

MASTER

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THE INITIATION TRANSIENT IN DILUTE EXPLOSIVES

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In the context of the shock-initiation problem, we study analytically the first effects of chemistry, treating a small chemical heat release as a perturbation on an inert flow. Specifically, we study the initial transient in plane-shock initiation in a dilute explosive where the chemical energy is small relative to the mechanical-thermal energy. The vehicle for the study is the mathematical analog for reactive flow recently proposed by the author.

The solution resembles a double refraction: to first order, the pressure or density is a superposition of two forward-going waves, both originating at the rear boundary, and carrying the same function, but running at different velocities. Surprisingly, this first-order solution is independent of the sensitivity of the reaction rate to the state, which appears only at second order.

I. INTRODUCTION

We study analytically a limiting case of the general question, "How does the process of plane-shock initiation depend on the properties of the reaction rate?" To fix ideas, consider a system obeying the usual equations of motion (the Euler equations for inviscid compressible flow with chemical reaction [1, Sec. 4A3]), with reaction proceeding according to a first-order Arrhenius rate law,

$$r = k(1 - \lambda)e^{-T^*/T} \quad (1.1)$$

Here k is the rate multiplier, T^* is the activation temperature, and λ is the composition or degree of reaction (for reaction $A \rightarrow B$, λ is the mass fraction of B). For the problem of interest here, the multiplier k is a trivial parameter, serving only to set the time scale. The significant parameter is T^* ; it determines the sensitivity of the rate to the state. (In this paper, we use the word "sensitive" only in this sense, and not in the more common sense of the sensitivity of the explosive to some initiating stimulus.)

Calculations show that the nature of the initiation process depends strongly on the sensitivity of the rate. Figure 1 contrasts calculated initiation transients for sensitive and insensitive rates [2]. The system is a polytropic gas with reaction $A \rightarrow B$ obeying the first-order Arrhenius rate (1.1). The detonation is produced by a constant-velocity piston, and is

overdriven, with a final steady-wave velocity D which is $\sqrt{1.6}$ times the CJ value. The insensitive rate has $T^* = 0$, and the sensitive one has $T^* = 40T_0$, with T_0 the initial temperature. The solution is presented as a sequence of snapshots of the pressure profile (h is a Lagrangian space variable), plus the shock-pressure history.

The results for the two cases are quite different. In the insensitive case, Fig. 1a, the reaction zone always has about the same shape as the final steady state, and the shock pressure rises to its final steady value in a smooth, monotonic fashion. In the sensitive case, most of the initial reaction takes place at the piston, where the shocked material has been hot the longest. This hot spot gives rise to a reactive compression pulse. The pulse accelerates the reaction locally by compression heating, and grows as it goes, feeding on the heat of reaction. The profiles become humped -- that is, they have pressure maxima -- as the pulse proceeds. As it overtakes the shock, the shock pressure rises rapidly and then falls, tracking the shape of the pulse.

A much-used tool for studying flows of this type is the shock-change equation [1, Sec. 4Ab]. We write it down here for later reference. It expresses the rate of change of the shock strength as the sum of a gradient term and a reaction term:

