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BEHAVIOUR AT THE WAVE HEAD OF A FINITE AMPLITUDE GASDYNAMIC DISTURBANCE IN A CHEMICALLY REACTING FLUID FLOW

V. D. SHARMA AND RADHE SHYAM

Applied Mathematics Section, Institute of Technology, Banaras Hindu University, Varanasi 221005

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The effects of thermodynamical properties and that of the wave front curvature on the growth and decay behaviour of a finite amplitude gasdynamic disturbance headed by a planar, cylindrical or spherical wave front propagating through a chemically reacting gas mixture are investigated. In case the medium ahead of the wave is one of uniform equilibrium, it is found that the chemical rate process in the flow as well as the initial wave front curvature cause a delay in the shock wave formation. On the other hand if the medium ahead is in a state of disequilibrium, it is shown that the reaction rate process in the flow leads to a rapid shock formation and the stabilizing influence of the wave front curvature is not strong enough to overcome the instabilities associated with the disequilibrium state.

1. INTRODUCTION

Papers by Bürger (1966), Rarity (1967), Coleman and Gurtin (1967), Becker (1970) and Chu (1970) deal with the analysis of the formation of plane shock waves in one-dimensional unsteady flow with discontinuities resulting from the motion of a piston. In these papers, the authors had limited their investigations to the equilibrium flows with a planar geometry. In a recent paper Clarke (1977) has discussed the growth and decay behaviour of plane waves propagating through a spatially uniform but time dependent chemically reacting gas mixture in a general state of disequilibrium. All of them considered only plane waves; they did not determine the effect of wave front curvature on the growth and decay properties of the waves. Our purpose here is to determine the relative strength of the decay induced by geometric factors and the growth induced by the instabilities associated with the disequilibrium states. In addition to the determination of the growth and decay properties at planar and non-planar wave fronts propagating through equilibrium flow regions of a reacting gas mixture, the present work also extends the results of Clarke (1977) to flows with non-planar geometries. We have considered, a one dimensional unsteady flow of a reacting gas mixture with discontinuities resulting from the motion of a plane, cylindrically symmetric or spherically symmetric piston. In the non-planar cases the motion of the piston is taken to be outwards from the central axis or point of symmetry so that the wave is diverging rather than converging.

It is noted that if the medium ahead of the wave is one of uniform equilibrium, then a compression wave steepens up into a shock after a finite time only if the initial discontinuity associated with the wave exceeds a critical value. It is found that the geometry of the wave affects the growth properties only indirectly in that the critical value of the initial discontinuity depends on the initial curvature of the wave front. The critical values of the initial discontinuities for cylindrical and spherical waves for which the respective waves never completely decay are found to be larger in magnitude than the corresponding values for plane wavès. It is shown that an increase in the initial curvature of the wave front causes this critical value to increase and thus delays the shock wave formation. On the other hand if the medium ahead of the wave is in a state of disequilibrium, then it is found that the reaction rate process in the flow leads to a rapid shock formation; compared with the equilibrium case. Further, it is found that an increase in the initial curvature of the wave front causes the shock formation time to increase but this stabilizing influence of the wave front curvature is unable to overcome the tendency of the wave surface to grow into a shock.

Let t denote time, r the distance of the axis or the centre of symmetry from a plane and u the gas velocity along the r-axis. Let the thermodynamic state of the medium be denoted by the pressure p, the density ρ and the mass fraction c of the reactant species X, which takes part in the simple reversible reaction $nX \rightleftharpoons Y$, where Y is the product species which can dissociate to produce n molecules of X. Then the equations governing the one dimensional unsteady motion of a reacting gas mixture, neglecting the various transport effects, are

$$\frac{\partial \rho}{\partial t} + u\frac{\partial \rho}{\partial r} + \rho\frac{\partial u}{\partial r} + \frac{\nu\rho u}{r} = 0 \qquad \ldots(1)$$

$$\rho\frac{\partial u}{\partial t} + \rho u\frac{\partial u}{\partial r} + \frac{\partial P}{\partial r} = 0 \qquad \ldots(2)$$

$$\frac{\partial p}{\partial t} + u\frac{\partial p}{\partial r} + \rho a_f^2\left(\frac{\partial u}{\partial r} + \frac{\nu u}{r}\right) = \rho(\gamma - 1)\, QWn\omega \qquad \ldots(3)$$

