On the structure of a class of aerothermodynamic shocks

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Some recent work on the existence of vibrational de-excitation shocks (δ -shocks) in expanding non-equilibrium nozzle flows is extended to include situations in which an adiabatic shock (α -shock) may be embedded within the de-excitation shock. A discussion of some further properties of the shock solution is given and some examples are worked out. Numerical solutions of the full equations are also presented. These solutions confirm the existence of the δ -shocks but bring to light certain anomalies in the simple approximate solution. The modifications necessary to remove these discrepancies are outlined, and the implications of the numerical results are briefly discussed. Finally, some comments on the nature of the asymptotic solution for an arbitrary rate process are made.

1. Introduction

In a paper by Blythe|| (1967) it was shown that a phenomenon closely analogous to a condensation shock may occur in expanding nozzle flows in a vibrationally relaxing gas. This phenomenon is characterized by a sudden and rapid de-excitation of the lagging internal mode; associated with the de-excitation is a weak compression. The bulk of the energy from the vibrational mode is fed into the translational and rotational degrees of freedom which are assumed to remain in a local equilibrium state. These de-excitation shocks, or δ -shocks, fall into the general class of aerothermodynamic shocks discussed by Polachek & Seeger (1958).

The analysis in the present paper is concerned with extending and clarifying some of the earlier work. Exact numerical solutions are presented which confirm the existence of this type of de-excitation shock. In addition, some new results are obtained for more general rate processes.

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^{||} The paper was in two parts: for convenience these will be referred to as I and Π respectively.

The shocks can occur in near-frozen flows when the local pseudo-entropy (Broer 1951 and I, II) $\int_{\sigma(x)} d\sigma$

$$S_{\alpha} = -\int^{\sigma(x)} \frac{d\sigma}{T} \tag{1.1}$$

becomes significant. Here σ is the vibrational energy, T is the translational temperature and x is a suitable axial co-ordinate. Johannesen (1961) has pointed out that continuum non-equilibrium flows are in general equivalent to the flow of some inert gas (the α -gas) with heat addition $\Delta q = -\Delta \sigma$. For vibrational relaxation (1.1) defines the entropy⁺ of this α -gas, and the shock region obviously corresponds to a local heat release or increase in S_{α} . As noted above and in II, an equivalence with condensation shocks is immediately apparent.

Although the growth of S_{α} provides a qualitative indication of the onset of any region of rapid de-excitation, detailed statements about the occurrence and position of the δ -shock can only be made if certain features of the nozzle geometry and rate of heat addition are specified. In particular, when the low-temperature behaviour of the relaxation time τ is given by

$$\tau^{-1} \sim \rho T^{\delta}, \tag{1.2}$$

where ρ is the density, it was shown in II that, for nozzles whose area A grows asymptotically as some power ν of the axial distance, δ -shocks exist in an ideal vibrationally relaxing gas if

$$\delta > 1, \tag{1.3}$$

and

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$$l = 1 - \nu \{2 - \gamma + (\gamma - 1)\delta\} > 0.$$
(1.4)

Here γ is the specific-heat ratio for the active modes.

Note, however, that the qualitative criterion on S_{α} suggests that there will be other situations in which δ -shocks occur, or at least in which significant deexcitation takes place (see below). The extension to more general rate processes is discussed in §5. (Consideration of other asymptotic nozzle shapes is given in §5.2.)

It is, in fact, condition (1.4) that corresponds directly to the qualitative statement on S_{α} , but δ -shocks exist only if the additional condition (1.3) holds. This latter requirement implies a restriction on the rate at which heat is added. The onset of de-excitation in the low-temperature, near-frozen, region far downstream can lead to an increase in the translational temperature which causes a local reduction in the relaxation time. This process is in some sense unstable since any reduction in τ leads to a further increase in the translational temperature, etc. It was shown in II that for $\delta > 1$ this process is limited by a rapid return to equilibrium conditions through a δ -shock. For $\delta < 1$ the process is limited both by a marked return towards an equilibrium flow and by the effects of the local area increase. This latter case corresponds to a gradual de-excitation region. Apart from a discussion of the asymptotic limiting solution in §5, the analysis in this paper is mainly confined to the shock case $\delta > 1$.

The possible existence of de-excitation shocks has been suggested earlier (see, for example, Feldman 1958) with specific reference to two-dimensional flow

[†] For other rate processes this definition is not necessarily as straightforward (see § 5 and appendix B), but the physical mechanism governing the δ -shocks is similar.

problems. Bartlma (1965) noted the apparent existence of both weak (oblique) and strong (normal) shocks in some approximate numerical solutions for twodimensional nozzle flows in a relaxing gas, though these results should be treated with caution because of the approximations involved. Mohammad (1967) and Johannesen (1968) have also observed a non-uniqueness in some characteristics calculations for one-dimensional unsteady flow. The shocks discussed in II differ from those reported by Bartlma and by Mohammad and Johannesen in that their structure is continuous: in this sense the shocks can be termed fully dispersed (Lighthill 1956). For the two-dimensional flows, the shocks are partly dispersed, and any local region of rapid de-excitation includes a conventional Rankine-Hugoniot shock (the α -shock). The precise connexion between the onedimensional δ -shock of II and these two-dimensional calculations is not clear. In this paper only the quasi-one-dimensional situation is examined.

Although the supersonic δ -shock solutions described in II were continuous discontinuous, (supersonic-subsonic) solutions of the equations are possible. It was assumed in II that the nozzle back pressure was zero, or at least less than the pressure at the downstream limit of the δ -shock. For finite back-pressures conventional adiabatic shocks (α -shocks) may be embedded within the de-excitation shock. Solutions applicable to this case are outlined in §3.

For this type of flow it is useful to consider the possible transitions through the δ -shock by means of a modified Rayleigh-line diagram. Instead of the conventional temperature, entropy co-ordinates, a more convenient transition diagram is the T, σ plane (see §3). In this diagram α -shocks occur at fixed values of the vibrational energy.

