/2\rho_0(\gamma - 1)$ for any other value of gamma. An interesting point is the distribution of energy as shown by equation 27). We see that $11/108$ or about 10% is kinetic energy which exists only in the right half of the cylinder. $65/108$ or about 60% is potential energy in the right half of the model. The remainder, about 30%, is potential energy in the left half of the cylinder. The distribution of energy is shown graphically in Figure 4. The distribution for γ slightly different than 3 should not be too different.

IV.   The Available Work in a Detonation (Model II)

A simpler approach to finding the energy in a detonation is now considered. As before we use a cylinder of unit cross-section and of unit length, Figure 5. A piston is moved at velocity, $u = u_1$, to confine the gaseous products of detonation
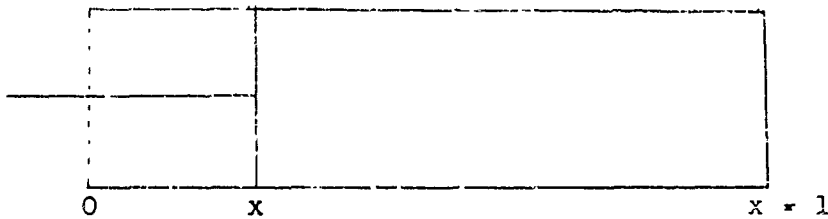
Figure 5

while the wave propagates to the right. In this way no expansion of the gas occurs so that at time $t = 1/D$ when the detonation front is at $x = 1$, the piston will be at $x = u/D = 1/(\gamma + 1)$. Pressure, density and particle velocity will be uniformly distributed in the space between the piston and $x = 1$. Work has now been done on the gas by the piston. If we sum up the potential and kinetic energy in the gas and subtract out the work done, the residual will be energy which must have been derived from the explosion. The kinetic energy for the unit volume is obviously $\rho_o u_1^2/2$. The potential energy is $p_1/(\gamma - 1)\rho_1$ per gram or $p_1\rho_o/(\gamma - 1)\rho_1$ for the unit volume initially used. The work done by the piston pushing with a force p_1 per unit area is $p_1 x$ or $(p_1/(\gamma + 1))$ when the detonation wave reaches $x = 1$. The energy which must have come from the chemical decomposition is therefore:

$$E = \rho_o u_1^2/2 + p_1 \rho_o/(\gamma - 1)\rho_1 - p_1(\gamma + 1) \qquad 28)$$

Substituting $p_1 = (\gamma + 1)\rho_o u_1^2$ and $\rho_o/\rho_1 = \gamma/(\gamma + 1)$ we get

$$E = p_1 \left[\frac{1}{2(\gamma + 1)} + \frac{\gamma}{(\gamma + 1)(\gamma - 1)} - \frac{1}{\gamma + 1} \right]$$

which simplifies to:

$$E = p_1 /2(\gamma - 1) \qquad\qquad 29)$$

per unit of initial volume.

10

The energy release per gram is:

$$e = p_1 / 2(\gamma - 1)\rho_0 \qquad \text{30)}$$

It is interesting to note that the result expressed in equation 30) is just the term e_0 in the Hugoniot relation, equation 6). This is seen as follows:

From equation 6):

$$e_0 = e_1 - p_1 (1/\rho_0 - 1/\rho_1)/2 \qquad \text{31)}$$

writing $e_1 = p_1/(\gamma - 1)\rho_1$ and $\rho_0/\rho_1 = \gamma/(\gamma + 1)$ we get:

$$e_0 = \frac{p_1}{\rho_0} \left[\frac{\gamma}{(\gamma + 1)(\gamma - 1)} - \frac{1}{2} + \frac{\gamma}{2(\gamma + 1)} \right]$$

which simplifies to:

$$e_0 = p_1/2(\gamma - 1)\rho_0 \qquad \text{32)}$$

It is therefore quite clear that we can associate the energy available to perform work with the e_0 term, i.e., the energy of detonation in the Hugoniot equation, irrespective of whether the release of energy is by a detonation process or not. A uniform constant volume explosion in which a wave is absent would, for example, result in the same quantity e_0 being converted from chemical energy to thermal energy. In this case $\rho_1 = \rho_0$ so that $e_1 = e_0$ in equation 6). By using the general sense of the equation of state, equation 2), we find that the pressure for a constant volume explosion is just 1/2 of the detonation pressure. This result which is independent of ρ agrees quite well with the answer obtained by the use of more elaborate equations of state.

