Growth of Discontinuities in Chemically Reacting Relativistic Fluids

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A relativistic theory is developed to study the growth of weak discontinuities propagating in a chemically reacting fluid mixture. The velocity of propagation is determined, which fully agrees with classical results in the nonrelativistic limit. The growth equation for the wave propagation in relativistic fluid flows with nonequilibrium effects is obtained and solved. The wave amplitude is determined as a function of time. The relativistic and relaxation effects on the global behavior of the wave amplitude are studied analytically. It is concluded that if the wave is of a compressive nature and its initial amplitude is greater than a critical value, then the discontinuity grows until it develops into a shock wave after a finite critical time t_c . But on the other hand if the initial wave amplitude is less than the critical one, the wave decays and damps out ultimately. It is shown that both relativistic and relaxation effects help in stabilizing the wave propagation by increasing the critical time t_c for the breakdown of the wave due to nonlinear steepening.

1. INTRODUCTION

The classical fluid flow theory based on the postulates of thermodynamic equilibrium may not be applicable to a flow field in which the density and pressure of individual fluid species change rapidly. For rapidly changing external conditions the concentrations of the various species in a fluid mixture are no longer functions of pressure and density alone, but they require an additional internal thermodynamic variable as an independent parameter of the relaxation process. With the advent of flights at very high speeds scientists are taking keen interest in studying the effects of relaxation processes in relativistic fluid flow theory. The relativistic theory of propagation of weak discontinuities and shock waves in a perfect gas has been extensively studied by Zumino (1957), Coburn (1961), Saini (1961), Kanwal (1966), and McCarthy (1969). Grot (1968) discussed wave propagation in nonlinear elastic media. Eckart (1940) and Taub (1948) provided the theoretical foundation of relativistic shocks. The shock relations in relativistic magnetohydrodynamics were presented by Lichnerowicz (1967). Recently Ram (1978) studied nonequilibrium effects on the breakdown of weak shocks. But the relaxation effects in the case of growth of discontinuities in relativistic fluid flows with varying internal structure do not appear to have been investigated. However, the study of the rates of chemical reactions is a complex and difficult science which is still in an incomplete state of development. We shall limit ourselves to homogeneous reactions in a perfect gas mixture in which the usual macroscopic conservation equations for nonviscous, nonconducting, and nondiffusing flow are applicable. For simplicity, we shall allow for only one nonequilibrium process of chemical reactions and neglect all photoreactions that depend on radiation. The main object of the present communication is to study such effects, and to determine the criterion for the formation of shock.

2. PRELIMINARIES

Let V_4 be an Einstein-Riemann space defined by four coordinates $x^{\alpha} = (x^i, x^4)$, where x^i are the Cartesian coordinates of a material point in three-dimensions and $x^4 = ct$, i = 1, 2, 3, and c is the constant speed of light in vacuum. Let a metric $ds^2 = g_{\alpha\beta} dx^{\alpha} dx^{\beta}$ be defined on V_4 with signature (+ + + -) and constant components given by

$$g^{\alpha\beta} = g_{\alpha\beta}, \qquad g^{ij} = g_{ij} = \delta_{ij}, \qquad g^{44} = g_{44} = -1$$

The range of Latin indices is 1,2,3 and that of Greek indices is 1,2,3,4.

The world velocity is defined by

$$U^{\alpha}(x^{\mu}) = \beta\left(\frac{v^{k}}{c}, 1\right), \qquad U^{\alpha}U_{\alpha} = -1$$
(2.1)

where

$$v^k = c \frac{\partial x^k}{\partial x^4}, \qquad \beta = \left(1 - \frac{v^k v_k}{c^2}\right)^{-1/2}$$

The invariant derivative of any function $\psi(x^{\mu})$ can be expressed in the

Growth of Discontinuities in Relativistic Fluids

form

$$D\psi \equiv U^{\alpha}\psi_{,\alpha} = \frac{\beta}{c} \left(\frac{\partial\psi}{\partial t} + v^{i}\psi_{,i} \right) = \frac{\beta}{c} \dot{\psi}$$
(2.2)

where $\dot{\psi}$ is the material derivative of ψ in classical mechanics.