A well-known result associated with the Rayleigh-line diagram for the flow of a perfect gas with heat addition concerns the existence of an upper bound to the magnitude of the heat input above which the flow chokes. A significant result derived in this paper shows that, irrespective of the amount of energy in the lagging mode, the present class of non-equilibrium flows do not break down in this way: choking is prevented by the strong coupling between the energy and rate equations.

There is apparently no experimental evidence, at least to the authors' knowledge, either to confirm or to deny the existence of δ -shocks in nozzle flows with vibrational relaxation. Moreover, numerical calculations, based on the full quasi-one-dimensional relations, were not available for the conditions under which the shocks should occur. In order to verify both that solutions of the full equations did possess regions of rapid de-excitation for appropriate conditions, and that the approximate solution did predict the structure and position of these regions, some numerical calculations for the full equations were carried out. At the same time detailed calculations based on the approximate solutions, which are outlined in §§2 and 3, were made.

The calculations were performed for the ideal vibrationally relaxing diatomic gas (Johannesen 1961). It should be stressed that this is a fairly severe test of the theory since the energy content of the vibrational mode may be quite small in comparison with the total internal energy. For rate processes in which this energy content is larger, the error terms in the approximate theory will be relatively smaller. However, the numerical solutions clearly show the existence of the δ -shocks and the agreement with the simple theory for the shock position is satisfactory. The shock structure is also predicted reasonably well by the theory, though values of the local maximum in the translational temperature at the downstream limit of the shock are, in general, noticeably different from the values given by the approximate solution. It is conjectured that, for sufficiently large values of ν , this discrepancy is mainly due to the effects of a finite area change through the shock. A similarity argument confirming this conjecture is presented in §4. If ν is small other factors have to be taken into account; the uniform channel limit, $\nu \to 0$, is also discussed in §4.

In II it was shown that the δ -shock occurs at 'large' distances downstream of the throat. A significant feature of the numerical calculations has been the magnitude of this distance. For a number of practical situations the shock position was typically 10⁵-10⁶ diameters downstream of the throat, but in some cases rather diffuse shocks were found to occur at around 10³ diameters. This latter distance is roughly equivalent to the maximum nozzle length of some current hypersonic facilities.

Although these results for vibrational de-excitation in a diatomic gas would seem to suggest that experimental verification would be difficult, this is not necessarily true for all rate processes. In cases where a considerable amount of energy is involved the shock may occur appreciably nearer the throat. It is relatively straightforward to obtain the dependence of the shock position on the energy content in the lagging mode for a fairly general class of rate processes (see $\S5$). It is perhaps worth remarking that in order to find the shock position the only knowledge of the rate equation required is its behaviour in a nearfrozen state. Unfortunately, the extension to include the shock structure depends strongly on the type of rate process considered, though some comments are made in \$5 on the asymptotic solution downstream of the shock. Throughout this paper it is assumed that the rate of change of internal energy depends only on local conditions and, if necessary, appropriate initial parameters (see \$5).

2. The shock equations

Unless otherwise stated, the notation used here is as in I and II. All basic variables are non-dimensionalized with respect to suitable reservoir conditions (see appendix A and I, §2.5). For the flow through the δ -shock (see II, §3) the governing equations can be written

$$\pi_1 u = u_0(\infty), \tag{2.1}$$

$$P_1 + \pi_1 u^2 = u_0^2(\infty), \tag{2.2}$$

$$\frac{\gamma}{\gamma - 1}T + \frac{1}{2}u^2 + \sigma = \frac{1}{2}u_0^2(\infty) + \sigma_{\infty}, \qquad (2.3)$$

$$\frac{d\sigma}{dy_1} = u_0(\infty) \,\pi_1 \,\frac{\Omega(T)}{u} \{ \overline{\sigma}(T) - \sigma \}, \tag{2.4}$$

$$u_0^2(\infty) = u_\infty^2 + \frac{2\gamma}{\gamma - 1},$$
 (2.5)

where

and u_{∞} is the initial speed far upstream of the shock. σ_{∞} is the initial (reservoir) value of the vibrational energy.

Here π_1 , P_1 and y_1 are related to the corresponding variables defined in II by

$$\pi_1 = \Pi Y_s^{\nu}, \quad P_1 = \pi_1 T, \quad y_1 = Y_s^{1-\nu} \left(\frac{u_0(\infty)}{m_0}\right)^{(\gamma-1)\delta} y. \tag{2.6}$$

In (2.6) the scaled density Π and the stretched variable y are related to the basic physical variables by (II, §§2, 3).

 $d = (\gamma - 1)\nu(\delta - 1)l^{-1}$.

$$\Pi = \lambda^{-\nu/l} \rho u_0(\infty) / m_0, \quad y = \lambda^{-d} \left(Y - Y_s \right), \quad Y = \lambda^{1/l} x, \tag{2.7}$$

where

$$Y = Y_{s} = \left\{ \frac{l}{(\delta - 1)(\gamma - 1)\sigma_{\infty}} \left(\frac{m_{0}}{u_{0}(\infty)} \right)^{\gamma - 1} \right\}^{1/l}$$
(2.9)

defines the shock position and

$$\lambda = \frac{\Lambda}{u_0(\infty)} \left(\frac{m_0}{u_0(\infty)} \right)^{1 + (\gamma - 1)\delta}$$
(2.10)

is a modified rate parameter. The non-dimensional rate parameter Λ (characteristic ratio of flow time to relaxation time) is defined with respect to reservoir conditions and the throat height (see appendix A). A derivation of the result corresponding to (2.9) for a more general rate process is given in §5. (The reader may wish to refer to that section for a brief discussion of the various scaling laws noted above.)

The conservation relations (2.1) to (2.3) are valid in the limit $\lambda \to 0$. According to the right-hand sides of these expressions, conditions ahead of the shock correspond to a low-temperature near-frozen state: $u_0(\infty)$ (see (2.5)) is apparently the fluid speed immediately upstream of the shock.

