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On the evolution of compression pulses in an exploding atmosphere: initial behaviour

By J. F. CLARKE

Department of Aerodynamics, Cranfield Institute of Technology,
Bedford MK43 0AL, England

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The development in space and time of a plane initial disturbance to a spatially uniform exploding atmosphere is analysed on the assumption that the disturbance amplitude is comparable in magnitude with the inverse (dimensionless) activation energy of the explosion reaction. Particular attention is focused on the shock-fitting problem, which has features that distinguish it from its inert-atmosphere counterpart.

Using the positive half of a sine wave to typify an isolated compression perturbation, it is found that the amplifying effect of the ambient reaction leads to very rapid shock wave development, which depends significantly on the spatial extent of the disturbance. The latter also influences the question of whether local explosion (local explosion is recognized here as a logarithmically unbounded growth of the disturbance amplitude; in other words as a local breakdown of the present approximations) occurs at the shock wave or some distance behind it. The subsequent evolution of these two states will no doubt be significantly different, but the answer to this speculation must await extension of the present theory to encompass the rapid events that ensue near the local explosion regions.

1. Introduction

The present paper is a further step in the study of the behaviour of finite amplitude disturbances propagating through a spatially uniform exploding atmosphere. An earlier work (Clarke 1978) has analysed the response of arbitrarily small amplitude plane disturbances in the absence of transport effects and also identified an important distinguished limiting case for which the disturbance amplitude is of the same order as the appropriately non-dimensionalized inverse activation energy of the ambient explosion reaction, assumed small of course. Some preliminary results for this distinguished limiting case were described and agree with the conclusions reached by Blythe (1978), who independently analysed the consequences of the same distinguished limit.

When the imposed initial disturbances to the ambient atmosphere are compressive in character (in other words when they represent local increases of gas temperature) the small disturbance solutions that result from the theory ultimately become multivalued and require the introduction of appropriate Rankine–Hugoniot shock discontinuities. Such a result is hardly a surprise, but the crucial role of the ambient explosion reaction as an amplifier of gasdynamic disturbances makes its presence felt in the general evolution of the perturbations and makes the shock-fitting exercise

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essentially more awkward than its now classical counterpart for chemically inert atmospheres. After a brief resumé of the general explosive-atmosphere results, the present work focuses its main attention on the two related questions of shock-fitting and the development of locally explosive behaviour.

2. General solutions

Consider the pair of dimensionless independent variables ξ, T defined so that

$$\xi = (a_{fi}t - x)/\epsilon a_{fi}\gamma t_{\mathrm{ign}}, \quad T = t/\gamma t_{\mathrm{ign}}, \tag{1}$$

where t is the time, x measures spatial location, a_{fi} is the initial ($t = 0$) frozen sound speed in the explosive gas mixture, γ is the frozen specific heat's ratio (assumed constant), t_{ign} is an ignition time, whose precise definition is not important at this particular stage of the work (but see Clarke 1978), and ϵ^{-1} is the dimensionless activation energy of the irreversible chemical reaction

$$nF \rightarrow P. \tag{2}$$

It has been shown by Clarke (1978) and also independently by Blythe (1978) that, when the gas velocity u in a planar disturbance superimposed upon an ambient homogeneous (adiabatic) explosion is $O(\epsilon)$, so that one can write

$$u(x,t) = \epsilon a_{fi} u^{(1)}(\xi, T) + \ldots, \tag{3}$$

then $u^{(1)}$ satisfies the nonlinear equation

$$2(1-\gamma T)\,(\partial u^{(1)}/\partial T)_\beta = \exp\left[(\gamma-1)\,u^{(1)}\right] - 1, \tag{4a}$$

$$(\partial\xi/\partial T)_\beta = -\tfrac{1}{2}(\gamma+1)\,u^{(1)} + \tfrac{1}{2}\ln(1-\gamma T), \tag{4b}$$

[see equations (60a, b) and (62) in Clarke (1978) or Blythe's (1978) equation (3.12)].

The dimensional pressure p and density ρ differ from their initial values p_{0i} and ρ_i as follows:

$$p - p_{0i} = \epsilon\rho_i a_{fi}^2 p^{(1)}(\xi, T) + \ldots, \tag{5a}$$

$$\rho - \rho_i = \epsilon\rho_i \rho^{(1)}(\xi, T) + \ldots, \tag{6a}$$

where

$$p^{(1)} = u^{(1)} - (1/\gamma)\ln(1-\gamma T), \tag{5b}$$

$$\rho^{(1)} = u^{(1)}. \tag{6b}$$

The mass fraction c of the reactant F behaves like $c_0(T) + \epsilon^2 c^{(1)}$ and so its additional gasdynamically induced variations play no part in the first-order theory that seeks to evaluate $u^{(1)}$ in the neighbourhood of the frozen wave-head. It also follows from the thermal equation of state

$$p = \rho R\Theta \tag{7}$$

that

$$\Theta^{(1)} = (\gamma-1)\,u^{(1)} - \ln(1-\gamma T), \tag{8a}$$

where the absolute temperature Θ is written in the form

$$\Theta = \Theta_{0i} + \epsilon\Theta_{0i}\,\Theta^{(1)}(\xi, T) + \ldots. \tag{8b}$$

For simplicity R is assumed not to depend significantly on the mass fraction c.

Equations (8) show that $(\gamma-1)u^{(1)}$ is the additional temperature that is superimposed on the ambient field by the gasdynamic disturbance. The terms in $\ln(1-\gamma T)$ in (5*b*) and (8*a*) represent a first approximation, the 'small-depletion' approximation as it is often called, to the progress of the ambient explosion. (It is evidently somewhat neater to work in terms of a time γT rather than T as defined in (1); the latter time, together with the other notation used here, appears in Clarke (1978) and so is retained in order to make reference back to that work more direct.)

