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Title: APPLICATIONS OF CLASSICAL DETONATION THEORY

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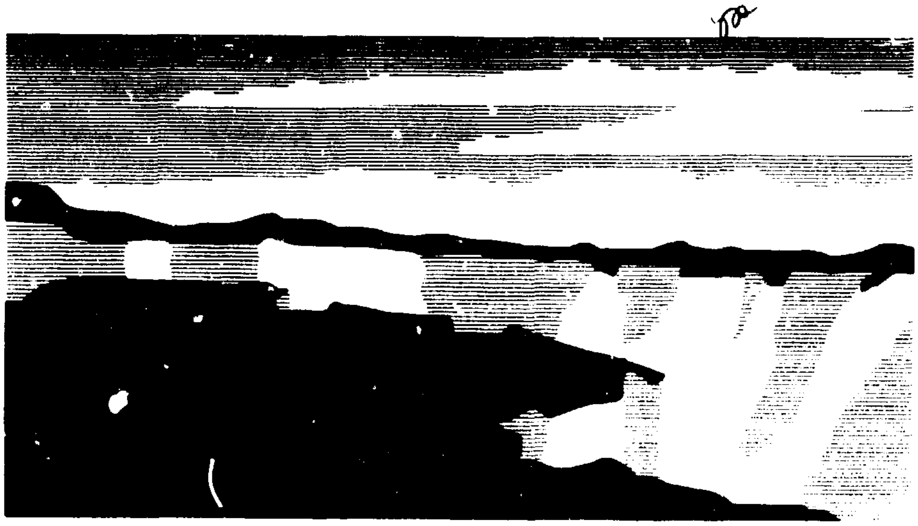

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PART 2

APPLICATIONS OF CLASSICAL DETONATION THEORY

William C. Davis

Abstract

Classical detonation theory is the basis for almost all calculations of explosive systems. One common type of calculation is of the detailed behavior of inert parts driven by explosive, predicting pressures, velocities, positions, densities, energies, etc. as functions of time. Another common application of the theory is predicting the detonation state and expansion isentrope of a new explosive or mixture, perhaps an explosive that has not yet been made. Both types of calculations are discussed.

In the preceeding paper Dr. Fauquignon has presented the classical theory of detonation. This simple theory is the basis for almost all calculations made for the design of devices driven by high explosives. Here we will examine how it is used, and describe some tests of the theory.

In some applications of explosives, say an aerial bomb, the important quantities for design are the velocity of the case fragments and the strength of the shock wave at relatively large distances for the bomb. The partition of energy between fragments and gas does not depend strongly on the details of the detonation and the interaction of waves with the metal, and is not at all sensitive to the method used to calculate the performance of the system. Many approximate methods[1] have been developed for such problems. Results of such calculations do not provide a test of the applicability of the theory. On the other hand, understanding small details of the system, such as spalling of the case of the bomb, require detailed calculations, and it is important to get the details of the flow of the detonation products reasonably correct. These calculations do provide a test of the applicability of the theory.

The classical model[2] gives the state of the detonation products at the end of the chemical reaction zone, and shows further that the state does not depend on the details of the chemical reaction, but simply on the energy released. The state, usually called the Chapman-Jouguet or CJ state and designated here by a subscript j, is described by

$$p_j = \frac{\rho_0 D^2}{\gamma_j + 1} \qquad \rho_j = \rho_0 \frac{\gamma_j + 1}{\gamma_j} \qquad u_j = \frac{D}{\gamma_j + 1} \qquad c_j = \frac{\gamma_j D}{\gamma_j + 1}$$

where p is the pressure, ρ is the density and subscript 0 denotes the initial state. D is the CJ detonation wave velocity, γ is the dimensionless sound velocity to be discussed below, u is the particle velocity, and c is the sound velocity. The dimensionless sound velocity γ is a thermodynamic state variable and is given by $\gamma = \frac{\rho c^2}{p}$, with the square of the sound speed defined as $c^2 = (\partial p/\partial \rho)_S$, for all ρ and p, not just at the CJ state. Note that γ in hydrodynamics is not the ratio of specific heats, and is not a constant except in special cases.