In the subsequent analysis we shall restrict ourselves to homogeneous reactions in a mixture of perfect gases in which macroscopic conservation equations for nonviscous, nonconducting, and nondiffusing flow are applicable. For simplicity, we shall allow for only one nonequilibrium process of chemical reactions and exclude all photochemical reactions that depend on radiation. The basic equations governing relativistic flow of a chemically reacting gas mixture under above-mentioned simplifying assumptions are (Saini, 1976)

$$(\rho U^{\alpha})_{,\alpha} = 0 \tag{2.3}$$

$$T^{\alpha\beta}_{,\beta} = 0 \tag{2.4}$$

$$Dq = \frac{\beta}{c} w(p, s, q)$$
(2.5)

where

$$T^{\alpha\beta} = (\omega + p) U^{\alpha} U^{\beta} + pg^{\alpha\beta}$$
$$\omega = \rho c^{2} \left(1 + \frac{e}{c^{2}} \right)$$

and a comma followed by an index denotes covariant differentiation. Here $T^{\alpha\beta}$, p, ρ , ω , s, and q, respectively, represent the energy momentum tensor, the scalar pressure, the mass density in the rest frame, the proper energy density, the entropy, and the relaxation parameter.

From (2.3), (2.4), and (2.5) we get

$$Dp + \rho a_f^2 U^{\alpha}_{,\alpha} + a_f^2 \left(\frac{\xi}{T}\rho_s + \rho_q\right) Dq = 0$$
(2.6)

$$\rho \sigma D U^{\alpha} + \frac{1}{c^2} S^{\alpha \beta} p_{,\beta} = 0 \qquad (2.7)$$

where

$$\sigma = 1 + \frac{h}{c^2}, \qquad S^{\alpha\beta} = U^{\alpha}U^{\beta} + g^{\alpha\beta}, \qquad TDS = Dh - \frac{1}{\rho}Dp + \xi Dq$$

and $a_f^2 = (\partial p / \partial \rho)_{s,q}$ is the square of the frozen speed of sound, h(p, s, q) is the enthalpy of the fluid mixture, and ξ is the affinity of internal transformation.

Let $\Sigma(x^{\mu})$ be a moving singular surface in the Einstein-Riemann space with parametric equations $x^{\mu} = \psi^{\mu}(b^1, b^2, b^3)$, where b^1, b^2, b^3 are the curvilinear coordinates on the timelike hypersurface $\Sigma(x^{\mu})$. Let N_{α} be the components of the unit normal vector to $\Sigma(x^{\mu})$; then we have

$$N^{\alpha}N_{\alpha} = 1, \qquad N_{\alpha} = \overline{\beta}(n_i, -G/c), \qquad N^{\alpha} = \overline{\beta}(n^i, G/c)$$
(2.8)

where

$$\overline{\beta} = \left(1 - \frac{G^2}{c^2}\right)^{-1/2}$$

 n_i are the components of the unit normal to a space-time surface S(t) in our rest frame and G is the speed of propagation of the moving surface S(t). From (2.1) and (2.8) we have

$$V \equiv U^{\alpha} N_{\alpha} = -\beta \overline{\beta} G_0 / c \tag{2.9}$$

where $G_0 = G - v^i n_i$ is the local speed of propagation of the surface S(t).

3. VELOCITY OF PROPAGATION

A timelike hypersurface $\Sigma(x^{\mu})$, across which the flow field variables are continuous, but their first and higher derivatives undergo finite jumps, is defined as a weak discontinuity. The compatibility conditions for a discontinuity can be expressed in the form (Truesdell and Toupin, 1960, pp. 492-498)

$$\left[Z_{,\alpha}\right] = BN_{\alpha} + g_{\alpha\beta}a^{\tau\phi}x^{\beta}_{,\phi}\left[Z\right]_{,\tau}$$
(3.1)

$$\left[Z_{,\alpha\beta}\right] = BN_{\alpha}N_{\beta} + 2N_{(\alpha}x_{\beta}^{\Gamma})\left(B_{,\Gamma} + b_{\Gamma}^{\theta}A_{,\theta}\right) + x_{(\alpha}^{\Gamma}X_{\beta}^{\theta})\left(A_{,\Gamma\theta} - b_{\Gamma\theta}B\right) (3.2)$$

where

$$A = \begin{bmatrix} Z \end{bmatrix} = Z_1 - Z_0, \qquad B = \begin{bmatrix} Z_{,\alpha} \end{bmatrix} N^{\alpha}, \qquad \overline{B} = \begin{bmatrix} Z_{,\alpha\beta} \end{bmatrix} N^{\alpha} N^{\beta}$$
$$b_{\Gamma\tau} = -g_{\alpha\beta} x^{\alpha}_{,\Gamma} N^{\beta}_{,\tau}, \qquad a_{\alpha\beta} = g_{\theta\tau} x^{\theta}_{,\alpha} x^{\tau}_{,\beta}$$
$$M_{(\alpha\beta)} = \frac{1}{2} (M_{\alpha\beta} + M_{\beta\alpha}), \qquad x^{\tau}_{\beta} = g_{\alpha\beta} a^{\tau\theta} x^{\alpha}_{,\theta}$$