The solution of the initial value problem for (4) is readily found to be

$$(\gamma-1)\,u^{(1)} = -\ln\{1-(1-\exp[-(\gamma-1)\,u_i])\,(1-\gamma T)^{-(\gamma-1)/2\gamma}\}, \tag{9}$$

where

$$\underset{\sim}{\xi} \equiv \xi+\frac{1}{2\gamma}\int_1^{1-\gamma T}\ln s\,ds = F(\beta,T), \tag{10}$$

$$F(\beta,T) \equiv \beta+\frac{(\gamma+1)}{(\gamma-1)^2}\int_1^{(1-\gamma T)^{-(\gamma-1)/2\gamma}}\ln[1-(1-\exp[-(\gamma-1)\,u_i])\,s]\,s^{-(3\gamma-1)/(\gamma-1)}\,ds, \tag{11}$$

and

$$u_i \equiv u_i^{(1)}(\beta) = u^{(1)}(\xi_{T=0},0) \tag{12}$$

is the given initial value of $u^{(1)}$.

Note that the parameter β has been selected so that $\beta = \xi$ at $T = 0 = t$; β is therefore related to $-x$, as can be seen from (1). It is convenient to work in terms of $\underset{\sim}{\xi}$ from now on [see equation (10)]. With the information that $a_f^2 = \gamma R\Theta$ it can be seen that $\underset{\sim}{\xi}$ is the co-ordinate

$$\left\{\int_0^t a_{fa}(s)\,ds-x\right\}\Big/\epsilon a_{fi}\gamma t_{1\mathrm{gn}},$$

where $a_{fa}(t)$ is the time-dependent ambient frozen sound speed, with the latter evaluated in accordance with the approximation in (8). Therefore $\underset{\sim}{\xi}$ is a label for the left-to-right propagating characteristics in the spatially uniform ambient atmosphere. Their change of shape with time is of course significant, but not crucially so in what follows, so that it is useful to be able to conceal this information within the variable $\underset{\sim}{\xi}$.

3. Comparison with inert-atmosphere results

In initial-value problems of the present type which deal with propagation through inert atmospheres the solutions corresponding to (9)–(12) are usually as far as one need go in order to acquire a satisfactory appreciation of the physical significance of the results. To be sure one may need to introduce shocks into the system, but the methods for doing this, together with numerous illustrative examples, are now well documented (e.g. Whitham 1974, especially chapter 2; Lighthill, 1978, §§ 2.10, 2.11) and the whole theory of discontinuous shock wave behaviour in inert systems is in a very satisfactory state, particularly for relatively weak waves. Thus, if u_i in (12) is known to be $f(\beta)$, the inert gas solution, in present terminology, is

$$u^{(1)}(\xi,T) = f(\beta);\quad \xi = \underset{\sim}{\xi} = F(\beta,T) = \beta-\tfrac{1}{2}(\gamma+1)f(\beta)\,T, \tag{13}$$

and it is clear that the solution is essentially simpler than (9) and (10) above.

One especially significant fact to note is that the quantity $F(\beta,T)-\beta$ in (13) is a *separable* function of β and T, whereas this is not so in the case of the explosive atmosphere (see equation (11)). This has an important effect on the shock-fitting problem, as will be shown below. The need to introduce a discontinuous shock wave into the field only arises when $F(\beta, T)$ is such that more than one value of β leads to the same value of ξ for a given T. This can only happen if $\partial F/\partial\beta$ vanishes somewhere (i.e. if the family of curves $\xi - F(\beta, T) = 0$ has an envelope). At the initial instant $\partial F/\partial\beta = 1$, with the consequence that a shock will first be required where $\partial F/\partial\beta$ and $\partial^2 F/\partial\beta^2$ vanish simultaneously.

Consider the particular case

$$u_i = f(\beta) = a\sin(b\beta), \quad 0 \leqslant b\beta \leqslant \pi, \qquad (14)$$
$$= 0, \quad b\beta < 0, \quad \pi < b\beta,$$

with $a \neq 0$ and $b > 0$.

For the inert gas (13) shows that

$$\partial F/\partial\beta = 1 - \tfrac{1}{2}(\gamma+1)\,ab\cos(b\beta)\,T, \qquad (15)$$

$$\partial^2 F/\partial\beta^2 = \tfrac{1}{2}(\gamma+1)\,ab^2\sin(b\beta)\,T. \qquad (16)$$

When $T > 0$ these quantities can only vanish simultaneously when $b\beta = 0$ or π and $\frac{1}{2}(\gamma+1)\,abT = \pm 1$ (which implies that $a \gtrless 0$, respectively). This is the familiar result that a shock wave will begin to form at the head, $b\beta = 0$, (tail, $b\beta = \pi$) of a compression (expansion) pulse after a particular lapse of time.

Making the substitution (14) into (11) demonstrates that there is no simple parallel to (15) and (16) in the case of disturbance propagation through an exploding atmosphere. However it *is* possible to evaluate $\partial F/\partial\beta$ and $\partial^2 F/\partial\beta^2$ exactly at $\beta = 0$. In the latter case it is convenient to leave the expression in the form

$$\left.\frac{\partial^2 F}{\partial\beta^2}\right|_{\beta=0} = -(\gamma+1)\,u_i'^2(0)\int_1^{Q^{-a}}\{s-1\}\,s^{-1/a}\,ds + \left(\frac{\gamma+1}{\gamma-1}\right)u_i''(0)\int_1^{Q^{-a}} s^{-1/a}\,ds,$$

where $$Q \equiv (1-\gamma T), \quad a \equiv (\gamma-1)/2\gamma > 0,$$

and $u_i'(0)$, $u_i''(0)$ are the first and second derivatives of u_i with respect to β evaluated at $\beta = 0$. With u_i given by (14) $u_i''(0)$ is zero and, since $Q^{-a} \geqslant 1$, it follows that $\partial^2 F/\partial\beta^2$ is essentially negative at $\beta = 0$ for all T.

