

# Detonation in miniature

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A mathematical analog for one-dimensional compressible flow in a chemically reacting fluid is constructed and used as a vehicle for a simplified introduction to such flows, with particular application to detonations. The presentation includes a concise self-contained introduction to the elements of nonreactive compressible flow.

## I. INTRODUCTION

Various aspects of the theory of compressible fluid flow have been discussed in this journal: history and overview,<sup>1</sup> hyperbolic partial differential equations and the method of characteristics,<sup>2-4</sup> supersonic flow,<sup>5-7</sup> shock waves,<sup>8-13</sup> and similarity methods.<sup>14</sup> The related kinematic wave equation, which we shall be using here, has been discussed and applied to other types of flow.<sup>15</sup> Not covered is our topic here—compressible flow in a chemically reactive fluid, with particular application to detonation. Also lacking is a concise introduction to nonreactive compressible flow in one dimension, which we present here in a self-contained fashion as a preliminary to the discussion of detonation.

For the purpose of more easily studying various topics in detonation theory, I have recently constructed a simple mathematical analog for the equations describing one-dimensional compressible flow in a chemically reacting fluid (hereafter *reactive flow*). This analog is an ideal vehicle for a simplified introduction to detonation theory, for, like other such analogs, it eliminates most of the complexity of the complete system of equations while retaining their essential features.

Some acquaintance with nonreactive flow is needed as background for this discussion, principally (i) the role of characteristics as information carriers, (ii) the nature of shock and rarefaction waves, and (iii) the degradation of a shock as it is overtaken by rarefaction. We therefore precede our discussion of detonation by a short introduction to nonreactive flow. Again an analog—in this case a well-known one—is the most appropriate vehicle. This discussion of nonreactive flow can stand alone as an introduction to that subject.

Because our entire presentation is based on mathematical analogs, a word about their nature is in order. An analog is a *qualitative* representation of the original. (There may of course be the added bonus that the original reduces to the analog in some special or limiting case, but this is by no means necessary.) The analog is constructed or designed, not derived. The design involves a trade off: one tries to maximize simplicity while minimizing the loss of important properties of the original. Simplicity is the analog's strong point. Specifically: (i) exact solutions are easier to find and more likely to exist, (ii) the tedium of routine mathematical manipulations is greatly reduced, and (iii) the essential ideas are less likely to be obscured by extraneous detail—in the full system one may fail to see the forest for the trees.

The construction of the analog is described in Sec. II. Section III is the introduction to nonreactive flow. Section IV is a discussion of some general properties of reactive flow

and of how wave motion is modified by the presence of chemical reaction. Sections V and VI constitute the introduction to detonation theory: Sec. V is a qualitative discussion and Sec. VI is a quantitative treatment, with results for the steady detonation wave. For reference, the complete set of equations for the physical system are set down in the Appendix.

## II. THE ANALOG

Our analog for reactive flow is an extension of the so-called kinematic wave equation, which is, among other things, one of the standard analogs for nonreactive flow. We review its construction in Sec. II A before extending it to the reactive case in Sec. II B.

### A. Nonreactive analog

The kinematic wave equation turns up in many places, but we are concerned here with its role as the simplest analog for compressible fluid flow. Johnson's paper<sup>15</sup> and the book by Whitham<sup>16</sup> may be consulted for background. To construct it, we retain the partial differential equation expressing the conservation of mass, but replace everything else—the equation of state of the material plus the partial differential equations expressing the conservation of momentum and energy—by a single algebraic relation.

Consider one-dimensional flow in a compressible fluid filling a channel of constant (unit) cross section. By assumption, all quantities are functions only of distance  $x$  along the channel and of time  $t$ ; these are our independent variables. An important quantity is the mass flux  $p$ ,

$$p = \rho u, \quad (1)$$

where  $\rho$  is density and  $u$  is particle velocity (we choose the symbol  $p$  because the mathematical role of mass flux in the analog resembles that of pressure in the physical system). Choose two fixed stations  $x_1$  and  $x_2$  in the channel. The time rate of change of mass in the volume between these stations must be equal to the net mass flux through its boundaries, that is

$$\frac{d}{dt} \int_{x_1}^{x_2} \rho(x,t) dx = p(x_2,t) - p(x_1,t). \quad (2)$$

Taking the time derivatives inside the integral sign and passing to the limit  $x_1 \rightarrow x_2$ , we obtain the equivalent partial differential equation expressing the conservation of mass

$$\rho_t + p_x = 0. \quad (3)$$

We would like to make a closed system from this single equation in the two unknowns  $p$  and  $\rho$ . One way to do this is to assume that the mass flux  $p$  and the density  $\rho$  are related by an "equation of state"

$$p = p(\rho). \quad (4)$$

If this is so then we have the determinate system

$$\rho_t + p_x = 0, \quad (5a)$$

$$p = p(\rho), \quad (5b)$$

which can also be written

$$\rho_t + c(\rho)\rho_x = 0, \quad (6a)$$

$$c(\rho) = p'(\rho). \quad (6b)$$

The quantity  $c$  turns out to be the sound speed, that is, the propagation speed of small disturbances. The partial differential equation (5a) or (6a), together with the algebraic relation (5b) or (6b), is the *kinematic wave equation*; it is the simplest analog for (inviscid) nonreactive flow.

In physical applications  $p(\rho)$  is chosen to give a good approximation to reality. Here we want the simplest form with the desired properties. For us,  $p(\rho)$  plays the mathematical role of an equation of state. As such, it should have the essential properties that both  $p$  and  $c$  increase with  $\rho$ , that is, that the function  $p(\rho)$  be monotone increasing and concave upwards. (The increase of  $c$  with  $\rho$  is what gives rise to nonlinear effects such as the steepening of a compression wave into a shock.) The simplest choice for  $p(\rho)$  satisfying these requirements is

$$p = (1/2)\rho^2, \\ c = \rho. \quad (7)$$

This choice gives the simplest nonlinear hyperbolic equation

$$\rho_t + \rho\rho_x = 0. \quad (8)$$

At this point we pause to comment on our terminology and the spirit in which we view the analog. Once we have constructed the analog, we will for the most part forget how we obtained it, and simply regard it as a given mathematical object put forward as an analog for the complete set of equations describing the physical system. As we study the analog, we see certain analogies between the quantities appearing in it and some of those in the physical system. We do not then hesitate to apply the terminology of the physical system to these quantities. In this sense, the quantities we have called  $\rho$ ,  $p$ , and  $c$  are the *mathematical* analogs of the physical density, pressure, and sound speed, and the functional relation  $p(\rho)$  plays the role of the equation of state. The relations between them in the analog are only similar to, and not identical with, those of the physical system. Thus, for example, in the physical system the sound speed is related to the equation of state by the relation  $c^2 = p'(\rho)$  [with  $p(\rho)$  an isentrope], whereas the corresponding relation in the analog is  $c = p'(\rho)$ , with  $c$  replacing  $c^2$ . (To retain dimensional consistency in the analog we must assign to the quantity  $p$  in it the dimensions of mass flux, that is  $[p] = [\rho u] = m l^{-2} t^{-1}$ .)