$$dp_s/dt = -\alpha p_s + \beta \bar{r} \quad (1.2)$$

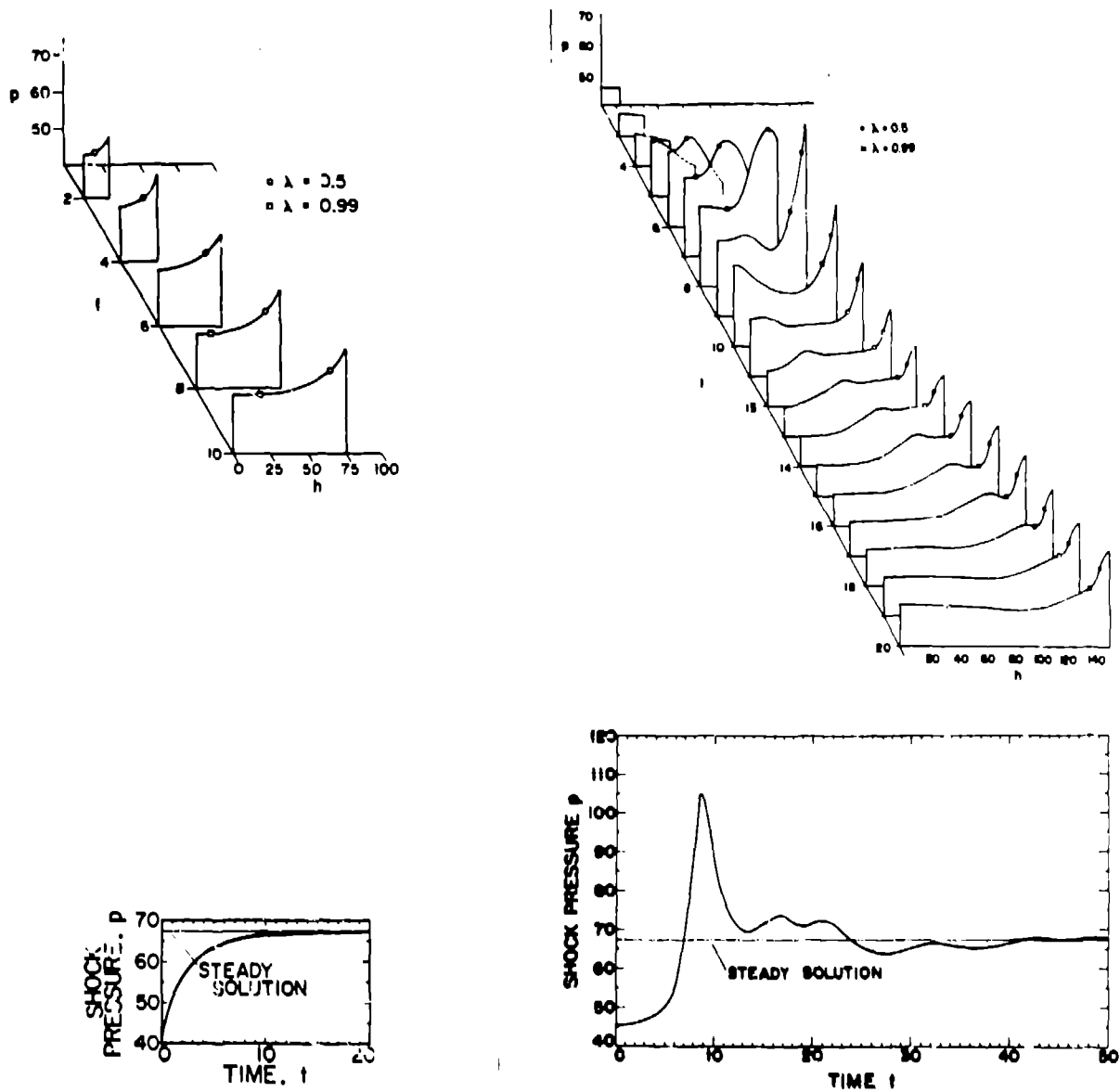


Fig. 1. Calculated shock initiation for (a) insensitive, and (b) sensitive reaction rate.

Here p_s is the shock pressure, $p_x = (\partial p / \partial x)_t$ is the pressure gradient, α is the thermicity of the reaction, r is the reaction rate, and a and B are positive-definite state functions. All quantities refer to the shocked state.

Some questions about the initiation problem are:

- (1) For what rates will some profiles have a hump?
- (2) What are the important parameters of the rate (e.g. sensitivity, λ -dependence)?
- (3) Which of the two terms of the shock-change equation is more important?

We answer these questions analytically, for

our mathematical analog (set of model equations) of reactive flow [3], in the limiting case of small heat of reaction q , with some restrictions on the form of the rate function. We use a perturbation treatment, with the inert ($q = 0$) case as the unperturbed reference flow, and the ratio of chemical to mechanical energy as the smallness parameter ϵ .

The solution resembles a double refraction: it is the superposition of two forward-going waves, both originating at the rear boundary, but traveling at different speeds. Both waves carry the same function: the (steady) composition history of the reference flow.

Examination of this solution (at first order of the perturbation) yields several interesting results:

(1) A precise criterion divides all rate functions into two classes: those which produce humped profiles and those which do not.

(2) The above criterion, and the solutions for density ρ and pressure p , depend only on the λ -dependence of the rate, and not on its sensitivity to the state. Dependence on the sensitivity appears only at second order.

(3) Of the two terms in the shock-change equation, the reaction term dominates: it is larger in magnitude than the gradient term at all times.

(4) In a comparison like that of Fig. 1, we give calculated results for a simple rate function from each class of the item (1) above. One resembles the insensitive case of Fig. 1; the other is more like the sensitive case. Appropriate λ -dependence of the rate produces results similar to those characteristic of high sensitivity.

How would we achieve our limiting case in practice? Dilution provides a dial on the chemical energy density, and the strength of drive provides a dial on the mechanical energy density. But there is a constraint: at CJ, the ratio of these two energies is of order one. To make this ratio small, we must overdrive the detonation. In practice, the available strength of drive is limited. A convenient way to get the desired small energy ratio (large overdrive) is to fix the mechanical energy by choosing a standard driver, and then make the chemical energy small by dilution. This is the approach used by Soloukhin and Brochet [4] in their study of the onset of instability in gaseous systems.

We state the problem in Sec. II, perform the analysis in Sec. III, give the results in Sec. IV, display the examples in Sec. V, and summarize the results in Sec. VI. The skimming reader should skip Sec. III (analysis) and possibly also Sec. II (detailed statement of the problem). The short recapitulation at the beginning of Sec. IV should help to bridge the gap.

II. PROBLEM

The analog [3] is:

$$\rho_t + p_x = 0 \quad (2.1)$$

$$\lambda_t = r$$

$$p = p(\rho, \lambda) \quad \text{equation of state}$$

$$r = r(\rho, \lambda) \quad \text{reaction rate.}$$

Here x and t are "distance" (better: particle label) and time, ρ and λ are density and composition, and p is "pressure." The choice of variable names is discussed in [3]. Those having a less direct connection with the original system

are in quotes here. Subscripts t , x , and (below) ρ and λ denote partial derivatives. Other subscripts (below) are part of the symbol.

The fixed-composition sound speed, which is also the (acoustic) characteristic speed, is $c = p_\rho$. For the equation of state we take

$$p = \frac{1}{2}(\rho^2 + q\lambda) \quad (2.2)$$

having

$$c = \rho \quad ,$$

and constant "heat of reaction" q .

