Growth and decay of weak discontinuities in a non-equilibrium flow of an ideal dissociating gas

V. D. SHARMA (VARANASI)

THE GROWTH and decay properties of weak discontinuities in a non-equilibrium flow of an ideal dissociating gas are investigated. The state ahead of the wave is considered to be spatially uniform and in a general state of disequilibrium. The singular surface theory is used to show that weak discontinuities propagate through this system at the frozen sound speed and, if the degree of disequilibrium is sufficient, are amplified by the non-equilibrium dissociation reaction. The strength of attenuation induced by the wave-front curvature relative to the growth induced by the non-equilibrium dissociation in the gas has been investigated.

Zbadano własności wzrostu i zaniku słabych nieciągłości w nierównowagowym przepływie dysocjującego gazu doskonałego. Stan gazu przed czołem fali założono jako przestrzennie jednorodny i znajdujący się w ogólnym stanie nierównowagi. Zastosowano teorię powierzchni osobliwych dla wykazania, że słabe nieciągłości rozchodzą się w takim układzie z prędkością zamrożonego dźwięku i, jeśli tylko stopień nierównowagi jest dostateczny, są one wzmacniane przez nierównowagową reakcję dysocjacji. Zbadano intensywność tłumienia wywołanego krzywizną czoła fali oraz rozwoju nieciągłości spowodowanego nierównowagową dysocjacją zachodzącą w gazie.

Исследованы свойства роста и затухания слабых разрывов в неравновесном течении диссоциирующего идеального газа. Состояние газа перед фронтом волны предполагается как пространственно однородное и находящееся в общем состоянии неравновесия. Применена теория особых поверхностей для показания, что слабые разрывы распространяются в такой системе со скоростью вмороженного звука и если только степень неравновесия достаточна, они усиливаются неравновесной реакцией диссоциации. Исследована интенсивность затухания, вызванная кривизной фронта волны, и развитие разрыва, вызванное неравновесной диссоциацией происходящей в газе.

1. Introduction

THE PROPAGATION of weak discontinuities has been discussed by several researchers who have applied the theory of singular surfaces to different material mediums. For example, THOMAS [1] and ELCRAT [3] considered sonic waves in ideal fluids. COLEMAN and GURTIN [4] studied acceleration waves in ideal fluids with internal state variables. CHEN [5–6] treated waves in elastic materials, while COLEMAN and GURTIN [7] waves in materials with memory. MCCARTHY [8] analysed second-order waves in relativistic gas dynamics and in other publications [9, 10] he treated acceleration waves in highly nonlinear deformable solids. RARITY [11], CHU [12] (pp. 41–46) and CLARKE [13] discussed wave propagation in relaxing or reacting fluids, using the method of characteristics; as they were concerned with plane waves only, they did not investigate the effects of curvature on the growth and decay properties of these waves. BECKER and SCHMITT [14] considered special cases of cylindrical and spherical waves but they did not consider the case when the medium

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ahead of the wave is in a state of disequilibrium. The purpose of this paper is to study these singular surfaces in the plane, cylindrical and spherically-symmetric motion of an ideal dissociating gas due to LIGHTHILL [15] and FREEMAN [16], taking into account the state ahead of the wave in disequilibrium.

2. Basic equations

For the Lighthill – Freeman ideal dissociating gas, the reaction rate is given by [17] (page 233)

(2.1)
$$\frac{d\alpha}{dt} = -\tau^{-1}\{-(1-\alpha)e^{-\theta/T} + \varrho\alpha^2/\varrho_d\} \equiv -\omega,$$

where $\tau = (C\varrho T^n)^{-1}$ is the characteristic time of the rate process. The quantities t, ϱ , T, α , ϱ_d and θ are respectively the time, density, temperature, degree of dissociation, characteristic density and characteristic temperature for dissociation. The constants C, n, θ and ϱ_d describe the rate and equilibrium properties of the gas.

The equations of continuity, momentum, energy and state for the ideal dissociating gas under consideration are

(2.2)
$$\frac{d\varrho}{dt} + \varrho \left(\frac{\partial u}{\partial r} + \frac{\nu u}{r}\right) = 0, \quad \varrho \frac{du}{dt} + \frac{\partial p}{\partial r} = 0,$$

(2.3)
$$\varrho \frac{dh}{dt} - \frac{dp}{dt} = 0, \quad p = \varrho(1+\alpha)RT, \quad h = R\{(4+\alpha)T+\theta\},$$

where $\frac{d}{dt} \equiv \frac{\partial}{\partial t} + u \frac{\partial}{\partial r}$, and the quantities *p*, *u*, *h*, and *R* denote respectively the pressure, velocity, enthalpy and the gas constant. The flow variables *u*, *p*, ρ , α , etc. are functions of the Eulerian coordinate *r* (the distance from a fixed origin) and the time *t*. The coefficient $\nu = 0, 1, 2$ refers to the case of a plane, cylindrical and spherical motion, respectively.