Johnson<sup>15</sup> and Whitham<sup>16</sup> discuss several applications of the system (6a) and (6b). Because it expresses mainly conservation of mass, it is often a good approximation in

those situations, such as river or glacier flow, in which momentum and energy changes are small. One must of course choose an appropriate  $p(\rho)$  for each application, guided by physical insight and empirical data. Interestingly enough, it can also be a good approximation in some situations in which momentum and energy changes are large. An example is a rarefaction wave moving into a compressible material (in an initially constant state). Here the analog becomes an exact description if we take for  $p(\rho)$  the appropriate isentrope of the material.

What are the shortcomings of the analog? The main one is that it has waves propagating in only one direction (toward positive  $x$ ). This of course restricts the class of problems to which it applies: wave reflections are excluded. Less serious is the absence of entropy production and thermal effects. In the physical system entropy is produced in the irreversible process represented by shock jumps. But entropy production and thermal effects are often relatively small, and a great deal of complexity is removed by omitting them.

## B. Reactive analog

We choose the simplest chemical reaction  $A \rightarrow B$ , which we allow to proceed only in the forward direction. We specify the composition of the system by the mass fraction of  $B$ , which we call  $\lambda$ . This dimensionless variable  $\lambda$  is a progress variable for the reaction, progressing from zero at no reaction to one at complete reaction.

We have then  $\lambda$  as a second dependent variable (in addition to  $\rho$ ). Now in the physical system, the addition of chemical reaction changes the governing equations in two ways: the pressure depends on the composition, as well as on other state variables, and there are one or more additional differential equations describing the rate of change of the composition with time. So here: to extend the nonreactive analog to include chemical reaction we do two things: (i) let the equation of state depend on  $\lambda$  as well as  $\rho$ , and (ii) add a second partial differential equation (the *rate equation*) describing the progress of the reaction.

We have then for the equation of state

$$p = p(\rho, \lambda). \quad (9)$$

For the rate equation, we take a simplified version of that for the physical system. By assumption each fluid element is a closed adiabatic system. The rate of change of  $\lambda$  within a particular fluid element, as seen by an observer moving with the element, is given by an ordinary differential equation

$$\frac{d\lambda}{dt} = r, \quad (10)$$

with  $r$  the *reaction rate*, usually taken to be a function of the local thermodynamic state. The corresponding partial differential equation in  $x$ - $t$  space is

$$\lambda_t + u\lambda_x = r, \quad (11)$$

the left-hand side being the convective derivative, that is, the directional derivative along a particle path. We use this equation, omitting the term  $u\lambda_x$  for simplicity, so that our rate equation becomes just

$$\lambda_t = r(\rho, \lambda), \quad (12)$$

where we have taken  $r$ , like  $p$ , to be a function of the local state  $(\rho, \lambda)$ .

Collecting these results, we have as our reactive flow analog the system

$$\rho_t + p_x = 0, \quad (13a)$$

$$\lambda_t = r, \quad (13b)$$

$$p = p(\rho, \lambda), \quad (13c)$$

$$r = r(\rho, \lambda). \quad (13d)$$

A broad study of variations on this theme is in progress.<sup>17</sup> Analogs of detonations in a wide variety of materials can be obtained by variations on these equations. For example, we can add a viscous term to (13a), consider additional chemical reactions by adding additional  $\lambda$ 's (with a new rate equation for each), and choose different forms for the functions  $p$  and  $r$ . We shall not pursue any of this here, but just stay with the simplest case, that is, the system (13) as it stands.

Throughout, we restrict our discussion to *well-behaved* equations of state, which we define as those satisfying the conditions

$$p_\rho > 0, \quad p_{\rho\rho} > 0, \quad p_\lambda > 0, \quad (14)$$

that is, having fixed- $\lambda$  curves which have positive slope and are concave upward in the  $p$ - $\rho$  plane, and which do not cross each other. The sound speed  $c$  turns out to be

$$c = p_\rho; \quad (15)$$

for a well-behaved equation of state, it increases with density. For purposes of illustration we take what we shall call our *standard equation of state*

$$p = (1/2)(\rho + q\lambda)^2, \\ c = \rho + q\lambda, \quad (16)$$

with positive constant  $q$  representing the heat of reaction. (To preserve dimensional consistency in the analog we must assign to  $q$  the same dimensions as  $\rho$ , that is  $\text{ml}^{-3}$ .) For  $q = 0$  this reduces to the nonreactive case (7),

$$p = (1/2)\rho^2, \\ c = \rho. \quad (17)$$

We restrict our discussion to reactions proceeding in the forward direction only, so that the rate  $r$  is positive everywhere except in the equilibrium state  $\lambda = 1$ , where it vanishes. We also consider only rates for which the reaction is complete in finite time. Again for purposes of illustration we define a *standard rate*

$$r = k(1 - \lambda)^{1/2}, \quad (18)$$

with constant multiplier  $k$ .

The limitations of this analog are essentially the same as those of the nonreactive one. A system with chemical reaction has two entropy-producing processes: the chemical reaction and shock jumps. But the effects of entropy production remain sufficiently small that their absence in the analog is not a serious defect.

### III. NONREACTIVE FLOW

We now return to the nonreactive system (5a) and (5b) or (6a) and (6b). In this section we use it for a brief intro-

duction to hyperbolic partial differential equations and nonreactive compressible fluid flow, the background needed for our study of detonations in Secs. V and VI.

#### A. Characteristics

The nature of the solutions of a system of hyperbolic partial differential equations, and also the role of the boundary conditions in determining a particular solution, is made clear by studying the *characteristic curves*, or *characteristics* for short, of the system.<sup>2,16</sup> A characteristic is, roughly, a curve in the dependent-variable (here  $t$ - $x$ ) space along which one of the equations of the system becomes an ordinary differential equation. For a system of  $n$  equations there are  $n$  families of characteristic curves. Our single Eq. (6a) has only one family of characteristics, easily obtained by noticing that the left-hand side is the derivative of  $\rho$  with respect to  $t$  in the direction  $dx/dt = c$ . Along any curve satisfying  $dx/dt = c$ , then, (6a) becomes the ordinary differential equation  $d\rho/dt = 0$ . We have then the *characteristic form* of this equation, usually written

$$\frac{d\rho}{dt} = 0 \quad (19)$$

on

$$\frac{dx}{dt} = c. \quad (20)$$

The solutions of  $dx/dt = c$  are the characteristics. Now the first equation of the pair (19) and (20) states that  $\rho$  is constant along each characteristic. Thus  $c(\rho)$  is also constant on each characteristic. From the second equation we then have that each characteristic is a straight line of slope  $c$ . The solution surface  $\rho(x, t)$  is thus a ruled surface whose contour lines are the family of linear characteristics. The  $x$ - $t$  slope of the characteristics, here  $c$ , is called the *characteristic speed*. It is easy to show, as may be seen by linearizing the equations for small disturbances, that the characteristic speed  $c$  is also the local sound speed.

