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ON THE PROPAGATION OF SONIC WAVES IN A DISSOCIATING GAS

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The effects of non-equilibrium dissociation and that of wave front curvature on the propagation of sonic waves and their consequent formation into shock waves are examined. Special attention is paid to waves of plane, cylindrical and spherical geometry propagating into regions of weak equilibrium or strong equilibrium. It is found that a state of strong equilibrium has a stabilizing influence in that not all compression waves will grow into shock waves. Further, it is interesting to note that in a weak equilibrium state, all compression waves, no matter how weak initially, always end up into a shock whereas all expansion waves decay but not completely unlike the situation that occurs in a strong equilibrium state.

1. Introduction

The growth and decay behaviour of sonic waves, following the analysis of THOMAS [2], has been investigated by several workers [1—7] in a variety of material media. Calling a state with a zero reaction rate and a non-zero affinity a weak equilibrium state, and one with both of these quantities zero a strong equilibrium state, BOWEN [8] has investigated the influence of these thermodynamical states on the propagation of plane acceleration waves in a mixture of chemically reacting elastic materials. In this paper, using the singular surface theory due to THOMAS [9, 10], we have investigated the growth and decay behaviour of sonic waves propagating into regions of strong and weak equilibrium of an ideal dissociating gas. It is found that in a strong equilibrium state there exists a critical value of the initial discontinuity such that all compression waves whose initial discontinuity is less than this critical value damp to zero and waves with initial discontinuity greater than this critical value grow without bound in a finite time. For the case of weak equilibrium state, it is found that all compression waves grow into a shock after a finite time whereas all expansion waves decay and ultimately take a stable wave form. It is found that the geometry of the wave front affects the growth properties indirectly in that the critical value of the initial discontinuity depends on the initial curvatures of the wave front. The critical values of the initial discontinuity for cylindrical and spherical waves for which the respective waves never completely decay are found to be larger in magnitude than the corresponding value for plane waves. The specific source of non-equilibrium effects considered here is the dissociation recombination reaction in a symmetrical diatomic gas; the present method can, however, be employed to vibrational excitation, ionization etc. Here we have considered the useful approximation of the ideal dissociating gas due to LIGHTHILL [13]. The species that make up the gas mixture are assumed to behave individually as thermally perfect gases. The temperature range is taken from 2500 °K to 4500 °K. In this temperature range, the contribution of energy from electronic excitation and ionization are both assumed negligible. The radiation heat loss from the mixture and the molecular transport effects leading to viscosity, diffusion and heat conduction are also neglected.

2. Basic equations

The equations governing the three-dimensional unsteady motion of an ideal dissociating gas are [14]

$$\frac{\partial \varrho}{\partial t} + u_i \varrho_{,i} + \varrho u_{i,i} = 0 \,, \tag{1}$$

$$\varrho \frac{\partial u_i}{\partial t} + \varrho u_j u_{i,j} + p_{,i} = 0 \,, \tag{2}$$

$$\varrho \left(\frac{\partial h}{\partial t} + u_i h_{,i} \right) = \frac{\partial p}{\partial t} + u_i p_{,i} \tag{3}$$

$$\frac{\partial \alpha}{\partial t} + u_i \alpha_{,i} = W \,, \tag{4}$$

where the summation convention on repeated indices is employed, and a comma followed by an index denotes the partial derivative with respect to a space variable. The range of Latin indices is taken to be 1, 2, 3. The symbols appearing in (1)—(4) are as follows: ϱ is the density; p is the pressure; u_i are the gas velocity components; h is the specific enthalpy; α is the mass fraction of the reactant species, which takes part in the simple reversible reaction

$$A_2 = X \rightleftharpoons A + A + X \,. \tag{5}$$

(The species X can be either the diatomic molecular species A_2 or the atomic species A) and W is the rate of progress of reaction (5), namely

$$W = \tau^{-1} \{ K(1 - \alpha) - \alpha^2 \} \,. \tag{6}$$

The quantities τ and K are the forward-reaction time,

$$\tau^{-1} = 4 \varrho^2 k_r (1 + \alpha)/m^2 \tag{7}$$

and the equilibrium constant,

$$K = \frac{\varrho_d}{\varrho} \exp\left(-T_d/T\right), \tag{8}$$

respectively. The quantities k_r, m, ϱ_d and T_d appearing in (7) and (8) are respectively the recombination rate coefficient, the molecular weight of A_2, the characteristic density for dissociation and the characteristic temperature for dissociation. In the temperature range 2500 °K $\sim$ 4500 °K, the variation in these quantities is very small and hence they will be treated as constants.