The inference is that the shock wave does not form at the head of this particular compression pulse (attention is focused on the case $a > 0$ from now on) when it propagates into an exploding atmosphere. The reason for this lies in the additional distortion of the pulse profile as a result of the chemical influences; the inert-atmosphere pulse only suffers distortion from the now familiar nonlinear convective effects, which are still present in the explosive atmosphere situation but which, as just remarked, are now augmented by the influence of the chemistry.

There is no simple analytical method of assessing just where a shock wave will form in the explosive situation but some general statements can be made, and illustrations provided, for particular values of the numbers a, b for example, as will shortly be demonstrated.

4. Shock-fitting

With the assumption that the time of passage of a fluid element through a diffusion-resisted shock wave is very small compared with the local chemical time it is correct to treat the discontinuities that may be required in the solution (9)–(12) as Rankine–Hugoniot discontinuities across which the chemical composition is constant, or frozen. When such waves are weak one can exploit the result that their propagation speed is the arithmetic mean of the frozen wavelet speeds on either side of the shock to a first order, and write

$$2\left(\frac{dx}{dt}\right)_{\text{shock}} = \left(\frac{\partial x}{\partial t}\right)_{\beta_2} + \left(\frac{\partial x}{\partial t}\right)_{\beta_1},$$

where β_1, β_2 are the frozen-wavelet labels ahead of and behind the shock respectively. From (1) and (10) a similar relationship holds with ξ in place of x and T in place of t and, in consequence, the shock wave location is found from the relations (N.B. ξ_s is the value of ξ on the shock)

$$\xi_s = F(\beta_1, T) = F(\beta_2, T), \tag{18}$$

$$\frac{\partial F}{\partial \beta_1}\frac{d\beta_1}{dT} + \frac{\partial F}{\partial \beta_2}\frac{d\beta_2}{dT} = 0. \tag{19}$$

When F takes the form $\beta - f(\beta)g(T)$ the function $g(T)$ can be eliminated from (19) and the result integrated to give the famous 'equal areas' rule

$$2\int_{\beta_1}^{\beta_2} f(a)\,da = (\beta_2 - \beta_1)\,[f(\beta_2) + f(\beta_1)] \tag{20}$$

(see Whitham (1974) and Lighthill (1978)).

With the non-separable form of $F(\beta, T)$ found in (11) the task of discovering the $\beta_1(T)$ and $\beta_2(T)$ relationships on the shock wave becomes much more awkward. If the shock propagates into the spatially uniform parts of the atmosphere $F(\beta_1, T)$ reduces to β_1, since $u_i \equiv 0$ in such regions [see equation (11)]. Elimination of β_1 between (18) and (19) is then possible, with the result that

$$\frac{d\beta_2}{dT} = -\frac{1}{2}\left\{\frac{\partial F(\beta_2, T)/\partial T}{\partial F(\beta_2, T)/\partial \beta_2}\right\}. \tag{21}$$

The partial derivatives of F with respect to β_2 and T can be found from (11) so that, although no analytical solution of this nonlinear first-order equation is possible here, it is in a suitable form for numerical integration, once its initial values are known.

The previous section has shown that the shock does not form at the leading edge $\beta = 0$ of the compression pulse, so that it does not propagate into spatially uniform gas, at least in the early stages of its history, and (21) therefore cannot be used at early times after shock formation. In the immediate neighbourhood of the shock-formation location, let us say β_f, T_f, a series development of the functions in (18) and (19) shows that

$$\Delta T \simeq -\frac{1}{6}\,\frac{\partial^3 F(\beta_f, T_f)/\partial \beta^3}{\partial^2 F(\beta_f, T_f)/\partial \beta\,\partial T}\,(\Delta\beta_n)^2, \tag{22a}$$

where $$T \equiv T_f + \Delta T; \quad \beta_n \equiv \beta_f + \Delta\beta_n, \quad n = 1, 2; \tag{22b}$$

and $$\Delta\beta_2 = -\Delta\beta_1. \tag{22c}$$

(If $\beta_n^0 = \beta_f + \Delta\beta_n^0$ denotes the values of β at the locus of vanishing $\partial F/\partial\beta$ it transpires that $\Delta\beta_n^0\sqrt{3} = \Delta\beta_n$; this fact provides a useful check on the numerical accuracy of subsequent numerical calculations.) Observing that $\partial^3F/\partial\beta^3$ and $\partial^2F/\partial\beta\,\partial T$ at β_f, T_f can be shown to be, respectively, positive and negative, it is possible to use (22*a*) to trace the approximate shock path until it intersects the pulse head at $\beta = 0$, *provided* that β_f is suitably small. It will be shown by example below that β_f *is* sufficiently small in several interesting cases, so that the task of locating the shock for such compression pulses is now accomplished, first, by evaluation of β_f, T_f from the conditions

$$\frac{\partial F}{\partial\beta} = 0 = \frac{\partial^2 F}{\partial\beta^2} \tag{23}$$

and, second, by integration of (21) with initial conditions

$$\beta_2 = 2\beta_f, \quad T = T_f + \frac{1}{6}\left|\frac{F_{\beta\beta\beta f}}{F_{\beta T f}}\right|\beta_f^2. \tag{24}$$

The results of some numerical calculations obtained in this way are given below.