The classical model has the detonation wave running at constant speed; therefore if one knows, or assumes, its location at an instant of time, one can calculate[3] its location and shape at a later time. The model gives the state of the detonation products at the wave front from the formulas above. The flow of the products, an inert flow with the only possible chemical changes being shifts in equilibrium composition as the state changes, can be computed from the usual equations[2] of hydrodynamics The only processes that produce appreciable entropy are shock waves in the flow of the products; if there are no shocks, the flow is isentropic. If there are shocks, they move the state off the isentrope, in most cases only slightly. The material description needed to complete the formulation of the flow of the products gases is required only near the isentrope through the CJ point (called the principal isentrope).

While it may seem straightforward to model detonation by advancing the wave at each time step, and setting the state to the CJ state at that position, this procedure often causes numerical difficulties[4]. Since the state at the end of the chemical reaction is independent of the details of the reaction, any method for reacting the explosive to its products will give the same end state. In modeling, any scheme that reacts the explosive quickly and does not introduce numerical difficulties will be satisfactory. Many schemes have been used; some work better than others. Most calculations are made using one of the schemes for burning the explosive; there is no attempt to model the real reaction zone.

Any thoughtful person must ask why it is necessary to introduce this artificiality. Why not just model the reaction zone following all the details of the chemical reactions? The answer is that it is not practical to do that. To get even a reasonably accurate model of the reaction zone requires at least 50 calculational cells in the reaction zone. The device will usually have a characteristic size that is 100 to 1000 or more reaction zone lengths, to be far enough from the critical size, or failure size, for the system to be robust. While one-dimensional calculations are possible with 10 000 or more cells, two- and three-dimensional calculations with 10^8 or 10^{12} cells, the ones of interest, are not. Attempts to model the reaction zone in a real system take more than a day on the fastest computers.

Whether the front is advanced and the state set using the classical theory, or by using an artificial burning, a description of the properties of the detonation products is required in every calculation. The explosive driven system must be considered as an engine, differing from more conventional engines in that the parts are deformed as well as moved and that the cycle is not repeated. The detonation products are the working fluid for the engine. The description[5-7] of the products is usually called an "equation of state". The quantities that are required are two derivatives:

$$\gamma(p,\rho) \equiv (\rho/p)(\partial p/\partial \rho)_S \qquad \Gamma(p,\rho) \equiv (1/\rho)(\partial p/\partial E)_\rho$$

where E is the specific internal energy. Values are needed only in the immediate neighborhood of the principal isentrope that passes through the CJ point, because little entropy is produced in the weak shocks that may occur in the system after detonation.

The material description for calculations is almost always obtained by calibrating a convenient fitting form to experiments as much like the system to be calculated as possible. Sometimes the fitting includes results from equations of state calculated by statistical mechanics using assumed intermolecular force laws, and other theoretical equations of state. Simple expansions of the equation of state such as a virial expansion are of limited use. The densities are so high that the intermolecular interaction energy is very large compared with the thermal energy. Typically in the region of most of the energy transfer from products to inert parts one has $p/\rho RT > 10$. The results are presented as

$$p = p(\rho,E)$$

and the necessary derivatives for the hydrodynamic calculations are obtained from this expression. The "equation of state" is incomplete (a function of ρ and E rather than of ρ and S) because it is calibrated from mechanical measurements that yield no information about temperature or entropy.

One sees from this description of how the classical theory is used, to provide a model for fitting the measurements, that its success for this purpose does not provide a real test of the theory. The fact that the calibration experiments can be quite different from the system being modeled indicates that the classical model is probably qualitatively correct. A definitive test must use other data.