The thermal and caloric equations of state for the gas mixture are [13]

$$p = \varrho(1 + \alpha) RT, \tag{9}$$

$$h = \{(4 + \alpha) T + \alpha T_d\} R, \tag{10}$$

where R is the gas constant for A_2.

Eq. (3) with the help of (1), (2), (4) and (6—10) is conveniently transformed into

$$\frac{\partial p}{\partial t} + u_i p,_i + \varrho a_f^2 u_{i,i} + \varrho a_f^2 \sigma W = 0, \tag{11}$$

where a_f is the frozen sound speed given by $a_f^2 = \frac{\Gamma p}{\varrho}$; Γ being the ratio of frozen specific heats given by $\Gamma = (4 + \alpha)/3$, and σ is a function of local thermodynamic properties given by

$$\sigma = \frac{1}{3\Gamma} \{(T_d/T) - (\Gamma - 1)^{-1}\}.$$

3. Kinematics of moving singular surfaces

In this Section, appropriate kinematics to describe the motion of a weak discontinuity surface is outlined. We shall assume that the reader has some familiarity with the kinematics of moving singular surfaces [9, 10]. We consider a moving singular surface Σ given by $f(x_i, t) = 0$, and that we denote by n_i the unit normal vector $f,_i/|\text{grad} f|$ and by $G = -\frac{\partial f}{\partial t}\Big/|\text{grad} f|$ the normal speed of advance of Σ. For definiteness, we require that the description of the surface Σ is such that G is always positive. This means that the normal n_i always points in the direction of propagation of Σ. The jump in any quantity across Σ is denoted by $[Z] = Z_1 - Z_0$, where Z_0 denotes the value of Z immediately ahead of the wave front, and Z_1 is the value of Z immediately behind it. If, across Σ, the function Z is continuous, while its first and second order partial derivatives with respect to x_i and t suffer jump discontinuities then it can be shown that [9, 10]

$$[Z,_i] = Bn_i\,; \quad \left[\frac{\partial Z}{\partial t}\right] = -GB\,, \tag{12, 13}$$

$$[Z,_{ij}] = \bar{B}n_i n_j + g^{\alpha\beta} B,_\alpha (n_i x_{j,\beta} + n_j x_{i,\beta}) - Bg^{\alpha\beta} g^{\gamma\delta} b_{\alpha\gamma} x_{i,\beta} x_{j,\delta}\,, \tag{14}$$

$$\left[\frac{\partial^2 Z}{\partial x_i\,\partial t}\right] = \left(-G\bar{B} + \frac{\delta B}{\delta t}\right) n_i - g^{\alpha\beta}(GB),_\alpha x_{i\beta}\,, \tag{15}$$

where $\beta = [Z,_i]\, n_i$, $\bar{B} = [Z,_{ij}]\, n_i n_j$ and $\frac{\delta(\ )}{\delta t}$ represent the rate of change of ( ) as seen by an observer fixed on Σ. A comma followed by a Greek index say (α) denotes partial derivatives with respect to the surface coordinate y^α. The range of Greek indices is 1, 2. Quantities $g^{\alpha\beta}$ and $b_{\alpha\beta}$ are the contravariant and covariant components of the first and second fundamental tensors of Σ respectively. We also recall the following relations which we shall be using in our further analysis

$$n_{i,\alpha} = -g^{\beta\nu} b_{\beta\alpha} x_{i,\gamma}\,; \quad 2\Omega = g^{\alpha\beta} b_{\alpha\beta} \quad \text{and} \quad \frac{\delta n_i}{\delta t} = -g^{\alpha\beta} G,_\alpha x_{i,\beta}, \tag{16, 17, 18}$$

where Ω is the mean curvature of Σ.