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial r} = -Wn\omega \qquad \ldots(4)$$

where the coefficient $\nu = 0, 1, 2$ refers to the case of a plane, cylindrical and a spherical motion respectively; W is the molecular weight of X; γ the frozen specific heat ratio; a_f is the frozen sound speed given by $a_f^2 = \frac{\gamma p}{\rho}$; Q the energy of formation per unit mass of X; and ω the reaction rate given by

$$\omega = \tau^{-1}\{c^n - (1 - c)\,\delta\} \qquad \ldots(5)$$

where the quantities τ and δ are, respectively, the forward reaction time and the equilibrium constant given by

$$\tau^{-1} = F \exp(-Ex\, \rho/p)$$

and

$$\delta = z \exp(-nQ\rho/p)$$

where Ex denotes the reaction's activation energy and F and z are constants depending on the physical properties of the gas only.

The reaction rate ω would be zero if the chemical time τ happened to be infinite, or if the thermodynamic state were one of chemical equilibrium.

2. Equations in Characteristic Form

Let us introduce characteristic parameters, α and β, which are functions of r and t and which are such that

$$\frac{dr}{dt} = r_\alpha/t_\alpha = u + a_f \text{ where } \beta(r, t) = \text{constant} \qquad ...(6)$$

$$\frac{dr}{dt} = r_\beta/t_\beta = u - a_f \text{ where } \alpha(r, t) = \text{constant} \qquad ...(7)$$

where, we have written r_α for $(\partial r/\partial\alpha)_\beta$ etc.

In terms of these new variables, eqns. (1), (2) and (4) may be written into the following equivalent form

$$a_f(\rho_\alpha t_\beta + \rho_\beta t_\alpha) + \rho(u_\alpha t_\beta - u_\beta t_\alpha) + 2\frac{\nu\rho u}{r} a_f t_\alpha t_\beta = 0 \qquad ...(8)$$

$$\rho a_f(u_\alpha t_\beta + u_\beta t_\alpha) + (p_\alpha t_\beta - p_\beta t_\alpha) = 0 \qquad ...(9)$$

$$(c_\alpha t_\beta + c_\beta t_\alpha) = -2Wn\omega\, t_\alpha t_\beta. \qquad ...(10)$$

Also, eqns. (2) and (3) with the help of (6) and (7) can be expressed as

$$p_\alpha + \rho a_f u_\alpha = \rho(\gamma - 1)\, QWn\omega t_\alpha - \frac{\nu\rho u a_f^2}{r} t_\alpha \qquad ...(11)$$

$$p_\beta - \rho a_f u_\beta = \rho(\gamma - 1)\, QWn\omega t_\beta - \frac{\nu\rho u a_f^2}{r} t_\beta. \qquad ...(12)$$

3. Conditions at the Frozen Wave Head

Assuming the region ahead of the wave to be spatially uniform and at rest, eqns. (1), (3) and (4) yield

$$\rho_0 = \text{constant} \qquad ...(13)$$

$$p_{0t} = \rho_0(\gamma - 1)\, QWn\omega_0 \qquad ...(14)$$

and

$$c_{0t} = -Wn\omega_0 \qquad ...(15)$$

where the subscript '0' indicates a value in the region ahead of the wave front $\beta(r, t) = 0$ or $r = R(t)$, where $R(t)$ denotes the position on the wave front at any time t. The perturbations of the state ahead are assumed to propagate through the mixture behind the wave front $\beta = 0$. Across the wave front $\beta = 0$, the parameters p, ρ, u and c are essentially continuous but the discontinuities in their derivatives are permitted. We infer that a_f, ω, τ and δ will behave similarlty and that they will have their subscript '0' values at the wave head. Furthermore, any derivative with respect to α is continuous, discontinuities can appear only in the β-derivatives.

Evaluating (8), (9) and (10) at $\beta = 0^+$, and using (13) – (15), and the fact that $u_0 = 0$, we get

$$a_{f_0}\rho_\beta^+ = \rho_0 u_\beta^+ \qquad ...(16)$$

$$t_{0\alpha} p_\beta^+ - p_{0\alpha} t_\beta^+ = \rho_0 a_{f_0} t_{0\alpha} u_\beta^+ \qquad ...(17)$$

$$t_{0\alpha} c_\beta^+ - c_{0\alpha} t_\beta^+ = 0 \qquad ...(18)$$

where the quantities with a superscript '+' are discontinuous at the wave front $\beta = 0$.