We study the initiation transient of an overdriven detonation driven by a constant rear-boundary condition (analogous to a constant-velocity piston). Using (2.2) in (2.1) and adding the appropriate initial and boundary conditions, we have as the governing equations for our problem,

$\rho_t + \rho p_x + \frac{1}{2}q\lambda_x = 0$	(2.3)
	$\lambda_t = r(\rho, \lambda)$
shock:	$\lambda_s = 0$
	$D = \frac{1}{2}\rho_s$
initial (on $t = 0$):	$\rho_i = \lambda_i = 0$
boundary (on $x = 0$):	$\rho = \rho_b(t)$
	$= 0, t < 0$
	$= \rho_0, t \geq 0$

Subscript s denotes the state immediately behind the shock, D is the shock velocity, subscript i denotes the initial state, subscript b denotes the (rear) boundary, and subscript o denotes the reference flow defined below. The initial condition $\rho_i = 0$ simplifies the shock relation (3, Sec. VID). The boundary condition $\rho_b(t)$ is a step function, with ρ jumping from zero to the constant value ρ_0 at $t = 0$.

We find the solution for small q , treating q as a small perturbation on the reference or unperturbed flow, for which we take the solution of the same problem with $q = 0$. We show in the next section, by scaling the equations, that the appropriate smallness parameter is:

$$\epsilon = q/c_0^2 \quad (2.4)$$

essentially the ratio of the chemical to mechanical energy.

The t - x diagram for the flow is shown in Fig. 2. The acoustic characteristics, marked (+) in the figure, carry information from the boundary to the shock. The other family of characteristics [3] are less important in the present problem and will not be mentioned further

here. The time τ shown in the figure is the time at each x after passage of the shock. It will be used in the frame transformation of the next section.

The reference flow is a flat-topped shock, steady for all time. The shock velocity is $D = D_0 = \frac{1}{2}c_0$, with constant state (behind the shock) $\rho = \rho_0$, $c = c_0 = \rho_0$, $p = p_0 = \frac{1}{2}\rho_0^2$. The characteristics and shock path of Fig. 2 are straight lines. Reaction proceeds behind the shock and λ increases with time, but this has no effect on the state because the system has been decoupled by taking $q = 0$. For the steady solution for λ , we first define the mathematical function $\lambda_0(y)$ (which will appear later with different arguments) as the solution of the ordinary differential equation:

$$\begin{aligned} d\lambda_0/dy &= r(\rho_0, \lambda_0) , \\ \lambda_0 &= 0 \text{ at } y = 0 . \end{aligned} \quad (2.5)$$

The steady solution for λ is $\lambda_0(\tau_0)$, where τ_0 is the time τ (Fig. 2) after shock passage at each x for the reference solution, that is,

$$\tau_0 = t - x/D_0 . \quad (2.6)$$

We call the function $\lambda_0(y)$ the reference composition function.

We place some restrictions on the form of the rate function: We assume that reaction proceeds in the forward direction only, so that $\lambda_0(\tau)$ is a monotone-increasing function, and that reaction is complete in finite time. We also make the slightly more restrictive assumption, not needed for all of the

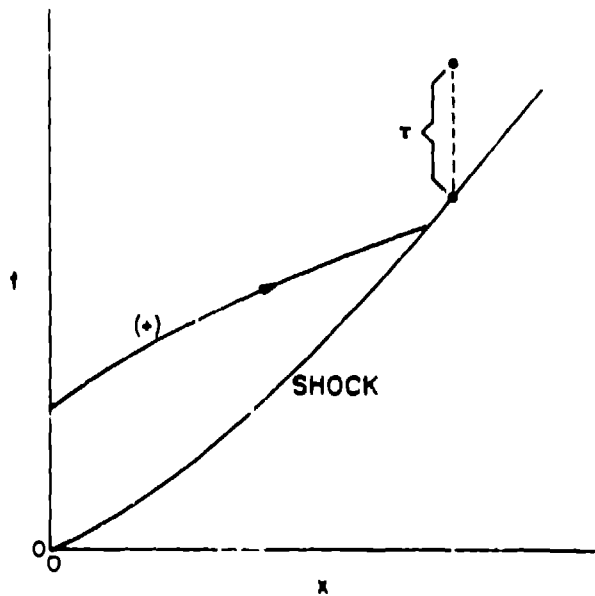


Fig. 2. Characteristic and shock paths.

conclusions, that $r(\rho, \lambda)$ be expressible, like (1.1), as the product of functions of ρ and λ , that is,

$$r(\rho, \lambda) = kf(\rho)g(\lambda) . \quad (2.7)$$

III. ANALYSIS

The plan is as follows. First we scale the equations to determine the appropriate smallness parameter. Then we transform to an accelerated frame in which time is measured from the shock. In the new frame, we linearize the equations about the reference (steady $q = 0$) solution. We solve these linear equations for the perturbations in ρ and λ by integrating along characteristics. Finally, we transform back to the original frame.

Scaling

We scale our equations (2.3) to determine the appropriate smallness parameter for the perturbation. Define a characteristic time t^* , a characteristic length x^* , and the corresponding implied characteristic velocity $v^* = x^*/t^*$. The substitution

$$x' = x/x^*, t' = t/t^*, r' = r(v^* \rho', \lambda) t^* \quad (3.1)$$

$$\rho' = \rho/v^*, q' = q/(v^*)^2$$

gives the identical set of equations for the primed variables.

We choose $v^* = c_0$, so that $\rho_0' = c_0' = 1$. Our dependent variables are thus of o -der one. We then take $t^* = 1$, and choose the rate multiplier k in (2.6) for unit reaction time in the reference flow (for which $f(\rho) = f(\rho_0) = f(c_0 \rho_0') = f(c_0) = \text{constant}$). This makes our independent variables of order one. The appropriate smallness parameter is then q' , which we call ϵ :

$$\epsilon = q' = q/c_0^2 , \quad (3.2)$$

as stated in (2.4). Our solution is valid for $\epsilon \ll 1$.