4. Derivation of the growth equation

A moving singularity surface Σ, across which the flow parameters are continuous but which is such that at least some of the first partial derivatives of these flow parameters suffer jump discontinuities at the surface, is called a weak discontinuity or a sonic wave. It follows from Section 2, that the quantities p, ϱ, α, u_i, a_f, τ, W and σ are continuous across Σ and they will have their subscript 0 values at the wave front. Assuming the state ahead of Σ to be uniform, it is shown in [1] that either $G - u_{n0} = \pm a_{f_0}$ or $G - u_{n0} = 0$, where $u_{n0} = u_{i0}\, n_i$ is the component of fluid velocity normal to the wave front Σ. The case $G - u_{n0} = 0$ which corresponds to a material surface is discarded as uninteresting, and we assume without loss of generality that

$$G = u_{n_0} + a_{f_0}\,. \tag{19}$$

When the medium ahead of the wave is uniform and at rest, it follows from (19) that the wave front Σ propagates through the medium with the frozen sound speed. As a result of which the successive positions of the wave front Σ at different instants form a family of parallel surfaces with straight lines as their orthogonal trajectories [11]. Thus given the wave surface at $t = 0$, say Σ_0, the position of the surface at any time $t > 0$ can be determined by measuring the distance traversed by the wave front along the normals to Σ_0. In the rest of the paper, we shall be concerned with the situation when the medium ahead of Σ is uniform and at rest. Then, on evaluating equations (1), (2) and (4) across Σ and using (12),(13) and (19), we get

$$\zeta = \frac{\varrho_0 \lambda}{a_{f_0}} = \xi / a_{f_0}^2, \quad \lambda_i = \lambda n_i, \quad \eta = 0, \tag{20, 21, 22}$$

where

$$\lambda_i = [u_{i,j}] \, n_j, \; \xi = [p,_i] \, n_i \, , \; \zeta = [\varrho,_i] \, n_i$$

and $\eta = [\alpha,_i] n_i$ are the quantities defined over Σ.

If we differentiate (2) and (11) with respect to x_k, take jumps across Σ, and multiply the resulting equations by n_k, we find, on using the relations (12)—(22), that

$$\varrho_0 \frac{\delta \lambda}{\delta t} = -(\bar{\xi} - \varrho_0 a_{f_0} \bar{\lambda}) \, , \tag{23}$$

$$\frac{\delta \xi}{\delta t} = a_{f_0} (\xi - \varrho_0 a_{f_0} \bar{\lambda}) - 2(\Lambda_0 - a_{f_0} \Omega)\xi - \frac{(\Gamma_0 + 1)}{\varrho_0 a_{f_0}} \xi^2, \tag{24}$$

where

$$\bar{\lambda} = [u_{i,jk}] \, n_i \, n_j \, n_k, \; \bar{\xi} = [p,_{ij}] \, n_i \, n_j$$

and

$$\Lambda_0 = \frac{1}{2} \left\{ 3\Gamma_0(\Gamma_0 - 1)\sigma_0^2 \left(W_0 + \frac{\alpha_0^2}{\tau_0} \right) + \frac{W_0}{3\Gamma_0} (3\Gamma_0 \sigma_0 - 1) \right\} .$$

Eqs. (23) and (24) can be combined to yield

$$\frac{\delta \zeta}{\delta t} + (\Lambda_0 - a_{f_0} \Omega) \zeta + \frac{(\Gamma_0 + 1) a_{f_0}}{2 \varrho_0} \zeta^2 = 0 \, , \tag{25}$$

where use has been made of (20).

Eq. (25) is the required growth equation for the discontinuity ζ which we have been seeking. In view of the relations (20), Eq. (25) yields a differential equation for λ and one for ξ. Thus, Eq. (25) is sufficient to predict the growth or decay of a discontinuity associated with the wave surface Σ. For a family of parallel surfaces, propagating with constant velocity, the mean curvature Ω has the representation [12]

$$\Omega = \frac{\Omega_0 - K_0 a_{f_0} t}{1 - 2\Omega_0 a_{f_0} t + K_0 a_{f_0}^2 t^2} \, , \tag{26}$$

where Ω_0 and K_0 are respectively the mean and Gaussian curvatures of Σ_0. Substituting for Ω in (25) and integrating, we get

$$\zeta = \frac{\zeta_0(1 - 2\Omega_0 a_{f_0} t + K_0 a_{f_0}^2 t^2)^{-\frac{1}{2}} \exp(-\Lambda_0 t)}{1 + \frac{(\Gamma_0 + 1)}{2\varrho_0} a_{f_0} \zeta_0 \int_0^t \{(1 - 2\Omega_0 a_{f_0} \hat{t} + K_0 a_{f_0}^2 \hat{t}^2)^{-\frac{1}{2}} \exp(-\Lambda_0 \hat{t})\} d\hat{t}}, \quad (27)$$

where ζ_0 is the value of ζ at the wave front at $t = 0$.