The first reassuring fact[8,9] is that most, but not all[10,11], detonations do in fact propagate with a leading shock wave that is reasonably smooth, followed by a decrease in pressure as the chemical reaction takes place, and then, if the back boundary condition is proper, followed by an expansion wave. These observations show that the classical model is at least qualitatively correct. The measured reaction zone in practical explosives ranges from about 10 μm to about 10 mm, a range of 1000. Explosives with reaction zones smaller than 10 μm are too dangerous to handle safely, and ones with reaction zones larger than 10 mm fail to propagate except in very large sizes.

Experiments[12] providing a severe test of the theory were carried out using liquid nitric oxide NO as a prototype explosive. The description of the detonation products was obtained from shock wave measurements made on liquid oxygen, liquid nitrogen, and liquid mixtures of oxygen and nitrogen. A careful study, using the best theory available to help the analysis was made. No calibration to detonation measurements was required. Then the results of detonation measurements were compared with the predictions of the theory, and the agreement was found to be very satisfactory. The really important conclusion to be reached, which could not be supported otherwise, was that the assumption that the detonation products reach chemical and thermal equilibrium in the detonation reaction zone is an excellent approximation.

Another set of experiments[13], however, testing the theory by the "inverse method", showed that the theory is not exactly correct. This method requires that the initial state of the explosive is varied to provide values for derivatives about a standard initial state. For TNT the energy was varied by using solid and liquid TNT so the energy was different by the heat of fusion, and the density was varied by using solid TNT pressed to different densities, or by varying the temperature of the liquid. For liquid nitromethane the energy was varied by mixing it with a mixture of nitric acid, acetonitrile, and water that had the same atomic composition but different energy, and the density was varied by changing the temperature. The results for the derivatives allowed the pressure to be calculated, and this inferred value was compared with detonation measurements. In these experiments agreement was not obtained; the values differed by several standard deviations.

The main support for belief that the classical theory is a good approximation to actuality comes from its use in predicting the behavior of an explosive, perhaps even an explosive that has never been made. It was recognized[14] at least 75 years ago that if the simple theory is correct one need know only the atomic composition of the explosive and its heat of formation to calculate its detonation properties. The atomic composition determines the composition of the products, since they are (by assumption) in chemical equilibrium. Most of the heat comes from the formation of the products, so the dependence on an exact figure for the heat of formation of the explosive is relatively weak. For most common explosives, the major products are N_2, H_2O, CO_2, CO, and C(soot), with minor amounts of NO, NH_3, CH_4, H_2, O_2, HCOOH, etc. Sometimes other elements besides CHNO are present. If an equation of state for each species is available, and a mixing rule is known, the free energy can be minimized to give the composition of the products and the state variables. There need be no calibration to detonation experiments.

While simple in concept, this procedure is complex and tedious in execution. Many workers[15-17] have made schemes for doing it, and many equations of state with various calibration data have been used, and different mixing rules have been tried. Other minor constituents have been considered. Obviously, different schemes give slightly different results. However, all reasonable schemes give surprisingly good predictions, usually within a few per cent of the measured values. Rarely in science and engineering has it been possible to make predictions of the detailed properties of complex materials as well as has been done for explosives. The value of the classical simple theory is proven by these results.

Reading the current papers on explosives one soon sees that workers are not satisfied with the available predictions. To make a decision about whether or not to invest the large amount of effort and funds needed to develop a new explosive for practical application, the accuracy of a few per cent is not good enough. The gain in performance from a new explosive is never more than a few per cent above the old ones. While refining the equations of state and the mixing rules, or trying new minor constituents, seems to help a little, studying the deficiencies and errors soon leads one to believe that there is an underlying additional cause of error. The most likely cause is that the products do not go completely to equilibrium in a short enough time in all explosives. There is strong evidence for very slow heat release near the end of the reaction zone. Perhaps the slow reactions can be identified and predicted, with subsequent improvement of the prediction of explosive performance.

This brief review describes how the classical theory of detonation, in its simplest form. is applied to practical problems. Almost all calculations of the behavior of explosive driven systems are based on the theory. Predictions of the performance of new explosives are based on the theory. The theory has been tested in many ways, not all of them described here. It is not perfect, nor is it complete, but it is extremely useful and is very widely used.

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