There is one particularly important feature of the shock waves that fit into the solution (9)–(12) that can be described in general, as opposed to particular (numerical), terms. However it does depend upon a number of facts, about the function F especially, and it is appropriate to accumulate these facts at this juncture. First note from (9) that there exists a time T_e, defined by

$$(1-\gamma T_e)^{-(\gamma-1)/2\gamma} = \{1-\exp[-(\gamma-1)\,u_i]\} \tag{25}$$

for any given value of β and hence of u_i, at which $u^{(1)}$ becomes logarithmically infinite. Such an event is similar to the one that is encountered in the simple 'small-depletion' (of the reactant F) model of a spatially homogeneous explosion (e.g. Clarke 1978). Since T_e depends upon spatial position through its dependence upon β it will be called the *local explosion time*. It is also important to observe from (11) and (25) that $\{F(\beta, T_e)-\beta\}$ depends only upon the value of u_i; also $F(\beta, T_e)$ is essentially finite with $\beta \geqslant F(\beta, T) \geqslant F(\beta, T_e)$ for $0 \leqslant T \leqslant T_e$.

The spatially homogeneous explosion ignition time T_{ign} is defined to be the value of T_e for a zero value of u_i, whence (25) shows that $0 < T_e < T_{\text{ign}}$ for compression waves, which have $u_i > 0$.

The derivative of F with respect to β plays an important part in fixing the location of a shock wave as can be seen from (19). Its value can be written in a reasonably concise form as follows:

$$\frac{\partial F}{\partial\beta} = 1-\frac{(\gamma+1)}{(\gamma-1)^2}\left(\frac{d\sigma}{d\beta}\right)\int_1^{(1-\gamma T)^{-a}} y^{-1/a}\{1-\sigma y\}^{-1}\,dy, \tag{26}$$

where
$$\sigma \equiv 1-\exp[-(\gamma-1)\,u_i(\beta)],$$
$$a \equiv (\gamma-1)/2\gamma.$$

It is apparent that, for a given value of β, $\partial F/\partial\beta$ diminishes monotonically in the interval $1 \geqslant \partial F/\partial\beta > -\infty$ as T increases in $0 \leqslant T < T_e$, *provided that* $d\sigma/d\beta > 0$. When $d\sigma/d\beta < 0$, $\partial F/\partial\beta > 0$ for all T in $0 \leqslant T < T_e$. When $T \to T_e$, $\partial F/\partial\beta \to \pm\infty$ for $d\sigma/d\beta \lessgtr 0$, respectively.

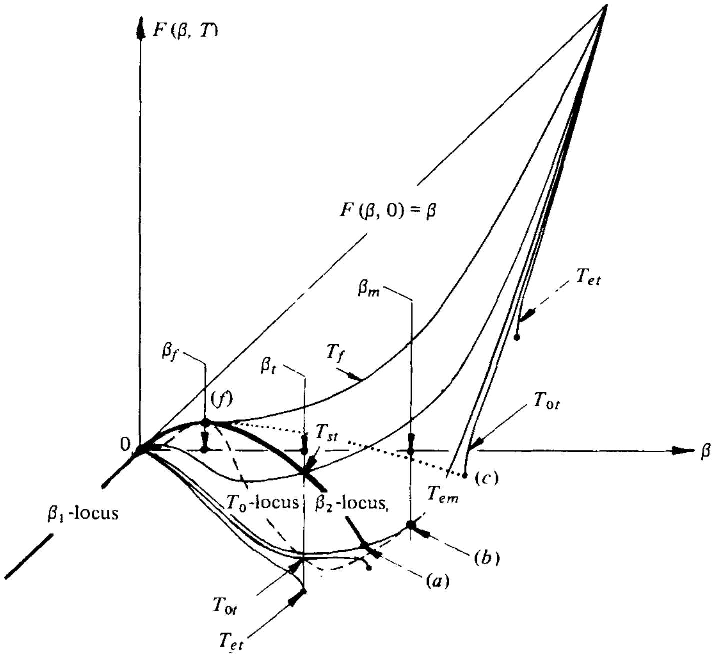

FIGURE 1. This figure illustrates schematically the variations of the function $F(\beta, T) = \hat{\xi}$ with β for a number of different times T for a simple initial compression pulse. The pulse has a single maximum for u_i at $\beta = \beta_m$. The sketch can only be properly comprehended by reference to the text, which defines all of the symbols that appear. The whole of § 4, especially from (24) onwards, can properly be thought of as an extended caption to this figure.

An exceptional case occurs at a stationary value of σ, and hence of u_i, when $\partial F/\partial\beta = 1$ for all T in $0 \leqslant T \leqslant T_e$. If the stationary value corresponds with a local maximum in u_i (> 0) the associated value, T_{es}, of T_e is locally a minimum.

If T_0 is the value of T at which $\partial F/\partial\beta$ vanishes for a given β the previous remarks show, first, that such a value exists for all situations that have $d\sigma/d\beta > 0$ and, second, that $0 < T_0 < T_e$ for any given permissible value of β. One can deduce that $\partial F/\partial\beta$ must be positive when $\beta = \beta_2$ (see (18), (19)) whence it follows that, *if* a shock exists at a given value of $\beta = \beta_2 = \beta_t$, say, its time of occurrence T_{st} must be such that $0 < T_{st} < T_{0t} < T_{et}$ *for the given* $\beta = \beta_t$. This state of affairs is illustrated in figure 1.