Since the explicit dependence of the shock solution on Y_s is eliminated, the present choice of dependent and independent variables is preferred to those used in II. For a given u_{∞} and γ the solution depends only on the parameters contained in the modified relaxation frequency $\Omega(T)$ and the energy term σ_{∞} . In this paper attention is confined to the case

$$u_{\infty} = 0. \tag{2.11}$$

For simplicity, it is also assumed that Ω can be described by its low-temperature behaviour $\Omega = T^{\delta}$ (2.12)

throughout the shock region. As observed in the introduction, the shock solution is appropriate for $\delta > 1$. If the flow is initially in equilibrium

$$\sigma_{\infty} = \overline{\sigma}_{\infty}(\theta_v) = \theta_v / (e^{\theta_v} - 1), \qquad (2.13)$$

where θ_{v} is the characteristic temperature of vibration.

It follows that for a given $\gamma (= \frac{7}{5}$ for a diatomic or linear molecule) the shock solution will depend on the parameters θ_v and δ only, and can be written

$$\frac{u(Q)}{u_0(\infty)} = \frac{1}{\pi_1} = \frac{\gamma \pm \sqrt{(1-Q)}}{\gamma+1},$$

$$\frac{T(Q)}{u_0^2(\infty)} = \frac{\gamma - (1-Q) \mp (\gamma-1)\sqrt{(1-Q)}}{(\gamma+1)^2},$$
(2.14)

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(2.8)

where the heat input

$$Q(\sigma; \theta_v) = 2(\gamma^2 - 1) \left(\sigma_{\infty} - \sigma\right) / u_0^2(\infty).$$
(2.15)

As usual the upper sign in (2.14) corresponds to a supersonic solution[†] and the lower sign to a subsonic solution. Q is given as a function of y_1 from the integrated form of the rate equation

$$y_1 + C = I(Q, Q_1; \delta, \theta_v) = \frac{\gamma - 1}{2\gamma} \int_{Q_1}^Q \frac{u^2(q) \, dq}{T^\delta(q) \{\overline{Q}(q; \theta_v) - q\}},\tag{2.16}$$

where the lower limit Q_1 has been inserted for convenience and $\overline{Q} = Q(\overline{\sigma}; \theta_v)$.



FIGURE 1. De-excitation shock profiles for $\delta = 1.5$.

The constant C in (2.16) is evaluated by matching with the solution valid upstream of the shock. This latter solution, termed the pseudo-entropy solution in II (see below §5), shows that for non-integer values of δ

$$C = \underset{Q \to 0}{F.P.} I(Q, Q_1; \delta, \theta_v).$$
(2.17)

For integer values there is an additional term

$$a_{\delta-1}(\gamma-1)^{\nu}l^{-1}\log\lambda,$$
 (2.18)

where $a_{\delta-1}$ is the coefficient of $Q^{\delta-1}$ in the expansion of the integrand as $Q \to 0$ (see Petty 1968).

The integral I has been evaluated numerically for a range of values of δ and θ_v . Figure 1 shows some typical results for the shock profile when $\delta = 1.5$ for various θ_v . As might be expected, an increase in the initial vibrational energy

† With respect to the frozen sound speed. This should be understood throughout.

leads to a steeper shock profile. Results for other values of δ show no qualitative difference. Comparison with exact numerical calculations for the full equations is deferred until §4.

3. The Rayleigh-line and related diagrams

Diabatic flows of the general kind considered here are usually discussed in the temperature-entropy plane. For the present class of non-equilibrium flows entropy, in its usual sense, is not clearly defined. However, as noted in the introduction, the quantity

$$\Delta_{\mathcal{A}} S_{\alpha} = S_{\alpha} - (S_{\alpha})_{\mathcal{A}} = -\int_{\sigma_{\mathcal{A}}}^{\sigma} \frac{d\sigma}{T}$$
(3.1)

can be referred to as the change in the pseudo-entropy: S_{α} is identifiable with the entropy of the α -gas of Johannesen. A convenient datum point for the pseudo-entropy is the point Q = 0 on the subsonic branch. From (2.14)

$$\Delta_0 S_{\alpha} = \frac{1}{\gamma - 1} \log \left\{ \left(\frac{\gamma \pm \sqrt{(1 - Q)}}{\gamma - 1} \right)^{\gamma} \frac{1 \mp \sqrt{(1 - Q)}}{2} \right\}.$$
(3.2)

The T, S_{α} diagram is shown in figure 2. Note that on the supersonic branch

$$\Delta_0 S_a \sim \frac{1}{\gamma - 1} \log T \tag{3.3}$$

as $T \rightarrow 0$.

In nozzle flows where δ -shocks occur, the initial conditions are always supersonic with Q = o(1). If the nozzle back-pressure is zero the solution remains supersonic; but if the back-pressure is finite any region of supersonic flow may be terminated by a conventional adiabatic shock (the α -shock). The solution downstream of the α -shock is defined by the subsonic branch of the δ -shock solution. (In the limit considered here the thickness of the α -shock, which is defined by the diffusive effects of viscosity and heat conduction, is negligible in comparison with the thickness of the δ -shock.)

The transition from the supersonic to the subsonic branches occurs at constant Q. A constant Q jump is shown in figure 2. Note that S_{α} increases across the α -shock. Since the transition across the α -shock is very simply defined in the (T, Q)-plane, it is convenient to use this diagram (see figure 3), when discussing solutions involving α -shocks.

Conditions at the downstream limit of the δ -shock are given by the equilibrium value $Q = \overline{Q}$. These equilibrium paths are

$$\theta_{v}/T = \log \{1 + \theta_{v}/(\sigma_{\infty} - cQ)\},$$

$$c = \gamma(\gamma + 1)^{-1}(\gamma - 1)^{-2}.$$
(3.4)

where

The intersection of these lines with the (T, Q)-curve defines both the final supersonic state and the final subsonic state (see figure 3).

In general, there are three main situations to consider for finite values of the back-pressure P_b :

(i) $P_e > P_b$, where P_e is the equilibrium pressure at the downstream limit of the 23-2

supersonic δ -shock. In this case any α -shock lies downstream of the δ -shock and the solution through the δ -shock remains supersonic.

(ii) $P_e \gtrsim P_b$. The α -shock is now embedded within the δ -shock.





(iii) $P_e < < P_b$. The α -shock terminates the region of supersonic frozen flow. Downstream of the α -shock there will be a return to equilibrium conditions.