It is clear from (27) that the temporal behaviour of the density gradient at the wave head will depend critically on the sign of Λ_0. Following BOWEN [8], it follows that for a state of strong equilibrium Λ_0 is non-negative whereas for a weak equilibrium state Λ_0 may be positive or negative. To make the exact result (27) more accessible, we discuss the following three cases of plane, cylindrical and spherical waves.

5. Discussion

Case (i): Plane waves

For a plane wave front $\Omega_0 = K_0 = 0$, the Eq. (27) reduces to the form

$$\zeta = \frac{\zeta_0 \exp(-\Lambda_0 t)}{1 + \frac{\zeta_0}{\zeta_c}\{1 - \exp(-\Lambda_0 t)\}}, \quad (28)$$

where

$$\zeta_c = 2\varrho_0 \Lambda_0/(\Gamma_0 + 1) a_{f_0}$$

Eq. (28) shows that if $\zeta_0 > 0$ (i.e. an expansion wave front) and $\Lambda_0 > 0$ then the denominator of (28) remains positive and $\zeta \to 0$ as $t \to \infty$, the wave damps out. Also if $\zeta_0 < 0$ (i.e. a compression wave front) and if it has the magnitude less than ζ_c then the denominator of (28) remains positive and $\zeta \to 0$ as $t \to \infty$, i.e. a compression wave decays and damps out ultimately. Further, if ζ_0 is negative and has a magnitude equal to ζ_c, then $\zeta = \zeta_0$ and the wave propagates without any growth or decay. But if ζ_0 is negative and has a magnitude greater than ζ_c then $|\zeta| \to \infty$ for a finite t^* given by

$$t^* = \frac{1}{\Lambda_0}\left\{\log\left(1 - \frac{\zeta_c}{\zeta_0}\right)^{-1}\right\}. \quad (29)$$

Thus at a finite time t^* the density gradient at the wave front becomes infinite and this signifies the appearance of a shock wave. Thus we find that ζ_c is a critical value of the initial discontinuity in the sense that all compression waves with initial discontinuity less than this value attenuate while all compression waves with initial discontinuity greater than this value grow into a shock wave after a finite time. It is evident from the expressions of ζ_c and t^* that they are increasing functions of Λ_0, i.e. the dissociation effects are to increase the shock formation time.

For $\Lambda_0 < 0$ (which can only occur in weak equilibrium state) it follows from (28) that if $\zeta_0 > 0$ then $\zeta \to |\zeta_c|$ as $t \to \infty$, i.e. all expansion waves decay and ultimately take a stable wave form. This interesting feature of expansion waves does not appear in the former case in which all expansion waves decay and damp out ultimately. But if $\zeta_0 < 0$ and $\Lambda_0 < 0$ then we have the criterion

$$\bar{t} = \frac{1}{|\Lambda_0|} \log \left\{ 1 + \frac{|\zeta_c|}{|\zeta_0|} \right\}, \tag{30}$$

for the shock formation at a finite time. Thus, in this case we find that a discontinuity, no matter how small, associated with a compression wave always grows into a shock. It is also evident from (30) that the weak equilibrium state causes the compression wave to steepen more swiftly than it does in an inert atmosphere (in which $\Lambda_0 = 0$).