Equation $(2.3)_1$ with the help of Eqs. (2.1), $(2.2)_1$, $(2.3)_2$ and $(2.3)_3$ can be written as

(2.4)
$$\frac{dp}{dt} + \varrho a_f^2 \left(\frac{\partial u}{\partial r} + \frac{vu}{r}\right) = \varrho a_f^2 \sigma \omega$$

where $a_f^2 = \Gamma p/\rho$ is the square of the frozen sound speed and $\sigma = \frac{1}{3\Gamma(\Gamma-1)} \left(\frac{\theta}{T}(\Gamma-1)\right)$ with $\Gamma = \frac{4+\alpha}{3}$.

3. Wave as a singular surface

Let r = R(t) or, for brevity, $\Sigma(t)$ denote the weak discontinuity surface, where R(t) is the position of the wave front at any time t. The description of the surface $\Sigma(t)$ is such

that its speed of propagation $G = \frac{dR}{dt}$ is always positive. Here we shall restrict our attention to the singular surface $\Sigma(t)$ across which the flow variables u, p, ϱ, α and T are essentially continuous but the discontinuities in their derivatives are permitted. We infer that a_f, σ and ω will behave similarly and that they will have subscript — 0 values at the wave front. A subscript — 0 indicates a value in the medium just ahead of the wave front. The unperturbed field ahead of the wave is assumed to be spatially uniform and at rest. Thus from Eqs. (2.1), (2.2)₁ and (2.4) we have

(3.1)
$$\varrho_0 = \text{const}, \quad \left(\frac{\partial p}{\partial t}\right)_0 = \varrho_0 a_{f_0}^2 \sigma_0 \omega_0 \quad \text{and} \quad \left(\frac{\partial \alpha}{\partial t}\right)_0 = \omega_0.$$

The reaction rate ω_0 will be zero if the chemical time becomes infinite or, more practically, if the state ahead of the wave is one of chemical equilibrium.

In our case, the geometrical and kinematical conditions of first and second order deduced by THOMAS [2] reduce to

(3.2)
$$\left[\frac{\partial z}{\partial r}\right] = A, \quad \left[\frac{\partial z}{\partial t}\right] = -AG,$$

(3.3)
$$\left[\frac{\partial^2 z}{\partial r^2}\right] = \overline{A}, \quad \left[\frac{\partial^2 z}{\partial r \partial t}\right] = -G\overline{A} + \frac{\delta A}{\delta t},$$

where the quantity z may represent any of the variables p, ρ , u, α and T. The square bracket stands for the value of the quantity enclosed immediately behind the wave surface minus its value just ahead of the wave surface. The quantities A and \overline{A} are defined over the singular surface $\Sigma(t)$ and the δ -time derivative of any quantity f is defined as $\frac{\delta f}{\delta t} = \frac{\partial f}{\partial t} +$

 $+G\frac{\partial f}{\partial r}$. Thus the δ -time derivative of any quantity which is considered to be expressed on $\Sigma(t)$ is identical with the ordinary derivative of the quantity. However, we shall choose to retain this notation in order to emphasize the fact that we are considering the time derivative of quantities which are only defined on the singular surface $\Sigma(t)$.

Taking jumps, across $\Sigma(t)$, in Eqs. (2.1), (2.2)₁, (2.2)₂ and (2.4) and making use of Eq. (3.1) and of the fact that $u_0 = 0$, we have

(3.4) $G\varepsilon = 0, \quad G\zeta = \varrho_0 \lambda, \quad \varrho_0 G\lambda = \xi, \quad G\xi = \varrho_0 a_{f_0}^2 \lambda,$

where $\varepsilon = \left[\frac{\partial \alpha}{\partial r}\right]$, $\zeta = \left[\frac{\partial \varrho}{\partial r}\right]$, $\lambda = \left[\frac{\partial u}{\partial r}\right]$ and $\xi = \left[\frac{\partial p}{\partial r}\right]$ are the quantities defined on the wave front $\Sigma(t)$.