Suppose that u_i has an absolute maximum positive value where $\beta = \beta_m$. The associated local explosion time T_e is an absolute minimum, say T_{em}, and $\partial F/\partial\beta = 1$ at β_m. With $T = T_{em}$ in (26) it is, for any given range of σ, always possible to find a disturbance with positive values of $d\sigma/d\beta$ so small that $\partial F/\partial\beta > 0$ for any β in $0 \leqslant \beta \leqslant \beta_m$. It follows from the monotone behaviour of $\partial F/\partial\beta$ described above that $\partial F/\partial\beta > 0$ for all $T < T_{em}$. Under such conditions, which broadly correspond with the initial perturbations being sufficiently stretched out in physical space, a *shock wave will not form before local explosion* takes place at the peak of the disturbance. This state of affairs constitutes case (iv) in the next section.

For any given range of values of u_i, and hence of σ, it is only necessary to reduce the length scale over which they initially arise in order to increase the positive values of $d\sigma/d\beta$ to levels which will make $\partial F/\partial\beta = 0$ for a whole set of values of T in

$$T_f \leqslant T < T_{em}$$

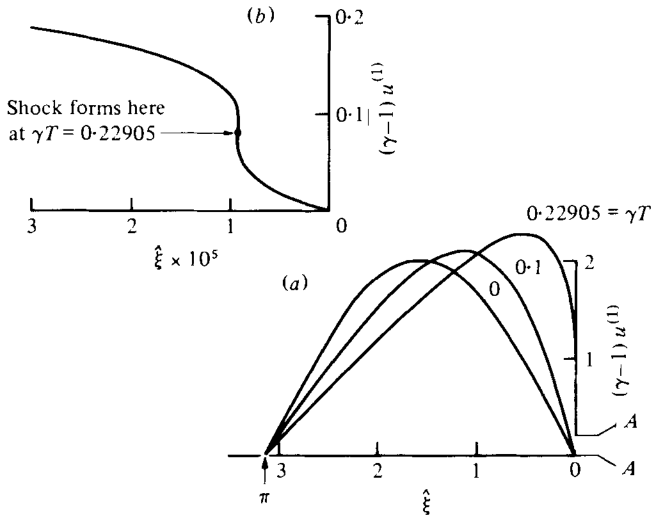

FIGURE 2. (a) Variations in the disturbance profile with $\check{\xi}$ (defined in (1) and (10)) for given times T prior to the formation of a shock wave. The initial profile is $2 \sin \hat{\xi}$ at $T = 0$. Note the growth in the amplitude of the disturbance peak. (b) Details at location AA.

[N.B. T_f is defined prior to (22)]. Frozen Rankine–Hugoniot shock discontinuities must be fitted into the field in these circumstances (figure 1 illustrates the multi-valuedness in the solution for $\hat{\xi} = F(\beta, T)$ that would result if a shock is not introduced) and it is important to observe that the relevant β_2-locus may lie in the range $\beta_2 < \beta_m$ for all times T in $T_f \leqslant T \leqslant T_{em}$. Figure 1 illustrates this condition, with the curve from (f) to (a) for a simple compression pulse with a single maximum for u_i; it is exemplified by case (iii) in the next section. Under such conditions the shock is physically separated from the region of local explosion at the peak of the disturbance, as can be seen from points (a) and (b) on figure 1.

Figure 1 also illustrates the rather unusual disposition of the various curves and loci that confirm the possibility of this relationship between the shock wave and the local explosion, which latter event takes place at the point (b) on the figure.

When the length scale of the disturbance is still further diminished the situation illustrated in figure 1 does not change qualitatively, save for the important case of the β_2-locus. As illustrated by the dotted line from (f) to (c) the shock can now cut off the peak of the initial disturbance, in which case the shock must ultimately encounter a point of local explosion, as depicted on figure 1 at point (c) at the time T_{0t}. This is exemplified by case (i) in the next section; case (ii) is very close to the particular circumstance for which the shock and the earliest local explosion at (b) coincide.

5. Typical compression pulses

Selection of an initial compression pulse shape as described in (14) enables one to make a number of computations which illustrate typical features of the pulse behaviour that can be encountered in an exploding atmosphere (N.B. $a > 0$ for compression pulses).

Prior to the formation of a shock wave, straightforward selection of a value for β enables one to calculate $u^{(1)}$ as a function of $\hat{\xi}$ for any chosen γT by using results (9)–(12).

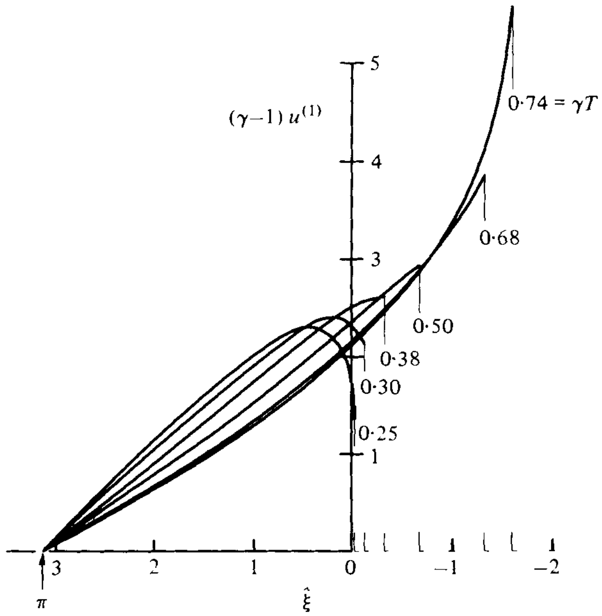

FIGURE 3. Continuation of figure 2 for times after shock formation. The shock grows in strength, 'swallowing' the disturbance peak shortly after $\gamma T = 0{\cdot}38$, and continuing to grow until shortly after $\gamma T = 0{\cdot}75$ when the disturbance becomes locally infinite (local explosion) *at* the shock.