From here on we drop the primes. Our governing equations are then just the set (2.3), with ϵ replacing q (and with the ρ -dependence of the rate rescaled as required by (3.1)).

Transformation to Accelerated Frame

We transform to the accelerated frame in which time is measured from the perturbed shock. The distance x is unchanged, but the new time τ at each x is measured from the shock, as indicated in Fig. 2. In the new frame, Fig. 3, the shock is the x axis, and the characteristics have negative slope. In the figure, the characteristics are drawn as straight lines, as they are for the linearized equations. The point τ^* is for later reference.

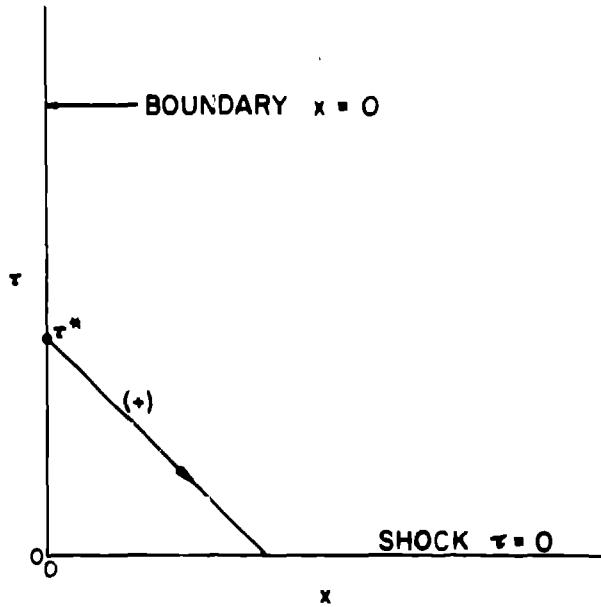


Fig. 3. Accelerated frame. Time τ is measured from the perturbed shock.

Define the shock path in the original frame by the function $t_s(x)$, the time of arrival of the shock at a given x , so that the shock velocity is $D(x) = 1/(dt_s/dx)$. The transformation equations are:

$$x = x, \quad \tau = t - t_s(x), \quad (3.3)$$

with partial derivatives $x_x = 1, x_t = 0, \tau_x = -1/D(x), \tau_t = 1$. Partial derivatives of $f = \rho$ or λ transform as follows:

$$f_x \text{ becomes } f_x - D^{-1}f_\tau \quad (3.4)$$

$$f_t \text{ becomes } f_\tau$$

In the new frame the system (2.3) becomes

$$(\rho - D)\rho_\tau - \rho D\rho_x = -\frac{1}{2}\epsilon(\lambda_\tau - D\lambda_x) \quad (3.5)$$

$$\lambda_\tau = r$$

$$\text{shock; } t = 0: \quad D = \frac{1}{2}\rho_s$$

$$\text{boundary, } x = 0: \quad \rho_b = \rho_0 = \text{constant, given,}$$

(with $\lambda_s = 0$; and $\rho_b = 0$ for $t < 0$ understood). Here D is $D(x)$, the unknown shock velocity; the transformation puts it in the coefficients of the first equation. The boundary condition is unchanged. The shock relation $\rho_s(x) = 2D(x)$ is also unchanged, but now applies on the new shock path (the x axis).

Linearization

The reference flow is the $\epsilon = 0$ solution: the steady flat-topped shock with $\rho_0 = c_0 = 1, D = \frac{1}{2}\rho_0 = \frac{1}{2}$, and $\lambda = \lambda_0(\tau)$. We write our dependent variables as perturbation expansions:

$$\rho(x, \tau) = \rho_0 + \epsilon\rho_1(x, \tau) + O(\epsilon^2) \quad (3.6)$$

$$\lambda(x, \tau) = \lambda_0(\tau) + \epsilon\lambda_1(x, \tau) + O(\epsilon^2)$$

$$D(x) = D_0 + \epsilon D_1(x) + O(\epsilon^2)$$

with perturbation functions ρ_1, λ_1 , and D_1 of order one, and order parameter $\epsilon \ll 1$. Substituting these into (3.5) gives to order ϵ

$$(\rho_0 - D_0)\rho_{1\tau} - \rho_0 D_{0x}\rho_{1x} = -\frac{1}{2}r_0 \quad (3.7)$$

$$\lambda_{1\tau} = a_0\rho_1 + b_0\lambda_1$$

where a_0 and b_0 are the partial derivatives of r with respect to ρ and λ , evaluated in the reference state. In obtaining the first equation we have used (2.5), $\lambda_{0\tau} = r_0$. We simplify by substituting the numerical values $\rho_0 = 1, D_0 = \frac{1}{2}$ in the first term, and $D_0 = \frac{1}{2}$ in the second. In the second term we replace ρ_0 by c_0 , but retain the symbol c_0 instead of the numerical value as reminder that the coefficient is a velocity. The complete set of linearized governing equations is then

$$\rho_{1\tau} - c_0\rho_{1x} = -r_0 \quad (3.8a)$$

$$\lambda_{1\tau} = a_0\rho_1 + b_0\lambda_1 \quad (3.8b)$$

$$\text{shock: } D_1 = \frac{1}{2}\rho_{1s} = \frac{1}{2}\rho_1(x, \tau=0) \quad (3.8c)$$

$$\text{boundary: } \rho_{b1} = 0 \quad (3.8d)$$

In these equations, r_0, a_0 , and b_0 are known functions of τ . For a given $r(\rho, \lambda)$ they can be calculated from the steady state equation (2.5). The two differential equations are uncoupled: (3.8a) can be solved by itself for $\rho_1(x, \tau)$, and then (3.8b) can be solved for $\lambda_1(x, \tau)$. The shock-velocity perturbation $D_1(x)$ is obtained from $\rho_1(x, \tau=0)$ through the shock relation (3.8c).