Now, if $G \neq 0$, then $\varepsilon = 0$ and it follows from Eqs. (3.4)₃ and (3.4)₄ that $\rho_0 \lambda (G^2 - a_{f_0}^2) = 0$, what suggests that either $G = \pm a_{f_0}$ or $\lambda = 0$, but λ cannot vanish, for if it does, then it follows from Eqs. (3.4)₂-(3.4)₄ that $\lambda = \xi = \zeta = 0$, which violates the basic assumption about $\Sigma(t)$. Hence, without any loss of generality, we assume

$$(3.5) G = a_{f_0}.$$

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4. Behaviour at the wave front

If we differentiate Eqs. $(2.2)_2$ and (2.4) with respect to r, take jumps across $\Sigma(t)$ and then make use of Eqs. (3.2) and (3.3), we get

(4.1)
$$\frac{\delta\lambda}{\delta t} = -\frac{1}{\varrho_0} (\overline{\xi} - \varrho_0 a_{f_0} \overline{\lambda}),$$

(4.2)
$$\frac{\delta\xi}{\delta t} = a_{f_0}(\overline{\xi} - \varrho_0 a_{f_0}\overline{\lambda}) - (\Gamma_0 + 1)\varrho_0 a_{f_0}\lambda^2 + 2\left(\Lambda_0 - \frac{\nu a_{f_0}}{2R}\right)\xi,$$

where

$$\xi = \left[\frac{\partial^2 p}{\partial r^2}\right], \quad \lambda = \left[\frac{\partial^2 u}{\partial r^2}\right]$$

and

$$(4.3) \quad \Lambda_0 = \frac{\omega_0 \sigma_0}{2} \{ (\Gamma_0 + 1) + n(\Gamma_0 - 1) \} + \frac{\omega_0 \theta}{6T_0} \left\{ \frac{(\Gamma_0 - 1)}{\Gamma_0} - \frac{\theta}{T_0} - 1 \right\} - \frac{\varrho_0 (1 + \alpha_0) \Gamma_0 \sigma_0^2 \alpha_0^2}{2\tau_0 \varrho_d}.$$

Inserting the term $(\bar{\xi} - \rho_0 a_{f_0} \bar{\lambda})$ from Eq. (4.1) into Eq. (4.2), and using Eqs. (3.4)₄ and (3.5), we get

(4.4)
$$\frac{\delta}{\delta t} \log\{(\varrho_0 a_{f_0})^{\frac{1}{2}}\lambda\} + \frac{(\Gamma_0 + 1)\lambda}{2} = \left(\Lambda_0 - \frac{\nu a_{f_0}}{2R}\right).$$

Integrating Eq. (4.4) between t_i (where $\lambda = \lambda_i$) and t yields

(4.5)
$$\lambda = \frac{\lambda_{i}(a_{f_{0l}}/a_{f_{0}})^{\frac{1}{2}} \exp\left\{\int_{t_{l}}^{t} \left(A_{0} - \frac{\nu a_{f_{0}}}{2R}\right) dt\right\}}{\left\{1 + \frac{\lambda_{i}}{2}\int_{t_{l}}^{t} \left(a_{f_{0l}}/a_{f_{0}}\right)^{\frac{1}{2}} (\Gamma_{0} + 1) \exp\left\{\int_{t_{l}}^{\tilde{t}} \left(A_{0} - \frac{\nu a_{f_{0}}}{2R}\right) d\hat{t}\right\} d\tilde{t}\right\}}$$

Equation (4.5) gives the variation of discontinuity λ associated with $\Sigma(t)$ as it moves into a non-equilibrium dissociating gas at rest. It is evident from Eq. (4.5) that the temporal behaviour of the velocity gradient at the wave head will depend critically on the sign of Λ_0 .

5. Discussion

Case I

If ω_0 is zero, so that the medium ahead of the wave is one of uniform equilibrium, Eq. (4.3) shows that $\Lambda_0 = -\frac{1}{2} \left\{ \frac{(1+\alpha_0)\Lambda_0 \alpha_0^2 \sigma_0^2}{\tau_0 \varrho_\alpha} \right\} < 0$. Then Eq. (4.5) reduces to (5.1) $\lambda = \frac{\lambda_t (R_0/R)^{*/2} \exp(-|\Lambda_0|t)}{\left\{ 1 + \frac{\lambda_t (\Gamma_0 + 1)}{2} \int_0^t (R_0/R)^{*/2} \exp(-|\Lambda_0|\tilde{t}) d\tilde{t} \right\}},$

where $R = R_0 + a_{f_0} t$ denotes the position of the wave front at any time t, R_0 being its initial position at t = 0. Here t_i has been set equal to zero for convenience.