A particular solution over some region of  $t$ - $x$  space is determined by specifying a *boundary condition*. This consists of specified values of  $\rho$  at every point of a *boundary arc*, such as arc  $AB$  of Fig. 1, which has nowhere the characteristic direction  $dx/dt = c$ . The boundary condition determines the solution everywhere in the band enclosed by the characteristics through the endpoints of the boundary arc. To see this, consider any point  $b$  ( $x_b, t_b$ ) on the boundary arc, having  $\rho_b$  as the specified value of  $\rho$ . From (20), the characteristic through this point is

$$x - x_b = c(\rho_b)(t - t_b), \quad (21)$$

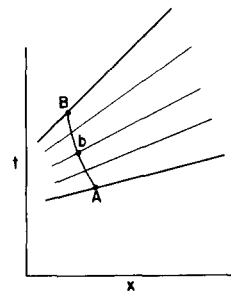


Fig. 1. Solution region determined by a boundary arc.

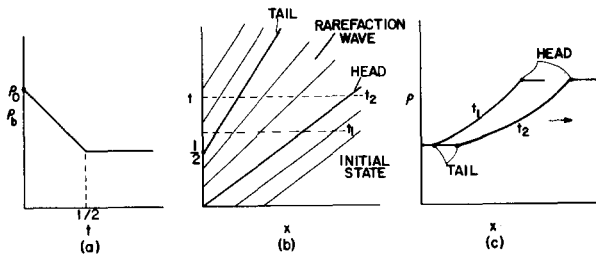


Fig. 2. Rarefaction wave. (a) Boundary condition; (b) characteristic diagram; (c) profiles at the times indicated in (b).

and  $\rho$  has the constant value  $\rho_b$  everywhere on this characteristic. Repeating this process for each point of the boundary arc, we see that the solution is determined everywhere in the band. Thus the value of  $\rho$  at each point of the boundary arc is “propagated” out along the characteristic through that point.

Throughout, we shall consider solutions only in the first quadrant of the  $t$ - $x$  plane. We also keep to a special choice of the boundary arc: the union of the positive  $x$  and  $t$  axes. Along the  $x$  axis (the *initial state*) we will always specify a constant state  $\rho = \rho_0$ . This leaves the  $t$  axis as the interesting part of the boundary arc. Along it we specify values of  $\rho$  in the form of a *boundary function*  $\rho_b(t)$ .

## B. Rarefaction waves

Let us consider the wave generated by a monotone decreasing boundary function  $\rho_b(t)$  such as the decreasing ramp function of Fig. 2(a),

$$\begin{aligned} \rho_b(t) &= \rho_0(1-t), \text{ for } 0 \leq t \leq 1/2, \\ \rho_b(t) &= \rho_1, \text{ for } t > 1/2. \end{aligned} \quad (22)$$

Such a wave is called a rarefaction wave.

The solution is divided into three parts by the *head* and *tail* characteristics emanating from the slope discontinuities in the boundary function, as shown in Fig. 2(b). The head characteristic is

$$x = c(\rho_0)t. \quad (23)$$

Ahead (to the right) of it, we have the initial constant state  $\rho = \rho_0$ , propagated up from the constant initial state on the  $x$  axis by characteristics parallel to the head characteristic. The tail characteristic is

$$x = c(\rho_1)(t - 1/2), \quad (24)$$

originating at the point  $t = 1/2$  on the  $t$  axis, which is the end of the ramp in  $\rho_b(t)$ . Behind (to the left of) it we have the constant state  $\rho = \rho_1$ . This is propagated to the right by the characteristics that leave the  $t$  axis from points above  $t = 1/2$ . These characteristics are parallel to the tail characteristic.

Between the head and tail characteristics we have the rarefaction wave, or rarefaction fan. It is easy to write this part of the solution in parametric form. The convenient parameter is the value of  $t$  between  $t = 0$  and  $t = 1/2$  on the  $t$  axis, which we call  $\tau$ . To obtain the solution in parametric form, we simply write down the solution on the characteristic through a point  $x = 0, t = \tau$  for arbitrary  $\tau$ . This is

$$\rho = \rho_b(\tau) = \rho_0(1 - \tau) \quad (25a)$$

on

$$x = c[\rho_b(\tau)](t - \tau). \quad (25b)$$

For our standard nonreactive equation of state (17) with  $c = \rho$ , we can eliminate  $\tau$  to obtain an explicit solution for  $\rho(x, t)$ . Solving (25b) for  $\tau$  and substituting for  $\rho_b(\tau)$  from (25a) gives

$$\tau^2 - (t + 1)\tau + (t - x/\rho_0) = 0. \quad (26)$$

The desired explicit solution is then, from (25a),

$$\rho(x, t) = \rho_0[1 - \tau(x, t)], \quad (27)$$

where  $\tau(x, t)$  is the solution of the quadratic equation (26). The wave gets longer and flatter as it runs, as indicated by the successive profiles in Fig. 2(c).

The response to a negative step function in  $\rho_b$  is a particularly simple configuration called a *centered rarefaction wave*. It may be obtained as the limit of the above solution as the ramp interval goes to zero, but more easily by noting that there is no longer any time scale in the problem. This suggests looking for a self-similar solution, that is, one having  $x/t$  as the single independent variable. Thus we try

$$\rho(x, t) = \rho(x/t) \quad (28)$$

in (6a). The result is immediate: either  $\rho = \text{const}$  or  $c(\rho) = x/t$ . The complete solution for a negative step in  $\rho_b(t)$  from  $\rho_0$  down to  $\rho_1$  at  $t = 0$  is then

$$\begin{aligned} \rho &= \rho_0, \text{ for } x/t > c(\rho_0), \\ c(\rho) &= x/t, \text{ for } c(\rho_1) \leq x/t \leq c(\rho_0), \\ \rho &= \rho_1, \text{ for } x/t < c(\rho_1). \end{aligned} \quad (29)$$

This solution, Fig. 3, has constant initial and final states as before, but now all characteristics of the fan emanate from the origin so that snapshots at different times are all identical provided we plot  $\rho$  against  $x/t$ . Note that for our standard nonreactive equation of state for which  $c = \rho$ , the state within the fan becomes  $\rho = x/t$ .