Solution

We first solve the equation of motion (3.8a). In characteristic form it is

$$d\rho_1/d\tau = -r_0(\tau) \text{ on } dx/d\tau = -c_0 \quad (3.9)$$

The characteristics are straight lines of slope $-c_0$ originating on the rear boundary $x = 0$ and running down to the shock $\tau = 0$, as shown in Fig. 3. We integrate (3.9) along a characteristic, starting at the boundary. Let τ^* , Fig. 3, be the starting point of a particular characteristic. Integration from τ^* to some τ on

the characteristic gives

$$\rho_1(\tau) - \rho_1(\tau^*) = -I(\tau, \tau^*) = -\int_{\tau^*}^{\tau} r_0(\tau') d\tau' \quad (3.10)$$

The boundary value $\rho_1(\tau^*)$ is zero by the boundary condition (3.8d). We can write I in terms of the reference composition function $\lambda_0(y) = \int_0^y r_0(y') dy'$ defined by (2.5) by writing it as the sum of two integrals:

$$I(\tau, \tau^*) = \int_0^{\tau} r_0(y) dy' - \int_0^{\tau^*} r_0(y) dy \quad (3.11)$$

$$= \lambda_0(\tau) - \lambda_0(\tau^*)$$

We want ρ_1 as a function of x and τ . For a given point (x, τ) , τ^* is the time at which the characteristic through the point intersects the x axis. Thus $\tau^* = \tau + x/c_0$. From (3.10) and (3.11) we have

$$\rho_1(x, \tau) = \lambda_0(\tau^*) - \lambda_0(\tau) \quad (3.12)$$

$$\tau^* = \tau + x/c_0$$

For the shock velocity, evaluate (3.12) at $\tau = 0$ and use the shock relation (3.8c). The second λ_0 in (3.12) vanishes because λ_0 is zero at the shock and we have

$$D_1(x) = \frac{1}{2} \lambda_0(x/c_0) \quad (3.13)$$

Knowing $\rho_1(x, \tau)$, we can solve (3.8b) for $\lambda_1(x, \tau)$. At each x , (3.8b) is an ordinary differential equation for λ_1 . Its solution is

$$\lambda(x, \tau) = a_0 e^{b_0 \tau} \int_0^{\tau} e^{-b_0 y} \rho_1(x, y) dy \quad (3.14)$$

For the pressure, we write p as $p = p_0 + \epsilon p_1$, and find that, to first order, the pressure perturbation p_1 is $p_1 = c_0 \rho_1$, so that p_1 is the same as ρ_1 .

Transformation to Original Frame

To return to the original t - x frame, we must replace τ by $t - t_s(x)$, see (3.3). Because the shock-velocity perturbation (3.13) is non-zero for all positive x , the displacement of the shock from its reference location becomes arbitrarily large as x increases, and the correction to $t_s(x)$ is secular; at large x we have

$$t_s(x) = x/D_0 + O(\epsilon x) \quad (3.15)$$

This property carries over into ρ_1 . Replacing τ in (3.12) by $t - t_s(x)$ and expanding each λ_0 function in powers of ϵ about the zeroth order argument $\tau_0 = t - x/D_0$, we find

$$\rho_1(x, t) = \lambda_0(\alpha) - \lambda_0(\tau_0) + O(\epsilon x) \quad (3.16)$$

$$\alpha = t - x/c_0$$

$$\tau_0 = t - x/D_0$$

The position error arising from the unbounded shock displacement gives rise to a secular second-order term with coefficient proportional to x . In the original t - x frame, then, our first-order result does not apply to arbitrarily large x (we have essentially the correct solution but at the wrong location). Because we are interested mainly in the initial transient, this is not a serious limitation. In any case, the nature of the solution is perfectly clear from the result (3.12) in the τ - x frame. The result (3.15) applies in either frame, since it depends only on x .

We will also need the gradient of ρ_1 . Taking the derivative of (3.16) with respect to x , and replacing the derivatives of each λ_0 function with respect to its argument by the function r_0 , we have

$$\rho_{1x}(x, t) = (1/D_0) [r_0(\tau_0) - \frac{1}{2} r_0(\alpha)] \quad (3.17)$$

IV. RESULTS

We recapitulate briefly. We have solved the initiation problem for small heat of reaction q by treating q as a small perturbation (subscript 1) on the reference $q = 0$ flow (subscript 0), writing the dependent variables as

$$\rho(x, t) = \rho_0 + \epsilon \rho_1(x, t) \quad (4.1)$$

etc. With suitable scaling, both ρ and ρ_1 are of order one; the results are valid for values of the smallness parameter $\epsilon = q/c_0^2$ much less than one. We discuss only the density perturbation ρ_1 and the shock-velocity perturbation D_1 ; these display most of the interesting physics. (For brevity, we use the term "perturbation" for ρ_1 and D_1 ; the actual perturbations are of course $\epsilon \rho_1$ and ϵD_1 .) The pressure perturbation is the same as the density perturbation, and the λ -perturbation can be calculated from (3.14) if desired. The reference flow is a steady, flat-topped shock with $\rho_0 = c_0 = \frac{1}{2} D_0$. The reference composition function $\lambda_0(y)$, which appears with two different arguments in the result, is the solution of the steady rate equation (2.5) for the reference flow. With argument $\tau_0 = t - x/D_0$ it is the composition history in the reference flow.