Case (ii): Spherical waves

If the wave front Σ at time $t = 0$ is a sphere of radius R_0, then at any time $t > 0$, Σ is a sphere of radius $R = R_0 + a_{f_0} t$. For such a wave $\Omega_0 = -\frac{1}{R_0}$ and $K_0 = \frac{1}{R_0^2}$ and thus the Eq. (27) reduces to

$$\zeta = \frac{\zeta_0 (R_0/R) \exp \{-\Lambda_0 (R - R_0)/a_{f_0}\}}{1 + \frac{(\Gamma_0 + 1)}{2\,\varrho_0} \zeta_0 R_0 \exp (\Lambda_0 R_0/a_{f_0}) \, E_i (\Lambda_0 R_0/a_{f_0}) \left\{ 1 - \frac{E_i(\Lambda_0 R/a_{f_0})}{E_i(\Lambda_0 R_0/a_{f_0})} \right\}}, \tag{31}$$

where $E_i(x) = \int_x^\infty t^{-1} e^{-t} dt$ is a tabulated function known as exponential integral function. For $\Lambda_0 > 0$, the term in the curly bracket in the denominator of (31) increases monotonically from 0 to 1 as R increases from R_0 to ∞. Hence in this case also there exists a critical value of initial discontinuity $\hat{\zeta}_c$, the magnitude of which is given by

$$|\hat{\zeta}_c| = \frac{2\varrho_0 \exp (-\Lambda_0 R_0 / a_{f_0})}{(\Gamma_0 + 1) R_0 \, E_i(\Lambda_0 R_0/a_{f_0})} \tag{32}$$

such that if $\zeta_0 < 0$ and has a magnitude less than $|\hat{\zeta}_c|$ then the denominator of (31) remains positive and finite and thus $\zeta \to 0$ as $R \to \infty$, the compression wave decays and damps out ultimately. Further, if $\zeta_0 < 0$ and has a magnitude equal to $|\hat{\zeta}_c|$, then $|\zeta| \to \zeta_c$ as $R \to \infty$. i.e. the wave does not completely decay and ultimately takes a stable wave form. But if $\zeta_0 < 0$ and has a magnitude greater than $|\hat{\zeta}_c|$, then we have the criterion

$$E_i(\Lambda_0 \hat{R}/a_{f_0}) = \left(1 - \frac{|\hat{\zeta}_c|}{|\zeta_0|}\right) E_i(\Lambda_0 R_0/a_{f_0}) \tag{33}$$

for the shock formation at a finite $R = \hat{R} = R_0 + a_{f_0}\hat{t}$. From the inequality $E_i(x) < e^{-x}/x$, it follows that $|\hat{\zeta}_c|$ (critical value of the discontinuity for the spherical wave) is greater than the corresponding value for a plane wave.

From the expression (32), it follows that $\frac{\partial|\hat{\zeta}_c|}{\partial \Lambda_0} > 0$ which means that the critical value of the initial discontinuity increases with Λ_0. Also $\frac{\partial|\hat{\zeta}_c|}{\partial R_0} < 0$ which implies that the initial curvature has a stabilizing effect on the tendency of the wave surface Σ to grow into a shock in the sense that an increase in the value of the initial curvature causes an increase in the critical amplitude. Further, it is also evident from (33) that $\frac{\partial \hat{t}}{\partial \Lambda_0} > 0$ which means that an increase in Λ_0 will cause the shock formation time $\hat{t}$ to increase, i.e. the non-equilibrium dissociation effects are to increase the shock formation time $\hat{t}$. On the other hand, if the wave is expansion ($\zeta_0 > 0$), then $\zeta \to 0$ as $R \to \infty$, the wave decays and damps out ultimately.

For $\Lambda_0 < 0$, the denominator of (31) reduces to

$$1 + \frac{(\Gamma_0 + 1)}{2\varrho_0} \zeta_0 R_0 \exp(\Lambda_0 R_0/a_{f_0}) \int_{-\Lambda_0 R_0/a_{f_0}}^{-\Lambda_0 R/a_{f_0}} x^{-1} e^x \, dx \,. \tag{34}$$

When $\zeta_0 > 0$, the denominator (34) remains positive and tends to infinity as $R \to \infty$. This happens because of the diverging nature of the integral involved therein. Also, numerator of (31), for $\Lambda_0 < 0$, tends to infinity as $R \to \infty$. Hence, by making use of L'Hospital's rule, we obtain that $\zeta \to |\zeta_c|$ (critical value for a plane wave) as $R \to \infty$. Also, (34) shows that if $\zeta_0 < 0$ then we have the criterion

$$\int_{-\Lambda_0 R_0/a_{f_0}}^{-\Lambda_0 \bar{R}/a_{f_0}} x^{-1} e^x \, dx = \frac{2\varrho_0 \exp(-\Lambda_0 R_0/a_{f_0})}{|\zeta_0|(\Gamma_0 + 1) R_0}$$

for the shock formation at a finite $R = \bar{R}$.