## C. Shocks

If we take  $\rho_b(t)$  increasing with time instead of decreasing, the characteristics are converging instead of diverging and we have a compression wave, Fig. 4. This wave becomes steeper and shorter with time instead of flatter and longer like the rarefaction wave. It can be shown that the earliest crossing of an adjacent pair of characteristics occurs in the interior of the quadrant, that is, at some nonzero positive  $t$  and  $x$ . After this time of first crossing, the wave profile will contain a growing triple-valued region, like an ocean wave breaking. In most applications, and certainly in ours, this is physically inadmissible, and we replace the triple-valued solution by a jump discontinuity, or shock, as

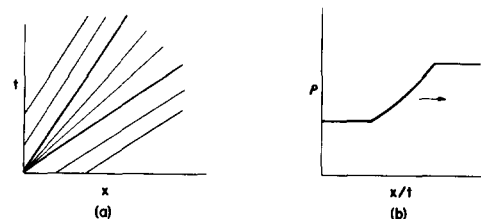


Fig. 3. Centered rarefaction wave. (a) Characteristic diagram; (b) profile.

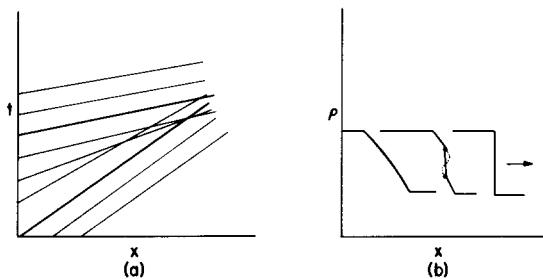


Fig. 4. Shock formation. (a) Characteristic diagram; (b) profiles.

indicated by the vertical segments in Fig. 4(b). A qualitative discussion of the process of shock formation may be found in Ref. 9. We shall be more interested here in the properties of the shock after it is formed.

The motion of the shock is governed by an algebraic relation. Although this relation can be derived directly from the differential equation (6a), it is simpler to appeal to the original physical mass-conservation requirement at the beginning of Sec. III. Figure 5 shows a profile and  $p$ - $\rho$  diagram. Denote the shock velocity by  $D$ , the state ahead (zero in the figure) by subscript zero, and the state behind (one in the figure) by a plain symbol. The mass flux into the shock ahead is  $\rho_0(D - u_0)$  and that out behind is  $\rho(D - u)$ . Equating these and solving for  $D$  gives

$$D = (\rho_1 u_1 - \rho_0 u_0) / (\rho_1 - \rho_0) \quad (30)$$

or

$$p_1 - p_0 = D(\rho_1 - \rho_0). \quad (31)$$

The construction for the shock state in the  $p$ - $\rho$  plane is as follows: The state must of course lie on the state curve  $p(\rho)$ . For a shock of specified velocity  $D$ , it must also lie on the straight line (31), which we call the *Rayleigh line* after the original (see Appendix A). The upper intersection 1 of these two curves in Fig. 5(b) is the shock state for the given value of  $D$ .

In Sec. III B we found that the response to a negative step function on the boundary is a centered rarefaction wave. What is the counterpart here, that is, the response to a positive step function, say  $\rho_b$  stepping from  $\rho_0$  up to  $\rho_1$  at  $t = 0$ ? It is the flat-topped shock shown in Fig. 5, a jump from  $\rho_0$  to  $\rho_1$ , followed by the constant state  $\rho = \rho_1$ . The shock velocity is given by (31), with  $p_1 = p(\rho_1)$ .

How is the shock affected by the flow around it? Let us compare the shock speed with the sound speeds before and behind, that is, at states 0 and 1 of Fig. 5. Recall that the shock speed is the slope of the Rayleigh line, and the sound speed is the slope of the state curve. For a well-behaved

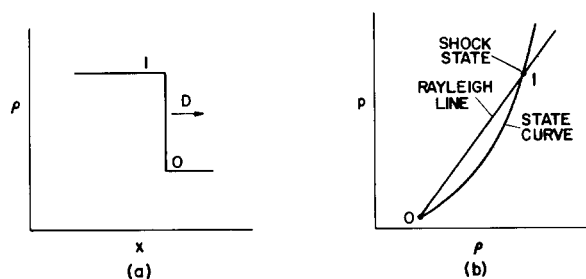


Fig. 5. (a) Shock profile; (b) Rayleigh line.

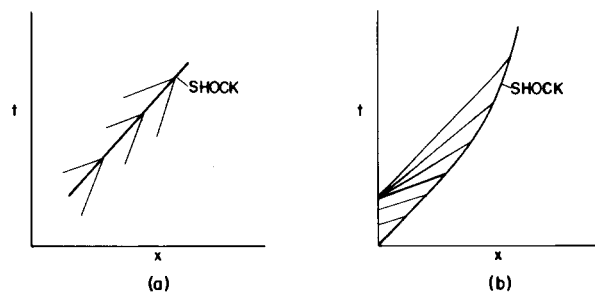


Fig. 6. Effect of neighboring flow on a shock. (a) The shock speed lies between the characteristic speeds ahead and behind. (b) Centered rarefaction wave overtaking and degrading a shock.

(concave upward) equation of state, we see by comparing these slopes in Fig. 5(b) that the sound speed behind (point 1) is greater than the shock speed, and that the sound speed ahead (point 0) is less than the shock speed. The shock is thus overtaken by characteristics from behind and overtakes characteristics ahead as indicated in Fig. 6(a). It is therefore affected by what is going on both ahead and behind. The standard equation of state (7) gives a particularly simple case. For it, the shock velocity is, from (31),

$$D = (1/2)(\rho_1 + \rho_0) = (1/2)(c_1 + c_0), \quad (32)$$

that is, the shock speed is the mean of the sound speeds before and behind.

As an example of how the flow behind affects a shock, consider the response to a boundary function  $\rho_b(t)$  consisting of a square pulse: a positive step generating a flat-topped shock, followed at a later time by a negative step generating a centered rarefaction, as shown in Fig. 6(b). The head of the rarefaction moves at the sound speed behind the shock. Because this sound speed is greater than the shock speed, the rarefaction wave overtakes the shock. As the process continues, characteristics carrying successively lower values of  $\rho$  overtake the shock and reduce its strength. Thus a shock is vulnerable to overtake and degradation by a following rarefaction wave.

#### IV. REACTIVE FLOW

In this section we follow the outline of Sec. III, limiting ourselves to stating those properties of reactive flow (as they appear in the analog) that are needed for the discussion of detonations to follow. From here on we will always take the constant initial state  $\rho = \rho_0$ ,  $\lambda = \lambda_0 = 0$ . The only shocks we consider are at the head of a wave, so that the state ahead of the shock is always the initial state.

##### A. Characteristics

There are two families of characteristics:  $dx/dt = c$  and  $dx/dt = 0$ , where  $c = p_\rho$ . As before, the characteristic speed is the local sound speed. These two families of characteristics represent right-going acoustic signals and (roughly) particle paths, respectively. We shall be concerned here only with the first family.

