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BRIEF NOTES

A note on shock waves in fluids with internal state variables

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THE OBJECT of this note is to derive a general expression which governs the behavior of the amplitude of a shock wave propagating in fluids with internal state variables. Two specific cases are discussed: (i) when the fluid ahead of the wave is well stirred, and (ii) when the fluid ahead of the wave is undergoing spinodal decompositions.

1. Introduction

IN THIS NOTE we consider the behavior of shock waves propagating in fluids with internal state variables. We derive a general expression which governs the behavior of the amplitude of a shock propagating in such a fluid without adopting any assumptions regarding the condition of the fluid ahead of the shock (1). After examining the implications of this equation, we specialize it to two specific cases: (i) when the fluid ahead of the wave is well stirred, and (ii) when the fluid ahead of the wave is undergoing spinodal decompositions.

2. Preliminaries

Here, we consider fluids whose internal energy e, pressure p and absolute temperature θ are determined by the specific volume v, the entropy η, and N internal state variables $a_1, a_2, \dots, a_N$:

$$e = \hat{e}(v, \eta, \mathbf{a}), \tag{2.1}$$

$$p = \hat{p}(v, \eta, \mathbf{a}), \tag{2.2}$$

$$\theta = \hat{\theta}(v, \eta, \mathbf{a}), \tag{2.3}$$

where $\mathbf{a}$ is the N-vector with components $(a_1, a_2, \dots, a_N)$ and is called the internal state vector. The material derivative $\dot{\mathbf{a}}$ of $\mathbf{a}$ obeys the constitutive relation

$$\dot{\mathbf{a}} = \mathbf{h}(v, \eta, \mathbf{a}). \tag{2.4}$$

Of course, it is well known that the response functions $\hat{e}$, $\hat{p}$ and $\hat{\theta}$ are not independent. Indeed, the Second Law of thermodynamics dictates that (2)

$$\hat{p} = -\hat{e}_v, \quad \hat{\theta} = \hat{e}_\eta, \tag{2.5}$$

(1) Our results generalize those given by CHEN and GURTIN [1] and CHEN [2].

(2) See, for example, COLEMAN and GURTIN [3].

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and that

$$\boldsymbol{\sigma}\cdot\mathbf{h} = \sigma_1 h_1+\sigma_2 h_2+\ldots+\sigma_N h_N \geqslant 0, \tag{2.6}$$

where $\boldsymbol{\sigma}$ is the N-vector defined by

$$\boldsymbol{\sigma} = -\hat{e}_{\mathbf{a}} \equiv -(e_{a_1}, e_{a_2}, \ldots, e_{a_N}). \tag{2.7}$$

In view of $(2.5)_1$ and (2.7), we see that

$$\boldsymbol{\sigma}_v = \mathbf{p}_{\mathbf{a}}. \tag{2.8}$$

In applications of our theory to chemically reacting mixtures each a_i is identified as the extent of reaction of a particular chemical reaction, $\dot{a}_i$ its reaction rate, and σ_i its chemical affinity.

In this paper, we are interested in the one dimensional motions of the fluids characterized by the constitutive relations (2.1), (2.2) and (2.3). Each such motion is described by the function χ giving the position x at time t of the material point X:

$$x = \chi(X, t). \tag{2.9}$$

Of course, we identify each material point with its position in a fixed homogeneous reference configuration with density ϱ_0. The specific volume v is, of course, given by

$$v = \varrho^{-1} = \varrho_0^{-1} x_X, \tag{2.10}$$

where ϱ is the present density.

We assume that the motion contains a shock moving with velocity $U(t) = dY(t)/dt > 0$, where $Y(t)$ is the material point at which the wave is to be found at time t. Hence, letting f denote v, ϱ, $\dot{x}$ or η, we have

(i) The motion χ is continuous.

(ii) f, $\dot{f}$, and f_X have jump discontinuities across the wave.

We also assume that

(iii) $\mathbf{a}$ is continuous, but $\dot{\mathbf{a}}$ and $\mathbf{a}_X$ have jump discontinuities across the wave.

In view of (2.1), (2.2), and (2.3), we see that e, p, and θ and their derivatives also have jump discontinuities across the wave. Further, we also have the following compatibility relations:

$$[\dot{x}] = -U[x_X] = -\varrho_0 U[v], \tag{2.11}$$

$$[\dot{a}] = -U[a_X], \tag{2.12}$$

$$\frac{d[f]}{dt} = [\dot{f}]+U[f_X], \tag{2.13}$$

whenever f is equal to v, ϱ, $\dot{x}$, η, e, p, or θ. Here, $[f] = f^- - f^+$ with $f^{\mp} = \lim\limits_{X\to Y(t)^{\mp}} f(X, t)$.