Growth of Discontinuities in Relativistic Fluids

In consequence of the compatibility condition (3.1) and the identity

$$a^{\tau\phi}x_{\tau}^{\alpha}x_{\phi}^{\beta} = g^{\alpha\beta} - N^{\alpha}N^{\beta}$$

we have

$$[DZ] = V[Z_{,\alpha}N^{\alpha}] + \delta[Z]$$
(3.3)

where

$$\delta[Z] = U^{\mu}[Z_{,\mu}] - V N^{\mu}[Z_{,\mu}]$$

Here $\delta[Z]$ is the generalized form of the δ_t derivative of Thomas (1957). In the local instantaneous rest frame we have

$$c\delta[Z] = \bar{\beta}^2 \delta_t[Z] \tag{3.4}$$

Using the jump conditions (3.1) in (2.3), (2.5), (2.6), and (2.7), we get

$$V\nu + \rho\lambda^{\alpha}N_{\alpha} = 0 \tag{3.5}$$

$$V\epsilon = 0 \tag{3.6}$$

$$V\mu + \rho a_f^2 \lambda^{\alpha} N_{\alpha} + a_f^2 \rho_q V \epsilon = 0$$
(3.7)

$$\rho \sigma V \lambda^{\alpha} + \frac{1}{c^2} \mu N_{\beta} S^{\alpha \beta} = 0$$
(3.8)

where

$$\lambda^{\alpha} = \begin{bmatrix} U_{,\beta}^{\alpha} \end{bmatrix} N^{\beta}, \qquad \mu = \begin{bmatrix} p_{,\beta} \end{bmatrix} N^{\beta}, \qquad \epsilon = \begin{bmatrix} q_{,\beta} \end{bmatrix} N^{\beta}, \qquad \nu = \begin{bmatrix} \rho_{,\beta} \end{bmatrix} N^{\beta}$$

and the jump in the reaction rate function w(p,s,q) across the weak wave is zero. Solving the equations (3.5)–(3.7) we get

$$\mu = a_f^2 \nu = -\rho \lambda a_f^2 / V, \qquad \lambda = \lambda^{\alpha} N_{\alpha}$$
(3.9)

Eliminating from (3.8) and (3.9) we have

$$\left[\sigma V^2 c^2 - (1+V^2)a_f^2\right]\lambda = 0$$

Since $\lambda \neq 0$, we have

$$V^{2} = \frac{a_{f}^{2}/c^{2}}{\sigma - a_{f}^{2}/c^{2}}$$
(3.10)

Ram and Singh

From (2.9) and (3.10) we get an expression for the speed of propagation G_0 in the form

$$G_0^2 = \frac{a_f^2}{\beta^2 \bar{\beta}^2 (\sigma - a_f^2 / c^2)}$$
(3.11)

In the instantaneous rest frame the equation (3.11) reduces to $G_0^2 = a_f^2 / \sigma$, which fully agrees with the earlier results of Ram (1978) and McCarthy (1969) as particular cases of this result.

If the medium is in a uniform state ahead of the wave front and if the motion is studied in the rest frame of this uniform state, then the speed of propagation G_0 is a constant.

4. THE GROWTH EQUATION

In this section we shall derive a fundamental equation which governs the growth and decay of weak discontinuities in relativistic gas flows with nonequilibrium effects. We assume that the wave is propagating into a gas at rest and of constant state. From the equations (3.8) and (3.9) we get

$$\lambda^{\alpha} = \frac{\lambda}{1 + V^2} N_{\alpha}^*$$

where $N_{\alpha}^{*} = S^{\alpha\beta}N_{\beta}$ are the spacelike components of N^{α} . Now we define the amplitude b of the wave $\Sigma(x^{\mu})$ by the relation

$$b = c\lambda = c\lambda^{\alpha}N_{\alpha} = c\lambda^{\alpha}N_{\alpha}^{*}$$

Differentiating (2.6) and (2.7) with respect to x^{β} and taking jumps across the wave front with the help of (3.1) and (3.2) and simplifying we get