##### B. Rarefaction waves

We will not need to consider rarefaction waves in which reaction occurs. However, we will need a rarefaction wave

similar to the nonreactive centered wave (29), but running into completely reacted material ( $\lambda = 1$ ) behind a detonation wave. If we fix  $\lambda$  at 1, the reactive equations (13a)–(13d) with the standard equation of state (16) become just the nonreactive set (6a) and (6b) with equation of state  $p = (1/2)(\rho + q)^2$ ,  $c = p + q$ . We have then just a nonreactive centered wave with this equation of state. Its head propagates at

$$\frac{dx}{dt} = c(\rho_0) = \rho_0 + q. \quad (33a)$$

In the fan we have  $x/t = c(\rho)$ , or

$$\rho = x/t - q. \quad (33b)$$

### C. Shocks

The Rayleigh-line relation (31) applies as before. We need to specify in addition how  $\lambda$  changes across the shock. Because the shock jump is instantaneous while the reaction rate is finite, we require that  $\lambda$  be unchanged through the shock, that is, that  $\lambda_1 = \lambda_0$ . The shock state will thus be on the intersection of the Rayleigh line and the  $\lambda = \lambda_0$  state curve.

As in the nonreactive case, shocks overtake characteristics ahead and are overtaken by characteristics from behind. The analogous question of the overtaking of a detonation wave by characteristics from behind is taken up in Sec. VI.

## V. DETONATION

In this section we return to the physical system for a qualitative description of the phenomenon of detonation. A detonation<sup>18–20</sup> is a shock wave driven by a closely following chemical reaction. A momentary impulse applied at the edge of a nonreactive material results in a shock that decays in the manner depicted in Fig. 6(b). A similar impulse applied to an explosive will, if strong enough, initiate a detonation wave. Here the heating and compression of the shock jump trigger an exothermic chemical reaction, which in turn supplies the energy to sustain the shock. An explosive, then, is a material that is potentially capable of strongly exothermic reaction, but is normally resting quietly in a state of metastable equilibrium. A stoichiometric mixture of hydrogen and oxygen gas at room temperature is an example. At this temperature, the true equilibrium state of the mixture is essentially pure water, but in the absence of strong perturbations, the reaction rate is so slow that it is, for all practical purposes, nonexistent. Reaction can, however, be triggered by a suitable stimulus such as a spark, which initiates a reaction wave that spreads through the material.

Depending on the mode and strength of initiation, the reaction wave can be one of two types: either a deflagration (flame) or a detonation. We consider here only one-dimensional waves. We can think of them as generated in an idealized experiment as follows. Confine the explosive in a long rigid tube of large enough diameter that edge effects can be neglected. Close one end of the tube by either a fixed end plate or a moveable piston. To generate a deflagration, use the fixed end plate, heating it suddenly and uniformly over its area. To generate a detonation, use the piston, giving it a strong blow.

A deflagration wave moves at slow subsonic speed—a few meters per second in gases. Although the pressure drops slightly through the wave, momentum changes are small; the important processes are diffusion, heat conduction, and viscosity. If the deflagration wave is confined, as by leaving the end plate in place after ignition in the above experiment, it will eventually change into detonation. We shall say no more here about deflagrations.

A detonation is very different. It runs at supersonic speed—1000 or 2000 m/sec in gases. The pressure (in gases) is on the order of 20 times the initial pressure, and the temperature is several thousand degrees. Momentum changes are controlling, because the reaction is over too quickly for other processes to have much effect; the reacting material is inertially confined in a thin layer behind the shock. Both detonation and deflagration waves convert chemical bond energy to translational energy. In a detonation wave, energy conversion is very rapid because the propagation velocity is so high. A 10-cm<sup>2</sup> detonation front in a solid explosive like TNT converts energy at a rate of 10<sup>11</sup> W, a figure comparable to the total electric generating capacity of the U.S.

The structure of a steady detonation wave is shown in Fig. 7. This structure, the so-called ZND model,<sup>18</sup> was proposed independently in the early 1940's by Zeldovich in Russia, von Neumann in the U.S., and Doering in Germany. The leading element is a shock, which instantaneously heats the material and triggers the reaction. Immediately behind the shock is the relatively short reaction zone in which the reaction proceeds to completion. The reaction zone is steady in the coordinate frame attached to the shock. Following the steady reaction zone is a time-dependent rarefaction wave that reduces the pressure down to the low value ordinarily obtaining at the rear boundary.

In Sec. VI we write down and solve the equations (in the analog) for a steady detonation wave.

## VI. STEADY SOLUTIONS

We pose the following problem: given a constant value of  $\rho_b$  at the rear of the wave, find a steady detonation solution of the ZND type, that is, one consisting of a shock and its attached steady reaction zone, both moving with a constant velocity  $D$ , and followed by a possibly unsteady nonreactive flow. We call the shock and its attached reaction zone at the front the *steady solution*, the complete-reaction state at the end of the reaction zone the *final state*,

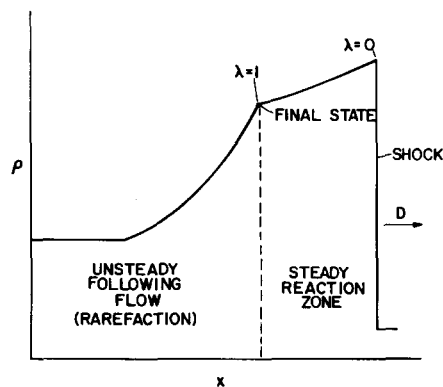


Fig. 7. ZND model of a detonation.

the nonreactive flow in the rear the *following flow*, and the constant propagation velocity  $D$  the *detonation velocity*.

The plan of attack is to divide the problem into two parts, addressing first the front part of the flow and then the back part. We call these the *velocity problem* and the *boundary problem*, respectively.

The *velocity problem* is the determination of all possible candidates for the steady part of the flow—the shock and its attached reaction zone—disregarding the requirements imposed by the rear boundary condition. As we shall shortly see, the equations governing this part of the flow contain the detonation velocity  $D$  as a parameter. For the complete problem,  $D$  is uniquely determined by the specified rear boundary condition, but for now we treat it as a free parameter. Choosing a given value of  $D$  (within a certain range) determines a particular steady solution. Varying  $D$  over the allowed range, we obtain the complete one-parameter family of all possible steady solutions. Of particular interest in each of these solutions is the final state to which the following flow must be joined.

The *boundary problem* is the choice of the appropriate steady solution from this family, plus the determination of the following flow such that the specified boundary condition is satisfied. This is essentially a two-point boundary value problem: the following flow is required to match the given value of  $\rho_b$  on the left, and the final state of the selected steady solution on the right. As we shall see, this is not as difficult as it sounds.