Density Perturbation

The density perturbation is

$$\rho_1(x, t) = \lambda_0(\alpha) - \lambda_0(\tau_0) \quad (4.2)$$

$$\alpha = t - x/c_0 = t - x/2D_0$$

$$\tau_0 = t - x/D_0$$

the shock-velocity perturbation is

$$D_1(x) = \frac{1}{2} \lambda_0(x/c_0) \quad (4.3)$$

The shock-velocity perturbation is just the composition history on the boundary, propagated to the shock along the unperturbed characteristics.

The density perturbation (4.2) is the sum of two traveling waves. We call them the transient or acoustic wave (argument α) and the steady wave (argument τ). The steady wave propagates the reference composition history $\lambda_0(\tau_0)$ at the reference shock velocity D_0 . Thus it is identical to the steady composition solution of the reference flow. The transient wave propagates the same function, but at the reference acoustic (= characteristic) speed, which is twice as large ($c_0 = 2D_0$). Thus the transient wave passes through the steady wave and overtakes the shock. This overtake is complete in unit time; from then on the transient is over and we have only the steady wave. Note that this first-order density solution is attached to the unperturbed shock path (see discussion at end of previous section).

Role of the Rate Sensitivity

From (4.2) we see that the first-order density perturbation does not depend on the rate sensitivity. The reference composition function $\lambda_0(y)$ is calculated in the constant-density field of the reference solution, so the dependence of r on p has no effect. (This statement is strictly correct only if the rate has the assumed product form (2.7).

Criterion for a Hump

By definition, we have a hump if the gradient $\rho_x = \epsilon \rho_{1x}$ changes sign with increasing x at some point of a fixed-time profile. From (3.17), ρ_{1x} is

$$\rho_{1x} = (1/D_0)[r_0(\tau_0) - \frac{1}{2}r_0(\alpha)] \quad (4.4)$$

where r_0 is the reaction rate in the reference flow. To see how this applies, consider a profile at fixed time. Both α and τ are linear decreasing functions of x . At the rear, $x = 0$, we have $\alpha = \tau_0 = t$. At the front, $x = D_0 t$, we have $\tau_0 = 0$, $\alpha = \frac{1}{2}t$. Thus we have $\alpha \geq \tau_0$ everywhere with equality at the rear. From (4.4) we see then that $\rho_{1x} \geq 0$ at the rear. What must r_0 do to make ρ_{1x} change sign at some point? Consider first an $r_0(y)$, Fig. 4a, which is monotone decreasing. At the rear, τ_0 and α are equal, so $r_0(\tau_0) = r_0(\alpha)$, and ρ_{1x} is positive. (In the figure, the rear point is shown for a profile at $t < 1$.) At the front, $\tau_0 = 0$ and $\alpha = \frac{1}{2}t$, so $r_0(\alpha)$ is less than $r_0(\tau)$, and ρ_{1x} is still positive. It is apparent that for this rate, ρ_{1x} will be positive for all x and there will be no hump. To have a hump, r_0 must increase sufficiently rapidly over part of its range, as in Fig. 4b. If the slope of $r_0(y)$ is large enough, and t is not too large, we can have $r_0(\alpha) > 2r_0(\tau_0)$ and thus negative ρ_{1x} over some range of x , and

therefore a hump in the profile.

Shock-Change Equation

The shock-change equation for the analog is

$$d\rho_s/dt = -(c - D)\rho_x + \frac{1}{2}cr/D \quad (4.5)$$

Linearization of this equation, with use of (4.4) for ρ_{1x} , gives

$$d\rho_{1s}/dt = \left[\frac{1}{2}r_0'(x/c_0) - r_0'(0) \right] + \left[r_0(0) \right] ,$$

the first square bracket being the gradient term and the second the reaction term. We see that:

- (1) The reaction term is always positive.
- (2) The gradient term can have either sign, depending on the form of the rate function.
- (3) The reaction term dominates: it is never smaller in magnitude than the gradient term.
- (4) The shock pressure is always monotone increasing; it does not overshoot.

V. EXAMPLES

We give two examples, one with, and one without, a hump. The rates are functions of λ alone, so the subscript 0 is unnecessary.

For no hump, we take a monotone-decreasing rate like that of Fig. 4a:

$$r = 2(1 - \lambda)^{1/2} \quad (5.1)$$

$$\lambda = 1 - (1 - \tau)^2$$

$$\tau = 1 - (1 - \lambda)^{1/2} .$$

This rate is shown in Fig. 5a. The corresponding solution (presented as a sequence of snapshots) is shown in Fig. 5b. Note the resemblance to Fig. 1a.