Differentiating (11) with respect to β and (12) with respect to α and then subtracting one from the other and evaluating the resulting equation at $\beta = 0^+$ making use of (5) – (7) and (16) – (18), we obtain

$$\frac{\partial}{\partial\alpha} \log \{(\rho_0 a_{f_0})^{1/2}\, u_\beta^+\} = \left\{\Lambda_1 - \frac{\nu}{2R}\, a_{f_0}\right\} t_{0\alpha} \qquad ...(19)$$

where

$$\Lambda_1 = \tfrac{1}{2}(\gamma - 1)\, QWn \left\{\frac{(\gamma - 1)\, Ex\rho_0}{p_0 a_{f_0}^2}\left(\omega_0 - (1 - c_0)\,\frac{\delta_0}{\tau_0}\, n\, \frac{Q}{Ex}\right) + \frac{\omega_0}{a_{f_0}^2}\right\}$$

which on integration yields

$$u_\beta^+ = u_{\beta_i}^+ \left(\frac{\rho_{0i} a_{f_{0i}}}{\rho_0 a_{f_0}}\right)^{1/2} \exp\left\{\int_{t_i}^{t}\left(\Lambda_1(\hat{t}) - \frac{\nu a_{f_0}(\hat{t})}{2R(\hat{t})}\right) d\hat{t}\right\} \qquad ...(20)$$

where $u_{\beta_i}^+$ is the value of u_β^+ at the initial time $t = t_i$. Now differentiating (6) with respect to β and (7) with respect to α and subtracting (7) from (6) and making use of (8), (11) and (12), the resulting equation when evaluated at $\beta = 0^+$ yields

$$t^+_{\beta\alpha} + \Lambda_2 t_{0\alpha} u^+_\beta + \frac{(\gamma + 1)}{4a_{f_0}} u^+_\beta t_{0\alpha} = 0 \qquad ...(21)$$

where

$$\Lambda_2 = \frac{\rho_0(\gamma - 1) QWn\omega_0}{2p_0}.$$

Equation (21), together with (20), can be integrated to yield

$$t^+_\beta = t^+_{\beta i} \exp\left\{-\int_{t_i}^{t} \Lambda_2(\hat{t})\, d\hat{t}\right\}$$

$$- u^+_{\beta i} \exp\left\{-\int_{t_i}^{t} \Lambda_2(\hat{t})\, d\hat{t}\right\} \int_{t_i}^{t} \frac{1}{4}\frac{(\gamma + 1)}{a_{f_0}} \left(\frac{\rho_{0i} a_{f_{0i}}}{\rho_0 a_{f_0}}\right)^{1/2}$$

$$\times \exp\left\{\int_{t_i}^{t} \left(\Lambda - \frac{\nu a_{f_0}}{2R}\right) dt\right\} dt \qquad ...(22)$$

where

$$\Lambda = \Lambda_1 + \Lambda_2.$$

Since the velocity gradient at wave head can be expressed as

$$u^+_r = -u^+_\beta / 2a_{f_0} t^+_\beta \qquad ...(23)$$

it follows from (20), (22) and (23), that u^+_r is equal to

$$\left(\frac{\rho_{0i} a^3_{f_{0i}}}{\rho_0 a^3_{f_0}}\right)^{1/2} \frac{u^+_{ri} \exp\left\{\int_{t_i}^{t} \left(\Lambda(\hat{t}) - \frac{\nu a_{f_0}}{2R}\right) d\hat{t}\right\}}{\left[1 + \frac{1}{2}(\gamma + 1) u^+_{ri} \int_{t_i}^{t} \left(\frac{\rho_{0i} a^3_{f_{0i}}}{\rho_0 a^3_{f_0}}\right)^{1/2} \exp\left\{\int_{t_i}^{t} \left(\Lambda(\hat{t}) - \frac{\nu a_{f_0}}{2R}\right) d\hat{t}\right\} dt\right]}. \qquad ...(24)$$

Equation (24) gives the variation of discontinuity in u^+_r at $\beta = 0$. It is evident from (24) that the temporal behaviour of the velocity gradient at the wave head will depend critically on the sign of Λ.

4. Discussion

For a plane wave $\nu = 0$, eqn. (24) reduces to the form as obtained by Clarke (1977) and, therefore, all his conclusions follow immediately.

Here we shall consider the following situations in which the wave front is of cylindrical or spherical geometry.