### A. Steady equations

The equations for a solution steady in a frame moving with a given constant velocity  $D$  are obtained in the usual way—by first transforming the time-dependent equations to this frame and then setting the time derivatives to zero.

Let  $\hat{x}$  denote position in the new steady frame. The transformation is

$$\hat{x}(y, t) = x - Dt. \quad (34)$$

The partial derivatives transform as follows:

$$\begin{aligned} \left(\frac{\partial}{\partial t}\right)_x &= \hat{x}_t \left(\frac{\partial}{\partial \hat{x}}\right)_t + \left(\frac{\partial}{\partial t}\right)_x, \\ \left(\frac{\partial}{\partial x}\right)_t &= \hat{x}_x \left(\frac{\partial}{\partial \hat{x}}\right)_t. \end{aligned} \quad (35)$$

Substituting  $\hat{x}_t = -D$  and  $\hat{x}_x = 1$  from (34), this transformation becomes

$$\begin{aligned} \left(\frac{\partial}{\partial t}\right)_x &= -D \left(\frac{\partial}{\partial \hat{x}}\right)_t + \left(\frac{\partial}{\partial t}\right)_x, \\ \left(\frac{\partial}{\partial x}\right)_t &= \left(\frac{\partial}{\partial \hat{x}}\right)_t. \end{aligned} \quad (36)$$

Under this transformation the governing equations (13a) and (13b) become, in the new frame

$$\begin{aligned} -D\rho_{\hat{x}} + \rho_t + p_{\hat{x}} &= 0, \\ -D\lambda_{\hat{x}} + \lambda_t &= r. \end{aligned} \quad (37)$$

For a steady solution, the dependent variables depend only on  $\hat{x}$  and the time derivatives vanish. We have then the following pair of ordinary differential equations

$$\frac{dp}{d\hat{x}} - \frac{Dd\rho}{d\hat{x}} = 0, \quad (38a)$$

$$\frac{d\lambda}{d\hat{x}} = \frac{-r}{D}. \quad (38b)$$

The first of these integrates immediately to

$$p(\rho, \lambda) - p_1 = D(\rho - \rho_1), \quad (39)$$

where the subscript one denotes an arbitrary point of the solution chosen as the initial point for the integration, and we have indicated explicitly the dependence of  $p$  on  $\rho$  and  $\lambda$  through the equation of state (13c). For a given value of  $D$ , this solution (39) gives the dependence of  $\rho$  on  $\lambda$  throughout the steady solution if any one point (point 1) is given. Note that its form is similar to that of the Rayleigh-line relation (31).

We can eliminate the unknown initial point 1 as follows: we take it to be the point immediately behind the shock, which we can then express in terms of the initial state via the Rayleigh-line relation (31),

$$p_1 - p_0 = D(\rho_1 - \rho_0). \quad (31)$$

If we solve (31) for  $p_1$  and substitute in (39), we find that  $\rho_1$  also drops out and we obtain an implicit expression for the steady solution  $\rho(\lambda; D)$  having  $\lambda$  as the independent variable and  $D$  as the only parameter

$$p(\rho, \lambda) - p_0 = D(\rho - \rho_0). \quad (40)$$

This equation states that in the  $p$ - $\rho$  plane the solution lies entirely on the Rayleigh line for the given  $D$ .

We now have the steady solution with the degree of reaction  $\lambda$  as the independent variable. To get it as a function of  $x$  we integrate the rate equation (38b). With  $\rho(\lambda)$  known this becomes a single ordinary differential equation for  $\lambda(\hat{x}; D)$ ,

$$\frac{d\lambda}{d\hat{x}} = \frac{-r[\rho(\lambda), \lambda]}{D}, \quad (41)$$

with the right-hand side a function of  $\lambda$  alone.

It turns out that we have no need of the  $\hat{x}$  dependence other than to actually exhibit the spatial profile. The important results require only the  $\lambda$  dependence and are independent of the choice of rate function.

### B. Velocity problem

We seek the complete one-parameter ( $D$ ) family of solutions of (40) encompassing the entire reaction zone. Each solution must satisfy two conditions: (i) it must lie on the Rayleigh line in the  $p$ - $\rho$  plane for the given  $D$ , and (ii) its final state must lie on the complete-reaction ( $\lambda = 1$ ) state curve.

Figure 8 shows three constant- $\lambda$  state curves. Recall the “well-behaved” properties given at the end of Sec. II: each fixed- $\lambda$  curve has positive slope and is concave upward, and the curves are displaced upward as  $\lambda$  increases, with no one crossing another. Now, the possible final states are the intersections of some Rayleigh line with the  $\lambda = 1$  state curve. Looking at the Rayleigh lines of Fig. 8, we see that there are zero, one, or two such intersections according as  $D$  is less than, equal to, or greater than the value at which the two curves are tangent. Thus the tangent value of  $D$  is the minimum possible steady propagation velocity.<sup>21</sup> In the standard terminology, the tangent velocity is called the

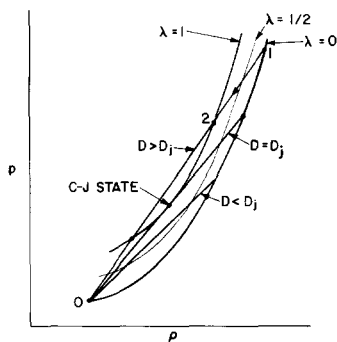


Fig. 8. The  $p$ - $\rho$  diagram for a steady detonation.

Chapman-Jouguet (CJ) velocity and the corresponding final state, the tangent point, the CJ state (point). We use subscript  $j$  to denote CJ quantities.

Of the two intersections for  $D > D_j$ , the lower one is readily eliminated by considering the nature of the solution. Consider the sequence of states in the  $p$ - $\rho$  plane, Fig. 8, as the wave sweeps over a fixed station. The shock raises the state instantaneously from the initial state 0 to the shock state 1, both on the  $\lambda = 0$  curve. As reaction proceeds, the state point moves in the direction of increasing  $\lambda$ , that is, down the Rayleigh line (as shown by the arrow in Fig. 8). It stops at the upper intersection 2, where the reaction is complete at  $\lambda = 1$ . Thus the upper intersection, and not the lower, is the final state actually reached. For  $D = D_j$ , the two intersections have coalesced into the CJ point, which is the final state for this case.

We have now determined the general nature of the steady solutions and determined their most important property: that there is a minimum possible propagation velocity, the tangent, or CJ, value. It remains to examine in more detail the properties of the final state, to which we must join the following nonreactive flow.