For a hump, we take a nonmonotone rate like that of Fig. 4b:

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

$$\lambda = 1 - a^2(1 - y^2)/(1 + y)^2 \quad ,$$

$$k\tau = 1 - b \tanh^{-1} \left\{ (1 - \lambda)^{1/2}/b \right\} \quad ,$$

$$y \equiv \left\{ (a - 1)/(a + 1) \right\}^{1 - k\tau}$$

$$a \equiv 1 + \delta \quad , \quad b \equiv \tanh^{-1} (1 + \delta) \quad .$$

$$k = -2a^{-1/2} \tanh^{-1} (a^{1/2})$$

Figure 6a shows this rate for $\delta = 0.05$. It mocks up a branching-chain mechanism with an induction zone, like that of hydrogen/oxygen and other gaseous systems. It is similar to one we have used earlier [5], but with a power of $\frac{1}{2}$ on the depletion term, to make the reaction time finite. The solution is shown in Fig. 6b. It is

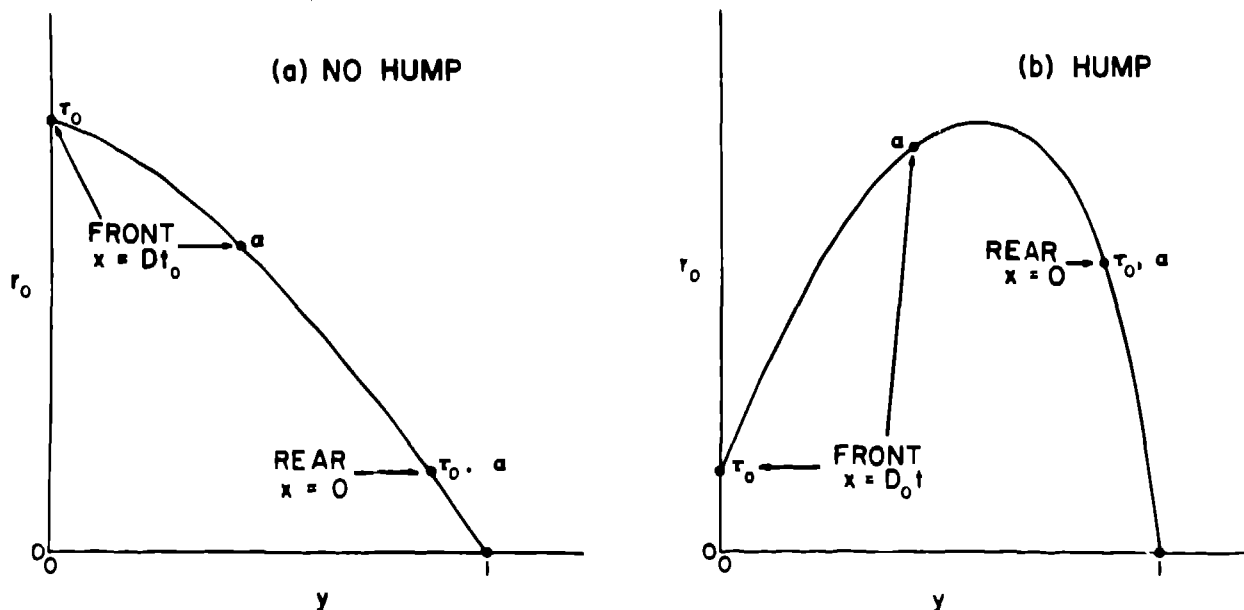


Fig. 4. General form of the reaction-rate λ -dependence for (a) no hump, and (b) hump.

similar to the sensitive-rate case, Fig. 1b, in having humped profiles and rise in shock pressure, but the shock pressure does not overshoot.

VI. SUMMARY

The reference (unperturbed) flow is a steady flat-topped shock in a material made inert by setting its heat of reaction q to zero. This flow has a steady reaction zone, but the composition variation has no effect on the state because the system has been decoupled by setting q to zero.

By turning on the heat of reaction (setting q to a small positive value), we make the system (roughly speaking) into an amplifier with gain $c = q/c_0^2$. It converts the composition signal of the reference flow into a two-component density signal, with steady component at the fundamental (original) frequency, and transient component at the first harmonic frequency (the exact factor of two being an accident of our particular choice of equation of state). The harmonic wave travels through the steady wave and disappears into the shock, giving the flow the character of a double refraction.

The wave shapes during the transient phase depend only on the λ -dependence of the rate (evaluated in the constant state of the reference flow). A monotone-decreasing $r(\lambda)$ produces monotone profiles and gently rising shock strength, as in Fig. 5. A sufficiently non-monotone $r(\lambda)$ produces humped profiles and

rapidly rising shock strength, as in Fig. 6.

The more complicated analysis of the same problem for the physical system, as described by the full Euler equations, is in progress. The results, although not so easily calculated, appear to have the same general nature as those given here. They suggest the possibility of learning something about the λ -dependence of the rate from pressure measurements in dilute explosives. In this instance, as in others [3], the analog has proved to be a reliable guide to the essential physics of the full set of equations, but much easier to work with.

ACKNOWLEDGEMENTS

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REFERENCES

1. Wildon Fickett and William C. Davis, Detonation (University of California Press, Berkeley, 1979).
2. Figure 1b is from W. Fickett, J. D. Jacobson, and W. W. Wood, "The Method of Characteristics for One-Dimensional Flow with Chemical Reaction," LASL Report 4269, July 1970, p. 38. Figure 1a is a similar unpublished calculation.
3. W. Fickett, "Detonation in Miniature," *Am. J. Phys.* 47, 1050-59 (1979).

4. R. I. Soloukhin and C. Brochet, "The Development of Instabilities in a Shocked Exothermic Gas Flow," *Combust. Flame*, **18**, 59-64 (1972). For a summary, see [1], Sec. 7B1.