$$\rho\sigma c^{2}V\bar{\lambda}^{\alpha}N_{\alpha} + (1+V^{2})\bar{\mu} + V\delta(\mu) + \rho\sigma c^{2}\delta(\lambda) + \rho\sigma c^{2}\lambda^{2} - \rho c^{2}(\sigma + a_{f}^{2}/c^{2})\lambda^{2} - 2\rho a_{f}^{2}\lambda^{2} = 0$$
(4.1)
$$V\bar{\mu} + \delta(\mu) + \lambda\mu + \frac{\rho}{1+V^{2}}a_{f}^{2}\lambda_{,\tau}N_{\alpha}^{*}x_{\alpha}^{\tau} + \rho a_{f}^{2}\left(\bar{\lambda}^{\alpha}N_{\alpha} - \frac{2\Omega\lambda}{1+V^{2}}\right) - \frac{\Gamma\rho a_{f}^{2}\lambda^{2}}{V^{2}}\frac{\rho a_{f}^{4}}{V}\rho_{q}\frac{\beta}{c}\left(\frac{\partial w}{\partial p}\right)\lambda = 0$$
(4.2)

where

$$\begin{split} \bar{\lambda}^{\alpha} &= \left[U^{\alpha}_{,\beta\gamma} \right] N^{\beta} N^{\gamma}, \qquad \bar{\mu} = \left[P_{,\beta\gamma} \right] N^{\beta} N^{\gamma} \\ \Omega &= \frac{1}{2} a^{\tau\phi} b_{\phi\tau} \end{split}$$

Here Ω is the mean curvature of the moving wave surface $\Sigma(x^{\mu})$ and Γ is the effective heat exponent given by

$$\Gamma = 1 + \rho \frac{\partial a_f^2}{\partial p}$$

Like all other thermodynamic variables Γ is a function of p,s,q and coincides with the adiabatic heat exponent γ for an ideal gas. Eliminating $\bar{\mu}$ and $\bar{\lambda}^{\alpha}N_{\alpha}$ between (4.1) and (4.2) with the help of (3.10) we obtain

$$\left(2\sigma - \frac{a_f^2}{c^2}\right)\delta(\lambda) + \lambda \left(\frac{\beta}{c}a_f^2\rho_q\frac{\partial w}{\partial p} - \frac{2V\Omega}{1+V^2}\right)\frac{1+V^2}{c^2V^2}a_f^2$$
$$+ \lambda^2 \left((1+V^2)(\Gamma+1)\frac{a_f^2}{c^2} - \frac{3a_f^2}{c^2}\right) - \frac{a_f^2}{c^2V}\lambda_{,\tau}N_{\alpha}^*x_{\alpha}^{\tau} = 0 \qquad (4.3)$$

which is the fundamental differential equation governing the growth and decay of a weak discontinuity.

Assuming the fluid to be in a uniform state before the arrival of the wave front and choosing the frame of reference to be the rest frame of this uniform state, we have

$$\beta = 1, \qquad \overline{\beta} = (1 + V^2)^{1/2}, \qquad N_{\alpha}^* = (1 + V^2)^{1/2} (n^i, 0), \qquad G_0 = a_f / \sigma^{1/2}$$
(4.4)

In consequence of (4.4) the equation (4.3) assumes a simple form

$$A_1 \frac{db}{d\eta} + (A_2 - \Omega)b + A_3 b^2 = 0$$
(4.5)

where

$$b = c\lambda, \qquad \eta = G_0 t$$

$$A_1 = \frac{1}{2\sigma} \left(2\sigma - \frac{a_f^2}{c^2} \right) \left(1 - \frac{a_f^2}{\sigma c^2} \right)^{-3/2}$$

$$A_2 = \frac{a_f \sigma^{1/2}}{2\tau a_e^2} \left(1 - \frac{a_f^2}{\sigma c^2} \right)^{-1/2} \left(1 - \frac{a_e^2}{a_f^2} \right)$$

$$A_3 = \frac{1}{2a\sigma^{1/2}} \left(1 - \frac{a_f^2}{\sigma c^2} \right)^{-1/2} \left((\Gamma + 1)\sigma - \frac{3a_f^2}{c^2} \right)^{-1/2}$$

Here a_f and a_e represent sound speed in the frozen state and the equilibrium state of the fluid, respectively, τ is the relaxation time, and η represents the distance traversed by the wave in time t. All parameters involved in A_1 , A_2 , and A_3 have been evaluated at the wave front. The mean curvature of the wave surface can be written in the form (Thomas, 1963)

$$\Omega = \frac{\Omega_0 - K_0 \eta}{1 - 2\Omega_0 \eta + K_0 \eta^2}$$
(4.6)

where

 $\Omega_0 = \frac{1}{2}(K_1 + K_2), \qquad K_0 = K_1 K_2$

Here K_1 and K_2 are the constant principal curvatures of the initial wave front. The solution of (4.5) is of the form

$$b(\eta) = F(\eta) \left(\frac{1}{b(0)} + \frac{A_3}{A_1} \int_0^{\eta} F(\eta') \, d\eta'\right)^{-1}$$

where

$$F(\eta) = e^{-A_2\eta/A_1} (1 - 2\Omega_0 \eta + K_0 \eta^2)^{-(1/2)A_1}$$

5. GLOBAL BEHAVIOR OF A DISCONTINUITY

The wave amplitude b can also be expressed as a function of time in the form

$$b(t) = \phi(t) \left(\frac{1}{b(0)} + \frac{A_3}{A_1} \int_0^t \phi(t) \, dt' \right)^{-1}$$
(5.1)