V. Discussion

The result of the foregoing calculations show that a detonation gets its energy to sustain itself from both chemical reaction and the isentropic expansion of the products of detonation. This expansion replaces the piston on which work must be done to sustain a steady pressure at the detonation front. The net energy released by the detonating explosive is the same as that released from the chemical process for a constant volume explosion as should be expected.

11

TABLE I

Explosive	$Q_v{}^{c)}$, kcal/gm		p_1, kilobars	ρ_o gm/cc	D m/sec	γ, (computed)	e_o kcal/gm
	H_2O^*	CO^*					
RDX[b)]	1.26	1.26	325	1.762	8322	3.03	1.083
TNT[b)]	1.055	0.678	178	1.640	6951	2.762	0.530
77/23 cyclotol[b)]	--	--	313	1.743	8252	2.790	1.200
Composition B[a)]	1.16	0.975	272	1.67	7868	2.825	1.067
Composition B[b)]	1.16	0.975	293	1.712	8022	2.762	1.16

*Arbitrary decomposition equations with H_2O or CO, respectively, as the first product. CO or H_2O become the respective second product. Carbon, CO_2 and N_2 are taken as the only other possible products.

a) Duff and Houston, ref. (3)
b) Deal, ref. (2)
c) Christian and Snay, ref. (8)

It is interesting to compare the energy term, e_0, derived from detonation pressure measurements with the energy of reaction given by arbitrarily writing down a chemical reaction for the explosive decomposition. Data for detonation pressures are available for a few explosives. These are tabulated in Table 1 and the value of energy. e_0 computed using equation 32) is compared with Q_v the energy of reaction as given by Christian and Snay[8] for two arbitrary reaction processes. The results are in good agreement except for TNT. It should be noted that Q_v is calculated leaving the products at standard state, that is, 298°K. e_0 on the other hand assumes a reference state of p = 0 which implies 0°K. A term must therefore be added to the values of Q_v for an assumed (ideal?) gas expansion to 0°K. This will increase these numbers by about 5-10%. On the other hand the assumption of constant γ throughout an isentropic expansion, (as we have done in deriving e_0) also tends to underestimate the value of e_0. The agreement is therefore brought into line by compensating errors, it might be said.

There are refinements that can be taken to arrive at more precise calculations. We are already working on a more suitable equation of state which, though arbitrary, will permit us to associate the low pressure points in the pressure-density relation along the isentrope with the temperature. The usual thermochemical standard state can then be established for this curve. In this equation γ will be a variable which approaches the ideal gas value at low pressure. Values of γ other than 3 should be tried in the present analysis to see the effect of γ on the energy distribution. This we expect to do.

By the introduction of a straightforward method to integrate the energy in a simple detonation model, we hope to have suggested the way towards the computation of efficiency of energy transfer in systems which may be closer to realistic.

VI. Conclusions

1. The energy and the energy distribution in a Taylor wave has been computed for a gamma law with gamma equal to 3.

2. The energy which must come from the chemical reaction has been computed for 2 models as well as for the Hugoniot relation and the results agree. The total energy of the explosion products above a ground state taken at p = 0 is

found to be equal to $p_1/2(\gamma - 1)\rho_0$ where p_1 is the detonation pressure and ρ_0 is the initial loading density to produce this pressure.

3. Energies calculated by the method given here using measured detonation pressure data give reasonable agreement to the energy of explosion at constant volume calculated from the chemical decomposition.

4. In the case of TNT, the energy calculated from detonation pressure is too low. This suggests that both the chemical reaction and the measured pressure should be reexamined. Possible sources of discrepancy are: a) an error in the pressure measurement; b) incomplete reaction; for example, atomic carbon may not crystallize quickly thus reducing the energy; c) the solid carbon may not transfer its energy to the gas on expansion so that the computed work may be lower than the thermal energy released by the reaction. More refined calculations by Fickett lead to a result in qualitative agreement with that found here.

5. The results obtained in this paper should be of assistance in understanding the detonation process in charges of finite size.

6. Use of a gamma law for explosives generalized to an energy relation which becomes a caloric equation of state is a practical simplification for the solution of thermohydrodynamic problems and is a means for obtaining answers which reasonably approximate the results of more involved assumptions.

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