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Equation (5.1) shows that if $\lambda_i > 0$ (i.e an expansion wave front), then $\lambda \to 0$ as $t \to \infty$ i.e. the wave decays and damps out ultimately. Also if $\lambda_i < 0$ (i.e a compression wave front) and $|\lambda_i| < \lambda_c$, where λ_c is a positive quantity given by

$$\lambda_{c} = \begin{cases} 2|\Lambda_{0}|/(\Gamma_{0}+1) & \text{for } \nu = 0 \text{ (plane wave),} \\ 2\left(\frac{|\Lambda_{0}|a_{f_{0}}}{\pi R_{0}}\right)^{\frac{1}{2}} \frac{\exp(-|\Lambda_{0}|R_{0}/a_{f_{0}})}{(\Gamma_{0}+1)\mathrm{erfc}(|\Lambda_{0}|R_{0}/a_{f_{0}})^{\frac{1}{2}}} & \text{for } \nu = 1 \text{ (cylindrical wave),} \\ \frac{2a_{f_{0}}\exp(-|\Lambda_{0}|R_{0}/a_{f_{0}})}{(\Gamma_{0}+1)R_{0}E_{I}(|\Lambda_{0}R_{0}/a_{f_{0}})} & \text{for } \nu = 2 \text{ (spherical wave),} \end{cases}$$

where $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-t^2} dt$, and $E_i(x) = \int_{x}^{\infty} t^{-1} e^{-t} dt$ are the well-known integrals,

then $\lambda \to 0$ as $t \to \infty$, the wave damps out ultimately. But if $\lambda_i < 0$ and $|\lambda_i| > \lambda_c$, then there exists a finite time t_s given by

$$t_{s} = \frac{1}{|\Lambda_{0}|} \log \left\{ 1 - \frac{2|\Lambda_{0}|}{|\lambda_{i}|(\Gamma_{0}+1)} \right\}^{-1} \quad \text{for} \quad \nu = 0,$$

and

$$\int_{0}^{t_{s}} (R_{0}/R)^{\nu/2} \exp(-|\Lambda_{0}|t) dt = \frac{2}{|\lambda_{t}|(\Gamma_{0}+1)} \quad \text{for} \quad \nu = 1, 2$$

such that $|\lambda| \to \infty$ 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 λ_c , one can see that $\frac{\partial \lambda_c}{\partial |\Lambda_0|} > 0$, which means that the non-equilibrium dissociation has a stabilizing effect on the tendency of the wave surface to grow into a shock in the sense that an increase in $|\Lambda_0|$ will cause λ_c to increase. Also $\frac{\partial \lambda_c}{\partial R_0} < 0$, which implies that the curvature has a stabilizing effect in that an increase in the initial curvature causes an increase in λ_c .

Case II

If $\omega_0 \neq 0$, and one consideres only short time interval, so that the quantities a_{f_0} , Γ_0 and Λ_0 do not change appreciably between t_i and t_i , it is evident that Eq. (4.5) can be written in the approximate form

(5.2)
$$\lambda \simeq \frac{\lambda_t (R_0/R_0 + \overline{a}_{f_0}t)^{\nu/2} \exp(\overline{A_0}t)}{\left\{1 + \frac{\lambda_t (\overline{\Gamma}_0 + 1)}{2} \int_0^t (R_0/R_0 + \overline{a}_{f_0}t)^{\nu/2} \exp(\overline{A_0}t) dt\right\}},$$

where \bar{a}_{f_0} , $(\bar{\Gamma}_0 + 1)$ and $\bar{\Lambda}_0$ indicate suitable mean values over the interval t_i to t_i and t_i has been set equal to zero for convenience.

An examination of Eq. (5.2) leads to the conclusion that if $\lambda_i < 0$ and $\Lambda_0 > 0$, then there exists a finite time t_s^* given by

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$$t_s^* = \frac{1}{\overline{A_0}} \log \left\{ 1 + \frac{2\overline{A_0}}{|\lambda_t|(\overline{T_0+1})} \right\} \quad \text{for} \quad \nu = 0,$$

and

$$\int_{0}^{r} (R_0/R_0 + \bar{a}_{f_0}t)^{\nu/2} \exp(\Lambda_0 t) dt = \frac{2}{|\lambda_i|(\Gamma_0 + 1)} \quad \text{for} \quad \nu = 1, 2$$

such that $|\lambda| \to \infty$ as $t \to t_s^*$, provided Eq. (5.2) remains valid over the required period. Thus we find that in a state of disequilibrium a discontinuity associated with a compression wave, no matter how small, always steepnes up into a shock after a finite time and 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 $\lambda_i > 0$ and $\overline{\Lambda}_0 > 0$, then using L'Hospital rule, it follows from Eq. (5.2) that for $\nu = 0, 1$ or 2, $\lambda \to \frac{2\overline{\Lambda}_0}{(\overline{\Gamma}_0 + 1)}$ as

 $t \to \infty$. Thus when the medium ahead of the wave is in a state of disequilibrium, 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. Of course the condition $t \to \infty$ means that this fixed wave form is attained only after a long time, the approximation (5.2) may not be valid up to this time, but the tendency towards a stable wave form is in no way less important.

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APPLIED MATHEMATIC SECTION INSTITUTE OF TECHNOLOGY, B.H.U., VARANASI, INDIA. PRESENT ADDRESS: DEPARTMENT OF AEROSPACE ENGINEERING UNIVERSITY OF MARYLAND, USA.

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