Case (ii) is probably of most interest. It was shown in II that on the supersonic branch the flow initially remains near to equilibrium downstream of the shock,

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where the effects of area change must again be taken into account. On the subsonic branch it can be shown that equilibrium flow is the only possible limiting solution. (In the supersonic case there may be an eventual departure from the equilibrium solution. Since this occurs exponentially far downstream of the primary δ -shock, it is of little practical interest.)

Typical paths in the (T, Q)-plane are shown in figure 4. It is apparent from figure 4, and the (P_1, T) -relation in the subsonic δ -shock, that the pressure may





FIGURE 5. Typical pressure distributions (schematic).

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initially decrease behind the α -shock, but for nozzles of sufficient length the pressure will always ultimately rise following the subsonic equilibrium curve (see figure 5). A simple inverse scheme for obtaining solutions in these cases is to define the shock position by a given value of $Q = Q_{\alpha}$ and then, for a given nozzle length, evaluate the back pressure P_b from the subsonic equilibrium solution.



FIGURE 6. (a) Adiabatic shocks and their relaxation zones for $\delta = 1.5$, $\theta_v = 1.5$. (b) Relaxation zone for $\delta = 1.5$, $\theta_v = 1.5$, (enlarged); the α -shock occurs at $y_1 = 0$.

Some calculations for the de-excitation region are shown in figures 6 (a) and (b). The passage through the α -shock leads to a marked decrease in the local value of the relaxation time and hence the width of the relaxation region behind the α -shock is very narrow in comparison with the upstream part of the δ -shock.

In the classical treatment of flows with heat addition, solutions do not exist for Q > 1: the sonic point, Q = 1, corresponds to thermal choking. However, for the non-equilibrium flows considered here the mechanism of the heat input is not independent of the flow. Moreover, it was noted in II that choking could not occur in a diatomic gas, though it is not immediately apparent that Q < 1 in a polyatomic gas with an arbitrary number of vibrational modes which relax together.

It is sufficient to consider initial equilibrium conditions with $u_{\infty} = 0$. (All flows, even with $\sigma_{\infty} \neq \overline{\sigma}_{\infty}$, are assumed to be derived from some equilibrium reservoir without any external heat addition. A slight modification in the argument given below leads to similar results for these cases.) Suppose, first, that no α -shock occurs. Upstream of the δ -shock $\sigma > \overline{\sigma}$ and it follows from the rate equation that σ is a monotonically decreasing function of x with a limiting value, in the δ -shock, defined by equilibrium conditions $\sigma = \sigma_e = \overline{\sigma}_e < \overline{\sigma}_{\infty}$. Since $\overline{\sigma}$ is a monotonically increasing function of T, it follows that $T_e < 1$. Hence from (2.14) and (2.5), Q < 1 if $\gamma < 1.839...$

If an α -shock occurs within the δ -shock then $Q_{\alpha} < (\bar{Q}_{e})_{\sup} < 1$ by definition. Since $T_{\sup} > T_{\sup}$ and Q is a monotonically decreasing function of T

$$(\bar{Q}_e)_{sub} < (\bar{Q}_e)_{sup}$$

and therefore Q < 1 on the subsonic branch.

Although the above argument establishes that Q < 1, irrespective of the number of vibrational modes n, it can be shown that as $n \to \infty$

$$1 - T_e = O(1/n).$$

4. Numerical solutions and higher approximations

4.1. Nozzle shapes and the shock-position

Probably the simplest way to check the analytical solutions described in II and in \S and 3 of this paper is to compare them with numerical solutions of the full equations. The numerical solutions used in this paper were found from an adaptation of the programme described by Wilson, Schofield & Lapworth (1967). For the analytical solutions the asymptotic nozzle shape has the form

$$A \sim C x^{\nu}. \tag{4.1}$$

The convergent-divergent nozzle shapes used in the numerical calculations belong to the family

$$A = 1 + x^2 \quad (x \le x_0), \tag{4.2a}$$

$$A = C(x-a)^{\nu} \quad (x \ge x_0). \tag{4.2b}$$

Both A and dA/dx are continuous at x_0 , or

$$a = x_0 - \frac{1}{2}\nu(x_0^{-1} + x_0), \quad C = (2x_0/\nu)^{\nu} (1 + x_0^2)^{1-\nu}.$$
(4.3)

Previous calculations reported in the literature have not, to the authors' knowledge, included cases in which weak compressions (δ -shocks) occur. A typical example from the present calculations is shown in figure 7. The region of frozen flow, prior to the collapse through the shock, is obviously extensive. Some comment on this point is made below in §4.3.

The analytical solution described earlier is also shown in figure 7. Agreement between this approximate solution and the exact solution is good, particularly for the shock position, though there is a significant difference in the values for the maximum temperature at the downstream edge of the shock. Apart from this shift in temperature, the initial equilibrium decay downstream of the shock agrees well with theoretical predictions.



FIGURE 7. A typical δ -shock. ——, numerical; ——, approximate analytical solution. $\theta_v = 1.0, \Lambda = 1.0, \delta = 1.5, x_0 = 1.0, \nu = 0.3.$

The δ -shock position for the numerical solutions is defined as the point at which the translational temperature attains the value corresponding to $y_1 = 0$ $(x = \lambda^{-1/l} Y_s)$ in the analytical solution. Equations (2.7) and (2.9) can be rearranged, for the asymptotic nozzle shape (4.1), to give

$$x_s = K X_s(\gamma, \nu, \delta), \tag{4.4}$$

$$X_s = \left\{ \frac{lu_0(\infty)}{\left(\delta - 1\right)\left(\gamma - 1\right)} \left(\frac{m}{u_0(\infty)}\right)^{(1-l)/\nu} \right\}^{1/l},\tag{4.5}$$

and
$$K = (\Lambda \sigma_{\infty} C^{(l-1)/\nu})^{-1/l}$$
. (4.6)

Note that in (2.7) and (2.9), m_0 must be replaced by m_0C^{-1} to account for the corresponding factor in (4.1) (see appendix A). In this form, for given γ and δ , $X_s = X_s(\nu)$: the dependence on the rate parameter, internal energy and matching point x_0 (i.e. C) are all contained in K.