Some typical profiles of $(\gamma-1)\,u^{(1)}$ (recall the significance of $(\gamma-1)\,u^{(1)}$ as a temperature perturbation; see (8)) *versus* $\hat{\xi}$ at fixed γT values appear in figure 2 (for $b = 1$) and figure 4 (for $b = \frac{8}{5}$), all for the single case of $(\gamma-1)\,a = 2$, $\gamma = \frac{7}{5}$. (Figure 3 is a continuation of figure 2 for times after shock formation.) Some pre-shock results for $(\gamma-1)\,a = 2$, $b = \frac{7}{15}$ have also been calculated by Blythe and are in general agreement with those exhibited here.

The usual steepening of the compressive and flattening of the expansive parts of the pulse are apparent but in addition it is clear, from the increase in peak values with increasing γT for example, that the disturbance is undergoing a general amplification (see e.g. figure 2). One effect of this is seen near the head of the pulse at $\gamma T = 0{\cdot}22905$ for $(\gamma-1)\,a = 2$, $b = 1$ (see figure 2) and at $\gamma T = 0{\cdot}55074$ for $(\gamma-1)\,a = 2$, $b = \frac{8}{5}$ (see figure 4), where the velocity profile first achieves the vertical slope that signifies satisfaction of conditions (23). From these times onwards shock waves must be introduced into the field and it is observed that, as a result of the explosion-induced amplification, they form, not at the wave head $\beta = 0$ but some way behind it; to be precise at the values of β_f listed in table 1. This exemplifies the statements made in earlier sections.

Calculation of β_f, T_f is most expeditiously made as follows. Both $\partial F/\partial\beta$ and $\partial^2 F/\partial\beta^2$ can be calculated analytically from direct differentiation of (11). A few numerical values of $\partial F/\partial\beta$ for different T at $\beta = 0$ quickly indicate the time for which this quantity vanishes. Further calculations of $\partial F/\partial\beta$ for fixed times near to the one just discovered permit simple interpolations to locate the desired simultaneous vanishing of both β-derivatives of F. The values of $F_{\beta\beta\beta f}$ and $F_{\beta Tf}$ required in (22a) or (24) then follow from substitution of β_f, T_f into the analytically determined derivatives.

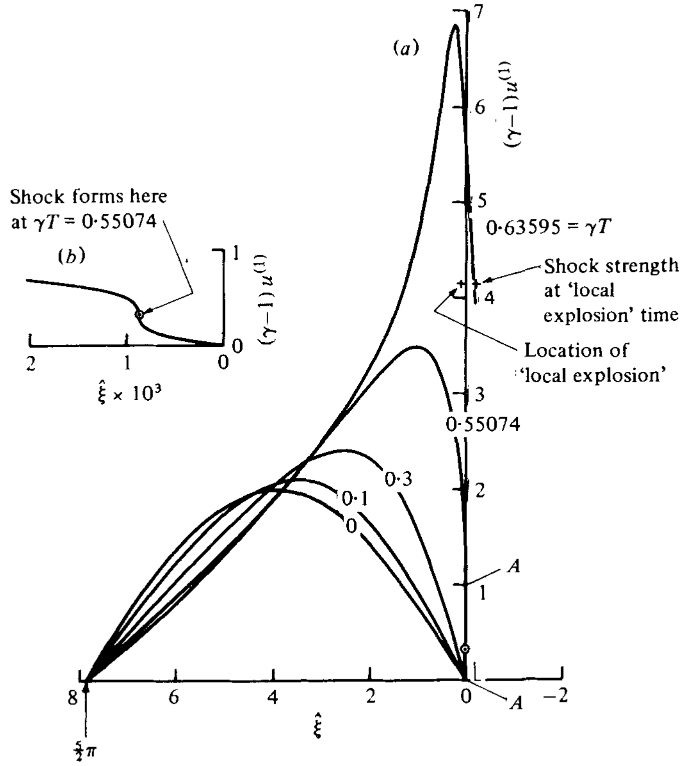

FIGURE 4. (a) Disturbance profiles evolving from $2\sin(\frac{2}{5}\hat{\xi})$ at $T = 0$. Local explosion occurs *behind* the shock shortly after $\gamma T = 0{\cdot}63595$ (see points marked +). (b) Details at location AA.

b	$b\beta_f$	γT_f
1	0·04000	0·22905
$\frac{1}{2}$	0·09761	0·44731
$\frac{2}{5}$	0·14156	0·55074

TABLE 1. Point of shock formation for various values of b.

Equation (21) with initial conditions (24) is now integrated using a simple fourth-order Runge–Kutta method, with Simpson's rule employed to evaluate the integral that appears in $\partial F/\partial\beta$. Very small step sizes are required initially, since β_2 grows very rapidly with T (N.B. $d\beta_2/dT \propto T^{-\frac{1}{2}}$ near β_f, T_f) but these are readily increased as the integration proceeds, especially as the computations can all be performed on a Texas Instruments TI 58 hand-held programmable calculator which allows immediate user control of quantities like step size.

The β_2, T relationship that results from these integrations can readily be converted into variations of ξ_s with T and also of the jump in $(\gamma-1)\,u^{(1)}$, written as $[(\gamma-1)\,u^{(1)}]$, at the shock; results are depicted in figures 5 and 6 respectively. They are also incorporated into figures 3 and 4 to complete those illustrations, of the profiles of $(\gamma-1)\,u^{(1)}$ versus $\hat{\xi}$ for various times, that began with figure 2.

Three values have been selected for b (see table 1) and the main results of the analysis are discussed for each in turn.