5. W. Fickett, J. D. Jacobson, and G. L. Schott, "Calculated Pulsating One-Dimensional Detonations with Induction-Zone Kinetics," *AIAA J.*, **10**, 514-16 (1972). For a summary, see [1], Sec. 6C1, pp. 283-284.

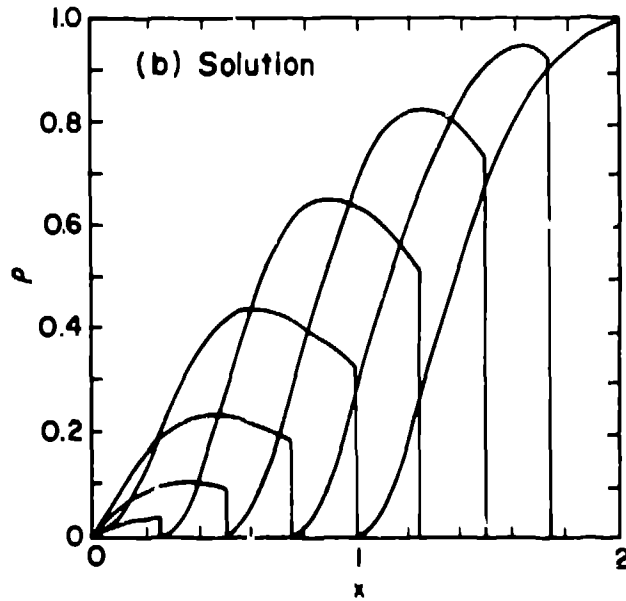
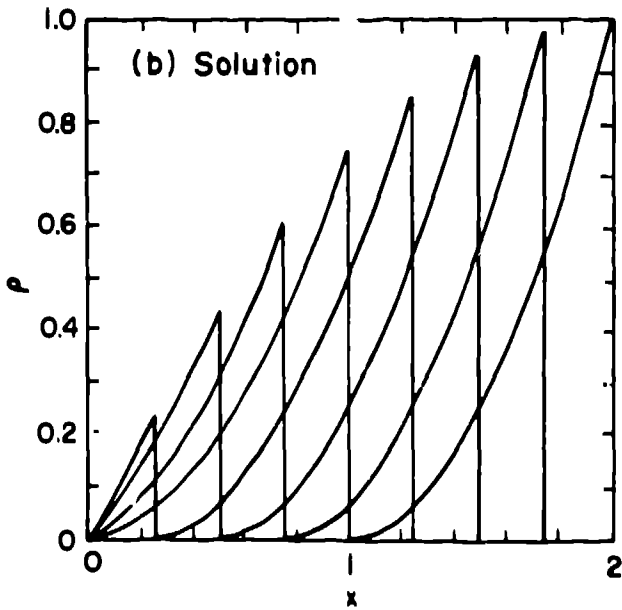
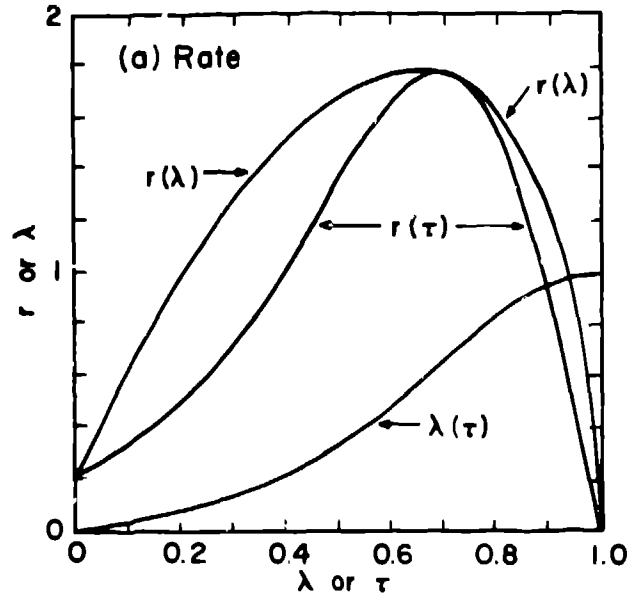
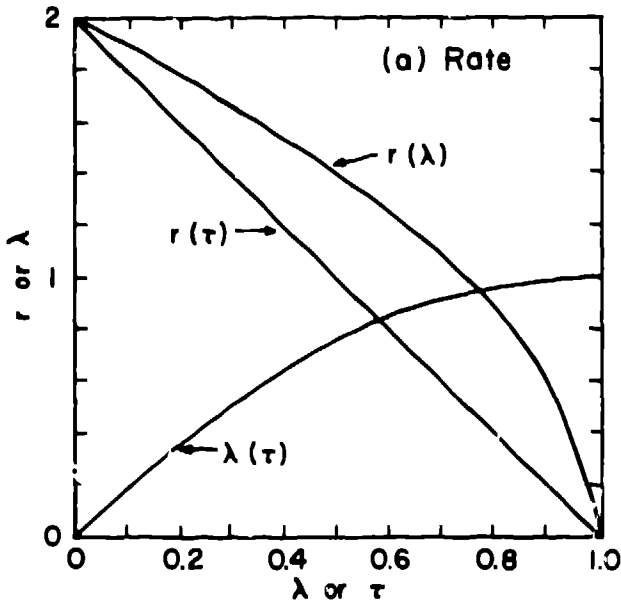


Fig. 5. No-hump example (monotone λ -dependence).

Fig. 6. Hump example (non-monotone λ -dependence).