Various tests of this similarity rule are shown in figures 8(a), (b) and (c). Only two cases are shown on each graph for reasons of clarity. For other values of the parameters the trends are very similar. The shock position is predicted reasonably well in most cases, and the various scaling laws appear to be correct except at small values of ν . Since $\nu \to 0$ corresponds to a straight channel, it is not sur-

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prising, in this limit, that the asymptotic state is dependent, in particular, on the initial conditions at the entrance to the channel, i.e. at x_0 . For a further discussion of this point, see §4.2.



FIGURE 8. (a) Comparison of X_s values for various Λ when $\delta = 1.5$, $\theta_v = 1.0$, $x_0 = 5$. \checkmark , $\Lambda = 0.1$; $\textcircled{\bullet}$, $\Lambda = 0.01$; \neg , theory. (b) Comparison of X_s values for various θ_v when $\delta = 1.5$, $\Lambda = 1.0$, $x_0 = 10$. \blacktriangledown , $\theta_v = 1.0$; \blacksquare , $\theta_v = 2.0$; \neg , theory. (c) Comparison of X_s values for various x_0 when $\delta = 1.5$, $\Lambda = 1.0$, $\theta_v = 1.0$. \blacktriangledown , $x_0 = 10$; \blacksquare , $\lambda_0 = 5$; \neg , theory.

4.2. Temperature profiles

The magnitude of the translational temperature T_e , at the downstream limit of the δ -shock, predicted by the approximate solution is significantly different from the corresponding value in the numerical solution. Figure 9 shows the variation of T_e with the shape parameter ν for several values of x_0 . Reservoir conditions, defined by Λ and θ , together with the gas parameter δ are fixed. The behaviour for other values of Λ , θ and δ is very similar.

Provided ν is not small it seems likely that this error in the approximate theory is mainly due to the effects of area change through the δ -shock. In order to account for these errors the continuity equation (2.1) is replaced by

$$\pi_1 u = (1 + \lambda^d Y_s^{\nu - 1} y_1)^{-\nu} \sim 1 - \nu \lambda^d Y_s^{\nu - 1} y_1 + \dots$$
(4.7)

Apparently the significant parameter in these perturbation calculations is

$$\alpha = \nu \lambda^d Y_s^{\nu-1}, \tag{4.8}$$

or, to first order, $\pi_1 = \pi_1(y_1; \alpha)$, etc. (4.9)

The actual evaluation of the perturbation terms is rather complex and does not seem to be necessary. To determine the validity of (4.9) it is sufficient to

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compare the numerical solutions at constant values of α . Lines on which $\alpha =$ const. are shown in figure 9. It is immediately clear that the similarity rule (4.9) is valid for sufficiently large values of ν .



FIGURE 9. Limiting temperatures in de-excitation shocks. ---, parallel pipe limit.

Not surprisingly the rule breaks down for smaller values of ν . In the parallel pipe limit, $\nu \to 0$, perturbations are presumably dominated by entry conditions at $x = x_0$. It can be shown that if conditions at x_0 are calculated by assuming frozen flow between the reservoir and x_0 , and, if for $x \ge x_0$ the one-dimensional relations without area change are used, values of T_e are obtained which are in reasonable agreement with the numerical computations (see figure 9 and Petty 1968). As $x_0 \to \infty$, these values converge on the δ -shock limit.

4.3. Comments

As noted in the introduction, the approximate theory is less accurate when the lagging mode contains only a small fraction of the total internal energy (see also $\S5$). Hence the comparison outlined above for a single vibrational mode is a reasonably severe test of the theory. Agreement with the numerical calculations is satisfactory.

In general the δ -shocks were found at least 10⁵ diameters downstream of the throat, though in certain situations, e.g. with larger values of λ , shocks may occur at 10³-10⁴ diameters but their structure becomes more diffuse in this limit (see figure 10). Obviously, in these latter cases, the approximate theory (valid as $\lambda \rightarrow 0$) can no longer be expected to hold. Moreover, since typical nozzle lengths in current hypersonic facilities are of the order of 10³ throat diameters, it would

appear that quantitative experimental confirmation of the theory is not feasible, but it may be possible, when λ is not small, to establish whether similar qualitative trends may occur.

For rate processes involving a large amount of energy, it can be shown that any δ -shock lies further upstream and an experimental investigation may be easier to carry out. Some discussion of the shock position, and of the asymptotic decay downstream of the shock, is given below in §5 for a fairly general family of rate processes.



FIGURE 10. A large Λ (diffuse shock) example for the nozzle shape defined by $x_0 = 5$, $\nu = 0.03$. $\theta_v = 0.5$, $\delta = 1.5$, $\Lambda = 10$.

5. General rate processes

5.1. δ -shocks for power law asymptotes

The analysis in this paper has so far been restricted to the ideal vibrationally relaxing gas, though it was noted in II that some of the results can easily be modified to include the case of a dissociating gas. One purpose of the present section is to obtain conditions under which δ -shocks occur for a general (single) rate process governed by $d\sigma$

$$\frac{d\sigma}{dt} = \Lambda F(\rho, T, \sigma), \tag{5.1}$$

where σ is again to be interpreted as the energy in the lagging mode. In order to compare directly the results of this section with the analysis for the ideal relaxing gas discussed earlier, it is assumed initially that at low temperatures and low densities[†]

$$F \sim -\rho^n T^{\delta} G(\sigma) \tag{5.2}$$

† Some restriction must obviously be placed on this double limit. The relative sizes of ρ and T are strictly defined by the local solution, but it is usually sufficient to suppose that $T = 0(\rho^{\alpha}), 0 < \alpha < 1$.

for finite values of σ . For this particular form of F the δ -shock position can be obtained explicitly and its dependence on the initial energy level σ_{∞} found. This *limiting* behaviour is possible in a number of rate processes. The extension to non-separable F is discussed in §5.2.