Case (iii): Cylindrical waves

In this case also the growth and decay phenomenon is very much similar to those of plane and spherical waves. If the diverging wave front Σ at $t = 0$ is a cylinder of radius R_0, then at any time $t > 0$, Σ is a cylinder of radius $R = R_0 + a_{f_0} t$. For such a wave $\Omega_0 = -\frac{1}{2R_0}$ and $K_0 = 0$ and thus Eq. (27) assumes the form

$$\zeta = \frac{\zeta_0 (R_0/R)^{1/2} \exp\{-\Lambda_0 (R - R_0)/a_{f_0}\}}{1 + \frac{(\Gamma_0+1)}{2\varrho_0} \zeta_0 \exp(\Lambda_0 R_0/a_{f_0}) \left(\frac{\pi R_0}{\Lambda_0 a_{f_0}}\right)^{1/2} \operatorname{erfc}(\Lambda_0 R_0/a_{f_0})^{1/2}} \times \left\{1 - \frac{\operatorname{erfc}(\Lambda_0 R/a_{f_0})^{1/2}}{\operatorname{erfc}(\Lambda_0 R_0/a_{f_0})^{1/2}}\right\} \tag{35}$$

where $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt$ is the complementary error function. For $\Lambda_0 > 0$, if $\zeta_0 > 0$ then ζ remains positive for all $R > R_0$ and monotonically approaches zero as $R \to \infty$. Also if $\zeta_0 < 0$ and has a magnitude less than $|\tilde{\zeta}_c|$, where

$$|\tilde{\zeta}_c| = \left(\frac{\Lambda_0 a_{f_0}}{\pi R_0}\right)^{1/2} \frac{2\varrho_0 \exp(-\Lambda_0 R_0/a_{f_0})}{(\Gamma_0+1) \operatorname{erfc}(\Lambda_0 R_0/a_{f_0})^{1/2}} \tag{36}$$

then $\zeta \to 0$ as $R \to \infty$, the wave damps out. Further, if $\zeta_0 < 0$ and has a magnitude equal to $|\tilde{\zeta}_c|$ then the wave decays and $\zeta \to |\zeta_c|$ (critical value for a plane wave) as $R \to \infty$, i.e. the wave ultimately takes a stable wave form. From the inequality $\operatorname{erfc}(x) < e^{-x^2}/x\sqrt{\pi}$, it follows immediately that $|\tilde{\zeta}_c|$ (for cylindrical wave) is greater than the corresponding critical value for a plane wave. But if $\zeta_0 < 0$ and has a magnitude greater than $|\tilde{\zeta}_c|$ then we have the criterion

$$\operatorname{erfc}\left(\frac{\Lambda_0 \tilde{R}}{a_{f_0}}\right)^{1/2} = \left(1 - \frac{|\tilde{\zeta}_c|}{|\zeta_0|}\right) \operatorname{erfc}\left(\frac{\Lambda_0 R_0}{a_{f_0}}\right)^{1/2}. \tag{37}$$

for the shock formation at a finite $R = \tilde{R}$. However, if $\zeta_0 > 0$ and $\Lambda_0 > 0$ then (35) shows that $\zeta \to 0$ as $R \to \infty$, the wave damps out. It is evident from (36) and (37) that the dissociation effects are to increase the shock formation time.

For $\Lambda_0 < 0$, the growth and decay phenomenon is again similar to those of plane and spherical waves, i.e. if $\zeta_0 > 0$ the $\zeta \to |\zeta_0|$ (critical value for a plane wave) as $R \to \infty$. But if $\zeta_0 < 0$, then we have the criterion

$$\int_{(-\Lambda_0 R_0/a_{f_0})^{1/2}}^{(-\Lambda_0 R^*/a_{f_0})^{1/2}} \exp(x^2)\, dx = \left(\frac{R_0 a_{f_0}}{|\Lambda_0|}\right)^{-1/2} \frac{\varrho_0 \exp(-\Lambda_0 R_0/a_{f_0})}{(\Gamma_0 + 1)|\zeta_0|}$$

for the shock formation at a finite distance $R = R^*$.

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