Case (i) — If the medium ahead is one of uniform equilibrium, in that case $\omega_0 = 0$, as a result of which p_0, a_{f_0} etc. are constants and $\Lambda < 0$. Since, the speed of propagation, a_{f_0} of the wave front is constant, the successive positions of the wave surface form a family of parallel surfaces and thus $R(t) = R_0 + a_{f_0} t$, where R_0 is the position of the wave front at time $t = 0$. Here t_i has been set equal to zero for convenience. Thus eqn. (24) reduces to

$$u_r^+ = \frac{u_{r_i}^+ (R_0/R)^{\nu/2} \exp(-\mid \Lambda \mid t)}{1 + \frac{1}{2}(\gamma + 1)\, u_{r_i}^+ \int_0^t \{(R_0/R)^{\nu/2} \exp(-\mid \Lambda \mid t)\}\, dt} \qquad \ldots(25)$$

which shows that if $u_{r_i}^+ > 0$ (i.e. an expansion wave front), then $u_r^+ \to 0$ as $t \to \infty$, i.e. the wave decays and damps out ultimately. Also if $u_{r_i}^+ < 0$ (i.e. a compression wave front) and $\mid u_{r_i}^+ \mid < (u_r^+)_c$, where $(u_r^+)_c$ is a positive quantity given by

$$(u_r^+)_c = \begin{cases} 2 \mid \Lambda \mid /(\gamma + 1) & \text{for } \nu = 0 \text{ (plane wave)} \\ 2\left(\dfrac{\mid \Lambda \mid a_{f_0}}{\pi R_0}\right)^{1/2} \dfrac{\exp(-\mid \Lambda \mid R_0/a_{f_0})}{(\gamma + 1)\,\mathrm{erfc}\,(\mid \Lambda \mid R_0/a_{f_0})^{1/2}} & \text{for } \nu = 1 \text{ (cylindrical wave)} \\ \dfrac{2 a_{f_0} \exp(-\mid \Lambda \mid R_0/a_{f_0})}{(\gamma + 1) R_0 E_i(\mid \Lambda \mid R_0/a_{f_0})} & \text{for } \nu = 2 \text{ (spherical wave)} \end{cases}$$

$\left(\mathrm{erfc}\,(x) = \dfrac{2}{\sqrt{\pi}} \displaystyle\int_x^\infty e^{-t^2} dt \text{ and } E_i(x) = \int_x^\infty t^{-1} e^{-t} dt\right)$, then $u_r^+ \to 0$ as $t \to \infty$, the wave damps out ultimately. But, if $u_{r_i}^+ < 0$ and $\mid u_{r_i}^+ \mid > (u_r^+)_c$, then there exists finite time t_s given by

$$t_s = \frac{1}{\mid \Lambda \mid} \log \left\{1 - \frac{2 \mid \Lambda \mid}{\mid u_{r_i}^+ \mid (\gamma + 1)}\right\}^{-1} \qquad \text{for } \nu = 0.$$

$$\int_0^{t_s} (R_0/R)^{\nu/2} \exp(-\mid \Lambda \mid \hat{t})\, d\hat{t} = 2/\mid u_{r_i}^+ \mid (\gamma + 1) \qquad \text{for } \nu = 1, 2$$

such that $\mid u_r^+ \mid \to \infty$ as $t \to t_s$, i.e. the wave terminates into a shock at an instant t_s. Thus we find that a compression wave steepens up into a shock after a finite time only if the initial discontinuity associated with the wave is sufficiently strong. From the above expressions of $(u_r^+)_c$, one can see that $\dfrac{\partial (u_r^+)_c}{\partial \mid \Lambda \mid} > 0$ which means that the chemical reactions in the flow have a stabilizing effect on the tendency of the wave surface to grow into a shock in the sense that an increase in $\mid \Lambda \mid$ will cause $(u_r^+)_c$ to increase and thus delays the shock wave formation. Also $\dfrac{\partial (u_r^+)_c}{\partial R_0} < 0$ which implies that the curvature has a stabilizing effect in that an increase in the initial curvature causes an increase in $(u_r^+)_c$. For $\mid u_{r_i}^+ \mid = (u_r^+)_c$, it follows from (25) that at a plane compression wave head the discontinuity propagates with the constant initial strength and at a cylindrical and spherical wave head they propagate according to

$$u_r^+ = -\frac{2}{(\gamma + 1)} \left(\frac{\mid \Lambda \mid a_{f_0}}{\pi R} \right)^{1/2} \frac{\exp(-\mid \Lambda \mid R/a_{f_0})}{\operatorname{erfc}(\mid \Lambda \mid R/a_{f_0})^{1/2}} \qquad \ldots(26)$$

and

$$u_r^+ = -\frac{2 a_{f_0} \exp(-\mid \Lambda \mid R/a_{f_0})}{(\gamma + 1) R E_i(\mid \Lambda \mid R/a_{f_0})} \qquad \ldots(27)$$

respectively.