570

Growth of Discontinuities in Relativistic Fluids

where

$$\phi(t) = e^{-A_2 G_0 t/A_1} \left[(1 - K_1 G_0 t) (1 - K_2 G_0 t) \right]^{-(1/2)A_1}$$

The wave geometry also plays an important role in the global behavior of the wave. If K_1 and K_2 are positive in the case of converging waves with curved surfaces, there are two possibilities. If the initial wave amplitude b(0) is negative in the case of a compressive wave and numerically less than a critical value b_c given by

$$b_{c} = \frac{A_{1}}{A_{3}} \left(\int_{0}^{t^{*}} \phi(t') dt' \right)^{-1}$$
(5.2)

where t^* is the least positive root of the equation

$$(1 - K_1 G_0 t)(1 - K_2 G_0 t) = 0$$

then the wave surface will form a caustics at a finite time t^* . When b(0) is numerically greater than b_c , then the wave amplitude becomes infinite at a finite critical time $t_c < t^*$ at the cusp of intersecting characteristics, and consequently a weak shock will become a strong shock due to nonlinear steepening as a result of infinite flow gradients. In the case of diverging wave surfaces, K_1 and K_2 are both negative, and therefore the solution (5.1) is valid for the whole interval $(0, \infty)$ except in the case of

$$|b(0)| > \frac{A_1}{A_3} \left(\int_0^\infty \phi(t') \, dt' \right)^{-1}$$
 (5.3)

When the condition (5.3) is not satisfied, the wave amplitude will decrease and the wave will be damped out ultimately. On the other hand if the condition (5.3) is satisfied, the nonlinear effect leads to steepening and consequently a breakdown occurs, which results in a shock formation after a finite time t_c given by

$$\int_{0}^{t_{c}} \phi(t') dt' = A_{1} / [A_{3}|b(0)|]$$
(5.4)

In the case of a plane wave front the solution (5.1) reduces to a simple form

$$b(t) = \exp(-A_2 G_0 t / A_1) \left(\frac{1}{b(0)} + \frac{A_3}{A_2} \left[1 - \exp(-A_2 G_0 t / A_1) \right] \right)^{-1} (5.5)$$

which fully agrees with the classical gas dynamic result of Ram (1978) in

Ram and Singh

the nonrelativistic limit. The critical value b_c of the initial wave amplitude and the critical time t_c are given by

$$b_c = \frac{\sigma}{\tau} \frac{a_f^2 / a_e^2 - 1}{(\Gamma + 1)\sigma - 3a_f^2 / c^2}$$
(5.6)

$$t_{c} = \frac{\tau a_{e}^{2} \left(2\sigma - a_{f}^{2} / a_{e}^{2}\right)}{a_{f}^{2} \left(1 - a_{e}^{2} / a_{f}^{2}\right) \left(1 - a_{f}^{2} / \sigma c^{2}\right)} \log \left(1 - \frac{b_{c}}{|b(0)|}\right)^{-1}$$
(5.7)

where τ is the relaxation time.

It is clear from (5.6) and (5.7) that if we neglect the relaxation effect, b_c vanishes. This shows that in equilibrium flows all compressive disturbances will grow into a shock wave, whereas in nonequilibrium flows there exists a critical line $b(0)=b_c$ below which all compressive disturbances will die out. The critical time t_c increases with relaxation and relativistic effects. This implies that in relativistic flows of chemically reacting fluids both relativistic and relaxation effects help in checking the growth of weak discontinuities. The relaxation process of internal transformation due to chemical reactions either disallows the shock formation or delays it (Ram, 1978). In the absence of nonequilibrium effects the critical time t_c can be expressed in the form

$$t_{c} = \frac{\left[2(\gamma-1) + (3-\gamma)a_{e}^{2}/c^{2}\right]\left[(\gamma-1) + a_{e}^{2}/c^{2}\right]}{\left[(\gamma-1) + (2-\gamma)a_{e}^{2}/c^{2}\right]\left[(\gamma+1)(\gamma-1+a_{e}^{2}/c^{2}) - 3(\gamma-1)a_{e}^{2}/c^{2}\right]}$$

which shows that t_c increases with relativistic effects.

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