If the total internal energy $e = e(\rho, T, \sigma)$, the energy equation can be re-written as

$$d(\log \rho) - (\Gamma - 1)^{-1} d(\log T) = (\Delta/T) d\sigma, \qquad (5.3)$$

where

as $T \rightarrow 0$. Here

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$$\Gamma = \gamma - (\gamma - 1) \left(1 - 1/\rho T \beta \right) \tag{5.4}$$

is an effective specific-heat ratio. Here γ is the frozen specific-heat ratio and

$$\beta = \left\{ \frac{\partial}{\partial T} \left(\frac{1}{\rho} \right) \right\}_{p,\sigma} \tag{5.5}$$

is the frozen expansion coefficient. In addition

$$\Delta^{-1} = c_v (\Gamma - 1) \left(\frac{\partial \sigma}{\partial e} \right)_{\rho, T}, \tag{5.6}$$

where c_v is the frozen specific heat at constant volume.

Near frozen solutions of (5.1) and (5.3), together with the usual continuity and momentum relations, can be found, apart from any non-uniformity in the reservoir region (see I), by the standard expansion

$$T = T_0(x) + \Lambda T_1(x) + \dots, \quad \sigma = \sigma_{\infty} + \Lambda \sigma_1(x) + \dots, \tag{5.7}$$

etc. From the zero-order frozen solution it follows that, subject to suitable restrictions on Γ and its derivatives,

$$\rho_0 \sim K T_0^{1/(\Gamma_{\infty} - 1)} \tag{5.8}$$

$$\Gamma_{\infty} = \Gamma(0, 0, \sigma_{\infty}), \tag{5.9}$$

and the limits $\rho, T \to 0$ are evaluated in the sense discussed above. (This should be understood throughout.) If $\Gamma_f = \Gamma(\rho, T, \sigma_{\infty})$ is independent of the density (e.g the ideal dissociating gas)

$$K = \exp\left(-\int_0^1 \frac{\Gamma_{\infty} - \Gamma_f}{(\Gamma_{\infty} - 1)(\Gamma_f - 1)} \frac{dT}{T}\right),\tag{5.10}$$

otherwise K must be found by numerical integration.

It is easily shown, as in II, that the expansion (5.7) is not uniformly valid if

$$\int_{0}^{\sigma_1(x)} \frac{\Delta_0}{T_0} \, d\sigma_1 \tag{5.11}$$

diverges for large x. (This condition implies that T_1/T_0 is unbounded as $x \to \infty$.) The corresponding result in II is easily interpreted in terms of the pseudo-entropy or entropy of the α -gas. In the general case considered here this interpretation is not as straightforward (see appendix B) but (5.11) is obviously associated with an effective heat addition. From the frozen solution and (5.2) it is found that (5.11) is divergent if

$$L = 1 - \nu \{ 1 + n - \Gamma_{\infty} + (\Gamma_{\infty} - 1)\delta \} > 0,$$
(5.12)

which is a generalization of the corresponding result in II (see equation (1.1) of the present paper).

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When

$$Y = \Lambda^{1/L} x \tag{5.13}$$

is O(1), the leading terms in the expansion (5.7) are of the same size, and an alternative solution must be sought. A principal feature of this region is the retention to zero order of the effective-heat-input term on the right-hand side of (5.3), though this domain still corresponds to a near-frozen, low-temperature, lowdensity state. Appropriate dependent variables are

$$u, \Lambda^{-\nu/L} \rho, \tag{5.14}$$

$$\hat{\Theta} = \Lambda^{-B} T, \qquad (5.15)$$

$$\hat{\Sigma} = \Lambda^{-B} (\sigma_{\infty} - \sigma), \qquad (5.16)$$

(5.16)

and where

$$B = (\Gamma_{\infty} - 1) \nu L^{-1}. \tag{5.17}$$

These dependent variables are equivalent, apart from some constant factors, to those used in II with b and l replaced by B and L respectively. Note that in (5.16) σ_{∞} should strictly include any frozen contribution of magnitude greater than $\Lambda^{\mathcal{B}}$ (see II, §2).

It follows that in this pseudo-entropy region F can be replaced by its asymptotic behaviour (5.2) with $G = G(\sigma_{\infty})$. Consequently any non-linearity in $G(\sigma)$ is not important in this domain.

It is easily shown that the governing equations are, to zero order,

$$u = U_0, \quad \rho = \Lambda^{\nu/L} m_0 U_0^{-1} \hat{Y}^{-\nu}$$
(5.18)

and

$$\frac{\nu}{\hat{Y}} + \frac{1}{\Gamma_{\infty} - 1} \frac{1}{\hat{\Theta}} \frac{d\hat{\Theta}}{d\hat{Y}} = \frac{\Delta_{\infty}}{\hat{\Theta}} \frac{d\hat{\Sigma}}{d\hat{Y}}, \qquad (5.19)$$

$$U_0 \frac{d\hat{\Sigma}}{d\hat{Y}} = \left(\frac{m_0}{U_0}\right)^n \hat{Y}^{-n\nu} \hat{\Theta}^{\delta} G(\sigma_{\infty}).$$
(5.20)

(These expressions should be compared with the corresponding relations in II, §2.) The constants U_0 and Δ_{∞} are defined by

$$U_0^2 = u_\infty^2 + 2\{h(1, 1, \sigma_\infty) - h(0, 0, \sigma_\infty)\} \Delta_\infty = \Delta(0, 0, \sigma_\infty).$$
(5.21)

and

As in II, the solution of the non-linear equations (5.19) and (5.20) for the temperature is easily obtained and can be written

$$\Theta = \hat{Y}^{-(\Gamma_{\infty}-1)\nu} \{ (m_0/U_0 K)^{\Gamma_{\infty}-1} - (\delta-1) (\Gamma_{\infty}-1) D \hat{Y}^L/L \}^{-1/(\delta-1)}, \quad (5.22)$$

$$D = \Delta_{\infty} G(\sigma_{\infty}) \ U_0^{-1} (m_0 U_0^{-1})^n, \tag{5.23}$$

where

and the arbitrary constant of integration has been determined by matching with the downstream behaviour of the conventional near-frozen solution. For $\delta > 1$, the pseudo-entropy solution (5.22) is singular at

$$x_{s} = \left\{ \frac{L(m_{0}U_{0}^{-1}K^{-1})^{\Gamma_{\infty}-1}}{\Lambda(\delta-1)(\Gamma_{\infty}-1)D} \right\}^{1/L}.$$
(5.24)

Note especially that the shock position is a monotonically decreasing function of σ_{∞} (in general $G'(\sigma) > 0$). The principal dependence of x_s on σ_{∞} is given by the factor $\{G(\sigma_{\infty})\}^{-1/L}$.