For the discussion of the boundary problem to follow, the important property is the ratio of  $c$  to  $D$  in the final state. Recall the nonreactive case discussed at the end of Sec. III C: Behind a shock the sound speed  $c$  is always greater than the shock speed, so rarefaction waves coming from behind always overtake and degrade the shock. Similar considerations arise here, and we need to know this same ratio in the final state at the end of the reaction zone. Recall that the sound speed is just  $p_\rho$ , the slope of a fixed- $\lambda$  curve in the  $p$ - $\rho$  plane, while the steady-wave velocity  $D$  is the slope of the Rayleigh line. From Fig. 8 we see that the fixed- $\lambda$  curve is the steeper of the two for all values of  $D$  of interest except the tangent value  $D = D_j$ , where their slopes are equal. Thus we have  $c > D$  for  $D > D_j$ , and  $c = D$  for  $D = D_j$ . A following rarefaction wave therefore travels at the same speed as the reaction zone for  $D = D_j$  but will overtake it for all larger  $D$ .

### C. Boundary problem

With the above family of steady solutions at our disposal, we want to choose one and join to it a suitable following flow so that the entire solution is consistent with the specified value of  $\rho_b$ . We do this for all values of  $\rho_b$ , beginning with an arbitrarily large value and working down.

Denote by  $\rho_f(D)$  the final-state value of  $\rho$  for the given  $D$ , and by  $\rho_j$  the CJ value of  $\rho_f$  that is,  $\rho_j = \rho_f(D_j)$ , the value of  $\rho$  at the CJ point. There are two cases:  $\rho_b \geq \rho_j$  and  $\rho_b < \rho_j$ .

As long as  $\rho_b \geq \rho_j$ , we have a very simple solution: that value of  $D$  for which  $\rho_f$  is equal to  $\rho_b$ . The following flow is then just the constant-state  $\rho = \rho_f = \rho_b$ , and  $\lambda = 1$ . This is called an *overdriven detonation*; because  $\rho_f(D)$  is a monotone increasing function, the harder the "push" (that is, the greater the value of  $\rho_b$ ) the faster it goes. In this respect the overdriven detonation is like a nonreactive shock.

For  $\rho_b < \rho_j$ , we cannot have such a simple solution, for  $\rho_j$  is the minimum possible value of  $\rho_f$  for any steady solution. We tentatively choose the minimum propagation velocity  $D = D_j$ . We must then choose a following flow which reduces the density from  $\rho_j$  at the final state to the smaller value  $\rho_b$  at the boundary. From the discussion of Secs. III and IV, the obvious choice is a rarefaction wave (with  $\lambda = 1$  throughout). We can place the head of the rarefaction wave at the final state of the reaction zone, because for  $D = D_j$  we have  $c/D = 1$  in the final state and the two waves propagate at the same velocity. This is the *CJ*, or *self-sustaining*, or *unsupported*, detonation. It runs at CJ velocity regardless of the value of  $\rho_b$  (as long as it is less than  $\rho_j$ ). The state at the tail of the following rarefaction is of course fixed by the specified value of  $\rho_b$ , as in Sec. III.

Had we chosen any value of  $D$  larger than  $D_j$  here, the rarefaction wave required to match the rear boundary would overtake the reaction zone (because  $c$  is greater than  $D$  in its final state as shown above). The consequent degradation of the steady solution is similar to that of a shock followed by a rarefaction wave, described in Sec. III C. The flow eventually approaches the CJ solution just described, with  $D = D_j$ .

In practice, detonations run so fast that the unsupported, or CJ, detonation is the usual case. The detonation front, consisting of a shock followed by a short reaction zone, runs at the minimum propagation velocity. This front, moving at supersonic speed, propagates without any help from behind, being driven by the energy of chemical reaction. The large-amplitude rarefaction wave which follows the front effectively isolates it from small-amplitude disturbances from the rear. By pushing very hard, that is, by giving a following piston a very high velocity, we can overdrive the detonation, raising both its pressure and velocity. The overdriven detonation is followed by a constant state and is, like a nonreactive shock, sensitive to disturbances from behind.

### D. Example

We calculate steady solutions for our standard equations of state (16) and rate (18). To simplify the equations, we choose  $\rho_0 = 0$  as the initial state. (This may be regarded as the limit of large heat of formation, with  $q/\rho_0$  approaching infinity.) Additional simplification results from taking  $c = \rho + q\lambda$  instead of  $\rho$  as the independent variable. Substituting the equation of state (16) into the Rayleigh-line relation (40) for the steady solution gives for  $c(\lambda; D)$

$$c/D = 1 + (1 - \lambda/\alpha)^{1/2}, \quad (42a)$$

$$\alpha = D/2q. \quad (42b)$$

This is the solution of a quadratic equation; we have suppressed the negative sign corresponding to the lower intersection of Fig. 8. The tangency condition for the CJ deto-



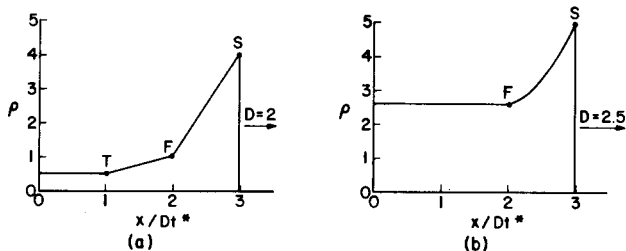


Fig. 9. Steady detonations for  $\rho_0 = 0$ ,  $q = 1$ . Here  $S$  is the shock,  $F$  the final state (end of the reaction zone), and  $t^*$  the reaction time. (a) CJ detonation (unsupported),  $\alpha = D/D_j = 1$ .  $T$  is the tail of the following rarefaction wave. (b) Overdriven detonation,  $\alpha = D/D_j = 1.25$ .

nation is that the radical vanish. This gives for the CJ velocity  $D_j = 2q$ . We can thus write the coefficient  $\alpha$  in (42b) as  $\alpha = D/D_j$ ; we call  $\alpha$  the degree of overdrive. Note that in the shock state ( $\lambda = 0$ ) the value of the quantity  $c/D$  is always 2, and that it decreases through the reaction zone. At  $\lambda = 1$  it is greater than 1 for  $D > D_j$  and equal to 1 for  $D = D_j$ , as it should be.

For the  $\hat{x}$  dependence, integration of the rate equation (38b) with our standard rate function (18) gives

$$\lambda = 1 - (1 - \tau)^2, \quad (43a)$$

$$\tau = -\hat{x}/Dt^*, \quad (43b)$$

$$t^* = 2/k, \quad (43c)$$

where  $t^*$  is the reaction time and  $Dt^*$  the reaction-zone length. Here  $\hat{x}$  is positive in the steady frame with origin  $\hat{x} = 0$  at the shock. The variable  $\tau$  is the time (in units of  $t^*$ ) for an observer watching the wave sweep past a fixed position in the original frame, with  $\tau = 0$  at the moment the shock arrives. Substituting (43a) for  $\lambda(\hat{x})$  into (42a) for  $c(\lambda)$  gives for  $c(\hat{x})$ ,

$$c/D = 1 + [1 - a + a(1 - \tau)^2]^{1/2}. \quad (44)$$

For  $D = D_j$ , this simplifies to

$$c/D = 2 - \tau. \quad (45)$$

We remark that  $dc/d\tau$  and  $d\rho/d\tau$  at the end of the reaction zone are  $-1$  for  $D = D_j$  and  $0$  for all  $D > D_j$ .