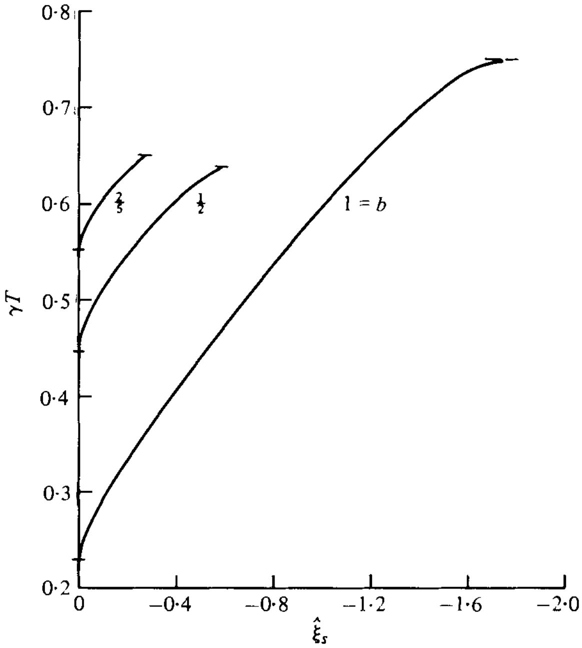

FIGURE 5. The development of shock position with time; $\hat{\xi}_s = 0$ is the locus of the *undisturbed* ambient atmosphere characteristic through the initial profile head. The initial profile is

$$(\gamma-1)\,u^{(1)}(\hat{\xi},0) = 2\sin b\hat{\xi}.$$

(i) $b = 1$. The variation with time γT of the jump in $(\gamma-1)\,u^{(1)}$ across the shock that forms at $\gamma T = 0{\cdot}22905$ is depicted in figure 6 and is also compared with the inert-gas result. The latter has the same initial pulse form of course but its strength is given, in general, by

$$[(\gamma-1)\,u^{(1)}] = 4(\gamma-1)\{\tfrac{1}{2}ab(\gamma+1)\,T-1\}^{\frac{1}{2}}\{b(\gamma+1)\,T\}^{-1}. \tag{27}$$

The inert-gas shock forms at a time T_{fi} such that

$$\tfrac{1}{2}ab(\gamma+1)\,T_{fi} = 1, \tag{28}$$

as already noted in §3, and achieves a peak strength of $u^{(1)} = a$ at the time $T_{\max}$, where

$$T_{\max} = 2T_{fi}. \tag{29}$$

As a result of the chemically induced amplification T_{fi} is here slightly later than T_f, but the most noteworthy feature of the development of shock strength in the present case is its monotone increase with increasing time. It can be seen from figure 3 that the shock wave 'swallows' the peak of the disturbance shortly after the time $\gamma T = 0{\cdot}38$, which is substantially earlier than the similar occurrence at $T_{\max}$ in the inert-gas case. Equation (29) shows that the latter is given by $\gamma T_{\max} = 0{\cdot}46$ when $b = 1$.

The shock in the exploding gas continues to grow in strength, but now with great rapidity and in such a way as to carry along the maximum temperature value immediately downstream of the shock. Figure 3 shows that $\partial T/\partial\hat{\xi}$ is now positive everywhere in the disturbance (recall the definitions of $\hat{\xi}$ and ξ in (10) and (1) respectively). At a γT of 0·75, where β_2 takes the value 2·11016, the shock strength $[(\gamma-1)\,u^{(1)}]$ achieves a value of 8·958... and very shortly (well within a γT interval of 10^{-3}) becomes

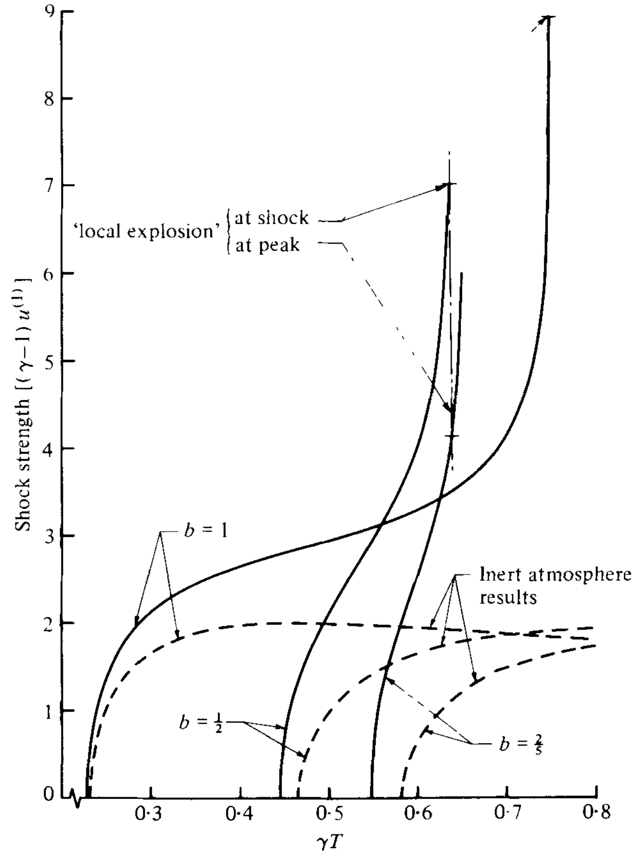

FIGURE 6. The growth of shock strength with time T for the initial profiles $(\gamma-1)\,u^{(1)}(\hat{\xi},0) = 2\sin b\hat{\xi}$ compared with behaviour from the same initial state in an inert atmosphere. Note the exceptional rapidity of the growth in the shock strength as the disturbance length increases (i.e. as b decreases), as well as the amount by which the explosive-atmosphere shock strength exceeds the inert-gas maximum value of 2 before local explosion intervenes.

logarithmically infinite. Evidently the compressive heating of the ambient explosive material has so progressed, in this case specifically through the agency of a Rankine–Hugoniot shock discontinuity, that a local explosion has taken place. Alternative descriptions of this event are 'ignition' or 'thermal runaway'; however one describes it, the breakdown of the present theory signifies that it is now necessary, certainly locally, to pay careful attention to the roles of transport effects and of the consumption of reactant material. The former have so far been ignored and the latter has not yet played a part in the theory, which is of first-order accuracy only, as can be appreciated from Clarke (1978).