5.2. δ -shocks for general F

Although the initial analysis described above was restricted to power-law behaviours, similar results can be obtained for quite general (non-separable) F with little change in the argument. In this section no restriction is placed on the asymptotic form of A other than dA/dx > 0.

It has already been observed that the first difficulty encountered with the conventional near-frozen expansion is the divergence of the pseudo-entropy integral. In the present context this is equivalent to the statement that

$$S_{a}(x) \to \infty \quad \text{as} \quad x \to \infty,$$
 (5.25*a*)

where the asymptotic growth of S_{α_1} is described by

$$S_{\alpha_1} \sim \int^x F\left(\frac{m_0 A^{-1}}{U_0}, \left(\frac{m_0 A^{-1}}{U_0 K}\right)^{\Gamma_{\infty} - 1}, \sigma_{\infty}\right) \left(\frac{m_0 A^{-1}}{U_0 K}\right)^{-(\Gamma_{\infty} - 1)} dx. \quad (5.25b)$$

The behaviour of this integral implicitly defines the stretching for the pseudoentropy régime. In general this stretching may be quite complex but it is apparent from the previous discussion that this region will correspond to a near-frozen, low-temperature, low-density state in which the heat-input term on the righthand side of (5.3) is significant.

Hence, in terms of the unstretched variables, the governing equations reduce to $\alpha = m/U - 4 - u = U$ (5.26)

$$\rho = m/U_0A, \quad u = U_0, \tag{5.26}$$

$$\frac{1}{A} + \frac{1}{\Gamma_{\infty} - 1} \frac{1}{T} \frac{dT}{dA} = -\frac{\Delta_{\infty}}{T} \frac{d\sigma}{dA}$$
(5.27)

and

$$\frac{d\sigma}{dx} = \Lambda F_{\infty}(m_0/U_0A, T, \sigma_{\infty}), \qquad (5.28)$$

where F_{∞} is the asymptotic expansion of F in the pseudo-entropy limit. These relations can be combined to give a single equation for the temperature distributions, and it follows from the form of this relation that a δ -shock is possible only if $F = \frac{|F|}{|T|} + \frac{|F|}$

$$|F_{\infty}|/T \to \infty$$
, as $T \to \infty$ (A fixed). (5.29)

Note that the functional form of F_{∞} corresponds to the low-temperature behaviour of F. In (5.29) T should strictly be replaced by a scaled temperature Θ which is O(1) in the pseudo-entropy domain. The limit in (5.29) then corresponds to $\Theta \to \infty$. (It should be stressed that it is the behaviour of F_{∞} for $\Theta \to \infty$ that is important and not the behaviour of F for finite temperatures.) Equations (5.25*a*, *b*) and (5.29) provide necessary and sufficient conditions for the existence of δ -shocks, replacing the simpler conditions L > 0, $\delta > 1$ which are true for the power law forms of F and A.

It is significant that throughout the analysis of this section only a knowledge of $F(\rho, T, \sigma_{\infty})$ is required, i.e. its behaviour near the initial energy state. The validity or otherwise of the ideal rate equation (2.4) used earlier in §§2–4 has been questioned from several points of view (Zienkiewicz & Johannesen 1963; Simpson & Chandler 1969; and for a review of nozzle data see Hall & Treanor 1968). In the context of the earlier sections, (2.4) should strictly be regarded as a simple model equation by means of which the perturbation analysis can be tested against exact numerical calculations. Here, it is sufficient to point out that the present analysis holds if the rate equation can be formulated in the near-

frozen limit in terms of local conditions and, if necessary, any initial parameters. (Thus a simple dependence on the flow history of the type $F = F(\rho, T, \sigma; \sigma_{\infty}, \epsilon_{\infty})$, where $\epsilon = \sigma - \overline{\sigma}$, can be permitted.) This restriction is rather less severe than the usual postulate that the rate of change of internal energy is a function *only* of local conditions for *all* values of σ .

However, it is important to note that, if the solution in the shock layer is required, the behaviour of the rate equation at all energy levels may be important. For the ideal gas discussed in II, the appropriate scaling in the shock layer is defined by the singular behaviour corresponding to (5.22) and by the statement that this behaviour is limited by the inclusion of the equilibrium factor $\overline{\sigma}$ in the rate equation. Since $\overline{\sigma}$ is a function of the translational temperature alone, this leads, in particular, to the result that $\sigma_{\infty} - \sigma = O(1)$ within the shock. For other rate processes in which the equilibrium curve is also density dependent the structure may be more complex.

5.3. Limiting solutions

Even though it is apparent that the shock structure for a specific F requires detailed calculations, some progress can be made with respect to the asymptotic decay downstream of the δ -shock. For finite back pressures, the downstream state is limited by the appearance of an α -shock (see §3). Downstream of the α -shock there is a return to a subsonic equilibrium state ($u \sim A^{-1}$). (The nozzle is assumed throughout to grow monotonically with x downstream of any geometric throat: an asymptotic return to a uniform duct can be permitted as a special case.)

Of more interest is the decay when the nozzle back pressure is effectively zero (alternatively this can be regarded as the behaviour upstream of any limiting α -shock). In II a discussion of the decay laws for the ideal rate equation showed that a wide variety of asymptotic states could exist. Cheng & Lee (1967, 1968) have examined similar limiting solutions for a dissociating gas. Here, an investigation of the decay laws is presented for the more general form (5.2) which includes the ideal relaxing gas and a dissociating gas as particular examples.