Since $\operatorname{erfc}(x) < \dfrac{\exp(-x^2)}{x\sqrt{\pi}}$ and $E_i(x) < \dfrac{\exp(-x)}{x}$, it follows from (26) and (27) that $\mid u_r^+ \mid \to \dfrac{2 \mid \Lambda \mid}{\gamma + 1}$ (critical value of the initial discontinuity for plane wave) as $R \to \infty$. Thus, all cylindrical and spherical compression waves for which $\mid u_{r_i}^+ \mid = (u_r^+)_c$ decay (but not completely) and ultimately take a stable wave form. In view of the above inequalities satisfied by the complementary error function and the exponential integral function, it follows from the expressions of $(u_r^+)_c$ that for cylindrical and spherical waves $(u_r^+)_c > \dfrac{2 \mid \Lambda \mid}{\gamma + 1}$ (critical value for the plane wave).

Case (ii) — If the medium ahead is in a state of disequilibrium, i.e. $\omega_0 \neq 0$, and one considers only a short interval of time, so that the quantities $a_{f_0}^{\cdot}$ and Λ do not change appreciably between t_i and t, it is evident that (24) can be written in the approximate form

$$u_r^+ \simeq \frac{u_{r_i}^+ (R_0/(R_0 + \bar{a}_{f_0} t))^{\nu/2} \exp(\bar{\Lambda} t)}{1 + \frac{(\gamma+1)}{2} u_{r_i}^+ \int_0^t \{R_0/(R_0 + \bar{a}_{f_0} \hat{t}))^{\nu/2} \exp(\bar{\Lambda}\hat{t})\} \, d\hat{t}} \qquad \text{...(28)}$$

where $\bar{a}_{f_0}$ and $\bar{\Lambda}$ indicate suitable mean values over the internal t_i to t, and t_i has been set equal to zero for convenience.

An examination of (28) leads to the conclusion that if $u_{r_i}^+ < 0$ and $\bar{\Lambda} > 0$, then there exists a finite time t_s^* given by

$$t_s^* = \frac{1}{\bar{\Lambda}} \log \left\{ 1 + \frac{2\bar{\Lambda}}{| u_{r_i}^+ | (\gamma + 1)} \right\} \qquad \text{for } \nu = 0 \qquad \text{...(29)}$$

$$\int_0^{t_s^*} (R_0/(R_0 + \bar{a}_{f_0} t))^{\nu/2} \exp(\bar{\Lambda} t) \, dt = \frac{2}{| u_{r_i}^+ | (\gamma + 1)} \quad \text{for } \nu = 1, 2 \text{ ...(30)}$$

such that $| u_r^+ | \to \infty$ as $t \to t_s^*$, provided (28) remains valid over the requisite period. Thus, we find that in a state of disequilibrium sufficiently far from equilibrium so that $\bar{\Lambda} > 0$, a discontinuity associated with a compression wave, no matter how small, always steepens up into a shock after a finite time. It follows from (29) and (30) that

$$\frac{\partial t_s^*}{\partial \bar{\Lambda}} < 0 \quad \text{and} \quad \frac{\partial t_s^*}{\partial R_0} < 0,$$

which mean that the chemical rate process in the flow accelerates the steepening tendency of a compression wave to grow into shock whereas, an increase in curvature causes the shock formation time to increase. We, thus, draw an important conclusion that in a state of disequilibrium, the stabilizing influence of the wave front curvature is unable to overcome the tendency of the wave surface to grow into a shock. On the other hand if $u_{r_i}^+ > 0$ and $\bar{\Lambda} > 0$, then, using l'Hospital's rule, it follows from (28) that for $\nu = 0$, 1 or 2, $u_r^+ \to \frac{2\bar{\Lambda}}{\gamma + 1}$ as $t \to \infty$. Thus, when the medium ahead of the wave is sufficiently far from equilibrium so that $\bar{\Lambda} > 0$, it is interesting to note that a discontinuity associated with an expansion wave tends towards a fixed value which is independent of its initial value.

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