It is interesting to observe that the local explosive event occurs substantially before the related inert-gas shock subsides into its $T^{-\frac{1}{2}}$ decay phase [see equation (27)]. The advance of the local explosion time ahead of the similar homogeneous event at $\gamma T = 1$ is also considerable enough to make the simple zero-depletion approximation to the *ambient* behaviour, which is inherent in the present first-order theory, quite acceptable (cf. Clarke 1978, figure 1*a*) for values of $\epsilon < 10^{-1}$, say.

(ii) $b = \frac{1}{2}$. For this value of b the compression pulse is initially stretched out to twice the length that it had in the previous example, with consequent reductions in initial slopes at given values of u_i, but it is otherwise unchanged. Figure 6 shows that the shock now does not form until $\gamma T = 0{\cdot}447\ldots$, but still noticeably earlier than its inert-gas counterpart, which has a γT_{fi} value [see equation (26)] of $0{\cdot}4\dot{6}$. Figure 6 also illustrates the fact that the shock's subsequent development is very much more rapid than for the $b = 1$ pulse. Indeed the present shock becomes stronger than the $b = 1$ shock for times γT in excess of about 0·56.

When $(\gamma - 1) u_i$ has its maximum value of 2 it can be seen from (9) that $(\gamma - 1) u^{(1)}$ becomes logarithmically infinite as $\gamma T \to 0{\cdot}638\ldots$. Evidently this signifies the development of a local explosion which grows from the peak of the imposed disturbance. In the previous, $b = 1$, case this peak was swallowed by the shock before local explosion could be achieved but in the present case the arrival of the shock wave at the (always amplifying) peak coincides almost exactly with the unimpeded occurrence of the local ignition. This state of affairs is illustrated in figure 6 where the shock-strength curve intersects the line drawn at $\gamma T = 0{\cdot}638\ldots$ when $(\gamma - 1) u^{(1)} \simeq 7$. Evidently the present Rankine–Hugoniot shock is not quite as strong at this time of the intervention of the local explosion as it is in the previous situation, but it is interesting to see that its time of growth to this point is only about 40% of the time taken in the initially sharper pulse. Figure 5 shows that the extent of the advance of the shock ahead of the line $\xi = 0$ is significantly smaller for $b = \frac{1}{2}$ than it is for $b = 1$.

(iii) $b = \frac{2}{5}$. Further spreading out of the initial disturbance by selection of the present value for b illustrates another feature of the evolution of compression pulses in an exploding atmosphere. Figure 6 shows γT_f at $0{\cdot}550\ldots$, compared with the inert-gas $\gamma T_{fi} = 0{\cdot}58\dot{3}$, followed by an even more rapid rate of growth of shock strength with time than appears with either of the two previous disturbance shapes.

A number of profiles of $(\gamma - 1) u^{(1)}$ *versus* ξ for fixed T values are shown in figure 4, which depicts conditions at the shock-formation time $\gamma T_f = 0{\cdot}550\ldots$, as well as the important new feature. This is the fact that the disturbance peak is now allowed to grow unimpeded towards its logarithmic increase near $\gamma T = 0{\cdot}638\ldots$, while the shock wave is still growing in the leading, or compressive, parts of the disturbance. The value and position of $(\gamma - 1) u^{(1)}(\beta_2)$ at the unimpeded local explosion time is indicated by a small cross on figure 6, with the similar small cross to its left on this figure marking the location of the local explosion point.

Comparison of the profiles for $\gamma T = 0{\cdot}63595$ (on figure 4) and $\gamma T = 0{\cdot}74$ on figure 3 is interesting, and hints strongly at different patterns of evolution of the gas dynamics and chemistry at and beyond the times of breakdown of the present theory.

The shock wave in the present, $b = \frac{2}{5}$, case continues to grow in strength until a local explosion occurs on its downstream side; the earlier advent of the explosion at the peak strictly invalidates such results and the portion of the $b = \frac{2}{5}$ curve that lies to the right of $\gamma T = 0{\cdot}638\ldots$ on figure 6 or above this γT value on figure 5 should properly be discounted.

(iv) *Smaller values of b*. Continued stretching-out of the disturbance by the selection of successively smaller values of b will ultimately lead to a situation for which no shock wave will form before the occurrence of local explosion at the disturbance peak. The evidence is that this occurs for b little smaller than $\frac{1}{3}$ and well before b is as small as $\frac{1}{4}$. It is of course true that the chemical amplification will produce a shock wave before *homogeneous* explosion takes place. However the occurrence of a *local* explosion strictly demands that the present theory should be discontinued at that time and replaced by one which takes more careful account of the behaviour near to, and as a result of, these dramatic chemico-gasdynamical events. The style and extent of the failure of the present theory will indicate how such a new theory is to be constructed.

REFERENCES

BLYTHE, P. A. 1978 *17th Symp. (Int.) on Combustion*, Leeds, England, 20–25 August. (In the press.)

CLARKE, J. F. 1978 *J. Fluid Mech.* **89**, 343–355.

LIGHTHILL, M. J. 1978 *Waves in Fluids*. Cambridge University Press.

WHITHAM, G. B. 1974 *Linear and Nonlinear Waves*. New York: Wiley.