It was shown in II that the asymptotic limiting states for zero back pressure could be found from a suitable model equation which was deduced by neglecting the equilibrium term in the rate equation. If δ -shocks occur this model equation is quantitatively incorrect, but it should be noted that it still predicts the appropriate qualitative behaviour.

In the present case, after making corresponding assumptions, the pseudoentropy and rate equations can be combined to yield

$$z^{\beta}\frac{d^{2}w}{dz^{2}} = -G'(\sigma)w^{-\beta}\frac{dw}{dz}$$
(5.30)

$$G(\sigma) = \frac{(L/\lambda)^{1/\delta}}{\Delta_{\infty}(\Gamma_{\infty} - 1)} \frac{1}{1 - \delta} \frac{dw}{dz},$$
(5.31)

and

where
$$w = (L/\lambda)^{1/\beta} \{ T x^{(\Gamma_{\infty} - 1)\nu} \}^{1-\delta}, \quad z = x^L$$
 (5.32)

and
$$\beta = \delta/(\delta-1).$$

The modified rate parameter λ includes factors due to the mass flow and the asymptotic constant speed. (The assumption that the speed is constant is consistent with possible limiting forms of the energy equation.)

It has been observed that the energy σ always decays asymptotically, even though in certain circumstances it does so through a series of de-excitation shocks. Since it is the decay downstream of any primary δ -shock, or local temperature maximum, that is of interest, it is sufficient to consider only the low-energy behaviour of G which is assumed to be

$$G \sim \sigma^r, \quad \sigma \to 0.$$
 (5.34)

(5.33)

It seems likely on physical grounds that $r \ge 1$. The case r = 1 was considered in II; only r > 1 is discussed here. For simplicity it is assumed that (5.34) holds for all values of σ . (A slight modification in the ensuing argument enables the analysis to be applied in the primary de-excitation region even if σ is not small there.)

From (5.30) and (5.31) it follows that the appropriate asymptotic behaviour is described by f_{θ}

$$\frac{z^{\beta}}{1-\delta}W_{zz} = -W^{-\beta} \left(\frac{1}{1-\delta}W_z\right)^{2-(1/r)},$$
(5.35)

where

$$= W\left\{\frac{r^{r/(r-1)}}{\Delta_{\infty}(\Gamma_{\infty}-1)} \left(\frac{1}{\lambda}\right)^{1/\delta}\right\}^{(r-1)(\delta-1)/(r+\delta-1)}.$$
(5.36)

Equation (5.35) is equivalent to the first-order equation

w

$$(1-\delta)\frac{d\eta}{d\zeta} = \frac{(1+\mu)\eta - \zeta^{-\beta}\eta^{2-1/r}}{\eta - \mu_1\zeta},$$
(5.37)

where

$$\eta = z^{1+\mu} \frac{1}{1-\delta} \frac{dW}{dz}, \quad \zeta = z^{\mu} W,$$
(5.38)

and

$$\mu = \frac{(Br-1)(\delta-1)}{(r+\delta-1)}, \quad \mu_1 = \mu/(\delta-1).$$
(5.39)

Phase-space trajectories follow immediately from (5.37). A detailed evaluation depends on the various parameters and the results are summarized in figure 11, which should be compared with the corresponding diagram in II. For r = 1 regions D and C have an upper barrier corresponding to an equilibrium decay. In general this decay is exponentially fast, and the power-law behaviour noted in figure 11 will always dominate away from any δ -shock transition.

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For region F, a cursory examination suggests that there may be three possible limiting states, corresponding respectively to those in C, D and E. In the limit $\Lambda \rightarrow 0$ it follows from the pseudo-entropy result (5.22) that the correct behaviour is $T_{L} = \sigma^{-(n\nu-1)/(1-\delta)}$ (5.40)

$$T \sim x^{-(n\nu-1)/(1-\delta)}$$
. (5.40)

(The temperature profile (5.22) is valid asymptotically for both regions F and E.) A careful examination of the integral curves of (5.37) also leads to this result in F for $\Lambda \rightarrow 0$.

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FIGURE 11. Asymptotic behaviour $(k = l - (\Gamma_{\infty} - 1) \nu)$.

Appendix A. Non-dimensional variables

If primes denote dimensional quantities, the non-dimensional variables used in the text are

$$\begin{array}{l} \rho = \rho'/\rho'_{\infty}, \quad T = T'/T'_{\infty}, \quad \Omega = \Omega'/\Omega'_{\infty}, \\ \sigma = \sigma'/RT'_{\infty}, \quad u = u'/\sqrt{(RT'_{\infty})}, \\ A = A'(x')/A'(h') \quad \text{and} \quad x = x'/h', \end{array} \right\}$$

$$(A 1)$$

where R is the gas constant, h' is the minimum nozzle height and the suffix ∞ denotes initial reservoir conditions.

The rate parameter Λ is defined by

$$\Lambda = \rho'_{\infty} \Omega'_{\infty} h' / \sqrt{(RT'_{\infty})}, \tag{A 2}$$

and the non-dimensional mass flow rate by

$$m = \frac{m'}{\rho'_{\infty}\sqrt{(RT'_{\infty})A'(h')}}.$$
 (A 3)

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Appendix B. Pseudo-entropy

The energy equation

$$de + pd(1/\rho) = 0 \tag{B1}$$

can be re-written as $TdS_{\alpha} = de_{\alpha} + pd(1/\rho) = -e_{\sigma}d\sigma$, (B 2)

where
$$de_{\alpha} = e_{\rho} d\rho + e_T dT$$
, (B 3)

and S_{α} corresponds to the pseudo-entropy defined in II.

For internal relaxation, where the various energies are additive $(e_{\sigma} = 1)$, S_{α} is simply entropy production in the active modes and, as noted earlier, is equivalent to the entropy of Johannesen's α -gas. For a reacting gas the situation is more complex: de_{α} is the internal energy change at constant composition and dS_{α} must be regarded as an entropy change relative to a frozen flow. It is useful to refer to S_{α} as the pseudo-entropy, though this definition in the reacting case is not unique, since it is apparent that the coefficient on the right-hand side of (B 2) will depend on the particular thermodynamic variables employed. However, the definition in no way affects the analysis of §5.

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