Profiles and  $t$ - $x$  diagrams for a CJ ( $\alpha = 1$ ) and an overdriven ( $\alpha = 1.25$ ) detonation are shown in Figs. 9 and 10. These are calculated from (44) with  $q = 1$ ; they are displayed in the original frame (in which the shock moves at velocity  $D$ ) with time and space units  $t^*$  and  $Dt^*$ .

For the CJ detonation, Figs. 9(a) and 10(a), we have chosen a boundary density  $\rho_b$  (for  $t/t^* > 1$ ) of zero, and a following flow consisting of a centered rarefaction wave, with center at  $t = 0$ ,  $x = 1$  so that its head coincides with the path  $F$  of the final state. The vertical extent of the reaction zone relative to that of the following rarefaction is larger than that usually seen in the physical system, which is more like Fig. 8.

The overdriven detonation, Figs. 9(b) and 10(b), requires a following constant state with  $\rho$  (and thus  $\rho_b$ ) equal to the final-state value, which is 2.168 for the degree of overdrive chosen.

## APPENDIX: PHYSICAL SYSTEM

The standard equations for inviscid, compressible flow with chemical reaction are the so-called Euler equations,

with chemical reaction added. In one dimension and for a system with a single chemical reaction, these are<sup>18,19</sup>

$$\dot{\rho} + \rho u_x = 0 \quad (A1a)$$

$$\dot{u} + v p_x = 0 \quad (A1b)$$

$$\dot{e} + p v = 0 \quad (A1c)$$

$$\dot{\lambda} = r \quad (A1d)$$

$$p = p(\rho, e, \lambda) \quad (A1e)$$

$$r = r(\rho, e, \lambda). \quad (A1f)$$

Here  $\rho$ ,  $u$ ,  $p$ , and  $e$  are the density, particle velocity, pressure, and specific internal energy, respectively;  $v (= 1/\rho)$  is the specific volume; and  $\lambda$  is the reaction progress variable, whose value determines the chemical composition of the system. The dot denotes a material derivative, that is, the total time derivative of the state of a fluid element. In  $t$ - $x$  space it is the derivative along a particle path (convective derivative) and is thus, for any function  $f(x, t)$ ,

$$f = f_t + u f_x. \quad (A2)$$

The first three equations express the conservation of mass, momentum, and energy, respectively. The fourth describes the progress of the reaction. To complete the description of a particular system we must specify the two constitutive relations (material-response functions): the equation of state (A1e) and the reaction rate (A1f). The equation of state gives the pressure  $p$  as a function of the local thermodynamic state  $(\rho, e, \lambda)$ , that is, as a function of density, energy, and composition. Similarly, the rate function gives the reaction rate  $r$  as a function of the same local state.<sup>22</sup>

This system of equations (A1a)–(A1f) is hyperbolic; that is, its solutions take the form of waves traveling through the material. These may contain moving jump discontinuities, or shocks. A shock is described by a set of algebraic relations, derivable from the differential equations (A1a)–(A1f), called the Rankine-Hugoniot conditions.<sup>10</sup> These relate the states immediately before the behind a shock to its propagation or shock velocity  $D$ . In a form commonly used, but not in precise one-one correspondence with (A1a)–(A1f), these relations are

$$u^2 = (p - p_0)(v_0 - v), \quad (A3a)$$

$$\rho_0^2 D^2 = (p - p_0)/(v_0 - v), \quad (A3b)$$

$$e - e_0 = (1/2)(p + p_0)/(v_0 - v), \quad (A3c)$$

$$\lambda = \lambda_0. \quad (A3d)$$

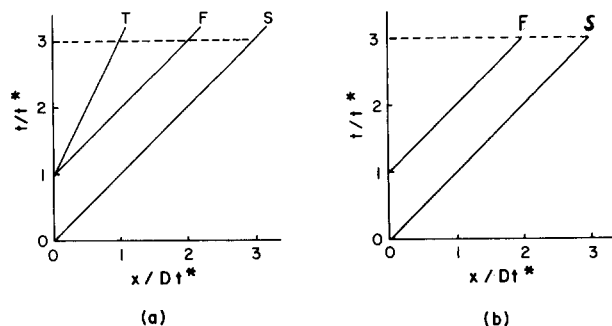


Fig. 10.  $t$ - $x$  diagrams for the detonations of Fig. 10. The profiles of Fig. 10 are at the times indicated by the dashed lines.

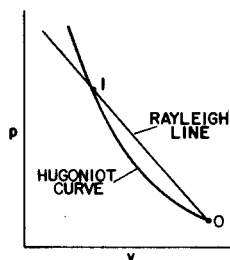


Fig. 11. Shock equations in the  $p$ - $v$  plane.

Here the subscript 0 denotes the state ahead of the shock, or *initial state*, and a symbol without a subscript the state behind, or *shocked state*. The first two equations together express the conservation of mass and momentum, and the third gives the conservation of energy. The fourth states that the composition does not change through the shock (because the shock jump is instantaneous while the reaction rate is finite). The most used of these relations are (A3b) and (A3c); they are customarily diagrammed in the  $p$ - $v$  plane, Fig. 11, for a given initial state. The *Rayleigh line* (A3b) is a straight line whose slope is proportional to the square of the shock velocity  $D$ . Substitution of the equation of state  $e(p, \rho, \lambda)$  into (A3c) [with the use of (A3d)] gives the *Hugoniot curve* in the  $p$ - $v$  plane, which is the locus of all possible shocked states, from a given initial state  $(p_0, v_0, \lambda_0)$ , for the given material. For a given shock velocity  $D$ , the shocked state, such as  $(p_1, v_1)$  in Fig. 11, is the intersection of the Rayleigh line for that  $D$  with the Hugoniot curve. The particle velocity in the shocked state is then given by (A3a).

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- <sup>21</sup>A possible solution that suggests itself for  $D$  less than the tangent value is one in which the reaction, incomplete at the end of the steady zone, is completed in a nonsteady following flow. It can be shown that such solutions do not exist.
- <sup>22</sup>The usual set of variables defining the local thermodynamic state is  $(\rho, T, \lambda)$ , with temperature  $T$  instead of internal energy  $e$ . Here  $e$  is more convenient because one of the equations expresses conservation of energy. Our equation of state  $p(\rho, e, \lambda)$  is "incomplete" in the sense that the temperature is not determined by local values of its partial derivatives. See M. Cowperthwaite, *J. Franklin Inst.* **287**, 379 (1969).