Balance of linear momentum and balance of energy imply that

$$[p] = \varrho_0 U[\dot{x}], \tag{2.14}$$

$$[p_X] = -\varrho_0[\ddot{x}], \tag{2.15}$$

$$\varrho_0 U\left[e+\frac{1}{2}\dot{x}^2\right] = [p\dot{x}], \tag{2.16}$$

$$[\dot{e}] = -[p\dot{v}]. \tag{2.17}$$

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By (2.11) and (2.14), we have

$$U^2 = -\frac{[p]}{\varrho_0^2 [v]} \tag{2.18}$$

for the velocity of the shock, and (2.14) with $f = v$ and $\dot{x}$, (2.2), (2.11) and (2.15) imply that (3)

$$2U\frac{d[v]}{dt} + [v]\frac{dU}{dt} = U^2[v_X] + \frac{1}{\varrho_0^2}[p_v v_X + p_\eta \eta_X + p_{\mathbf{a}} \cdot \mathbf{a}_X]. \tag{2.19}$$

Further, (2.17) with (2.1), (2.4), (2.5) and (2.7) implies that

$$[\theta\dot{\eta}] = [\boldsymbol{\sigma} \cdot \mathbf{h}]. \tag{2.20}$$

3. The governing equation of the amplitude

Here, we shall derive the governing differential equation of the shock amplitude without adopting any assumptions regarding the condition of fluid ahead of the wave. First, we note that the jump $[AB]$ in the product AB may be rewritten in the form (4)

$$[AB] = A^-[B] + B^+[A].$$

With this in mind, (2.19) becomes

$$2U\frac{d[v]}{dt} + [v]\frac{dU}{dt} = \left(\frac{p_v^-}{\varrho_0^2} + U^2\right)[v_X] + \frac{1}{\varrho_0^2} v_X^+ [p_v] + \frac{1}{\varrho_0^2} p_\eta^- [\eta_X] + \frac{1}{\varrho_0^2} \eta_X^+ [p_\eta] + \frac{1}{\varrho_0^2}[p_{\mathbf{a}} \cdot \mathbf{a}_X]. \tag{3.1}$$

Before we can fully evaluate (3.1), we need expressions for $[\eta_X]$ and dU/dt. The derivations of these expressions are rather lengthy; however, we shall only outline the procedure, the interested reader may consult other papers in which special cases of these results are derived.

First, we note that (2.16) with (2.11) may be rewritten in the form

$$[e] + \frac{1}{2}(p^- + p^+)[v] = 0. \tag{3.2}$$

Taking the d/dt derivative of (3.2), substituting the result into (2.13) with $f = e$ and using (2.1), (2.5), (2.17) and (2.20), we have

$$[\eta_X] = \frac{p_v^-(1-\mu)}{p_\eta^- U(2\tau-1)}\frac{d[v]}{dt} + \left(\frac{2p_v^-(1-\mu)}{p_\eta^- U(2\tau-1)} - \frac{[p_v]}{p_\eta^- U(2\tau-1)}\right)\frac{dv^+}{dt} + \left(\frac{p_\eta^- + p_\eta^+}{p_\eta^- U(2\tau-1)} + \frac{2[\theta]}{p_\eta^- U[v](2\tau-1)}\right)\frac{d\eta^+}{dt} - \frac{1}{U}[\dot{\eta}] + \left(\frac{p_{\mathbf{a}}^- + p_{\mathbf{a}}^+}{p_\eta^- U(2\tau-1)} - \frac{2[\boldsymbol{\sigma}]}{p_\eta^- U(2\tau-1)[v]}\right)\cdot\frac{d\mathbf{a}}{dt} \tag{3.3}$$

(3) Cf. CHEN and GURTIN [1].

(4) Cf. CHEN [2, 4].

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where we have introduced the definitions

$$\mu = -\frac{\varrho_0^2 U^2}{p_v^-}, \qquad \tau = -\frac{\theta^-}{p_\eta^- [v]}. \tag{3.4}$$

Now, differentiating (2.18) and using (3.3) and (3.4), we obtain

$$\begin{aligned} \frac{dU}{dt} = &-\frac{\tau p_v^- (1-\mu)}{\varrho_0^2 U (2\tau-1)[v]} \frac{d[v]}{dt} - \left\{ \frac{p_v^-(1-\mu)}{\varrho_0^2 U[v](2\tau-1)} + \frac{(\tau-1)[p_v]}{\varrho_0^2 U[v](2\tau-1)} \right\} \frac{dv^+}{dt} \\ &- \left\{ \frac{[p_\eta]}{2\varrho_0^2 U[v]} + \frac{p_\eta^- + p_\eta^+}{2\varrho_0^2 U[v](2\tau-1)} + \frac{[\theta]}{\varrho_0^2 U(2\tau-1)[v]^2} \right\} \frac{d\eta^+}{dt} \\ &- \left\{ \frac{[p_{\mathbf{a}}]}{2\varrho_0^2 U[v]} + \frac{p_{\mathbf{a}}^- + p_{\mathbf{a}}^+}{2\varrho_0^2 U[v](2\tau-1)} - \frac{[\sigma]}{\varrho_0^2 U[v]^2(2\tau-1)} \right\} \cdot \frac{d\mathbf{a}}{dt}. \end{aligned} \tag{3.5}$$

If we substitute (3.3) and (3.5) into (3.1), it can be shown that the resulting relation may be written in the form([5])

$$\frac{d[v]}{dt} = \frac{U(2\tau-1)(1-\mu)}{(3\mu+1)\tau - (3\mu-1)} \{\lambda - [v_X]\}, \tag{3.6}$$

where

$$\begin{aligned} \lambda = &-\frac{1}{p_v^-(2\tau-1)U(1-\mu)} \Bigg\{ \{3p_v^-(1-\mu) + (\tau-2)[p_v]\} \frac{dv^+}{dt} \\ &+ \left\{ \left(\tau - \frac{1}{2}\right)[p_\eta] + \frac{3}{2}(p_\eta^- + p_\eta^+) + \frac{3[\theta]}{[v]} \right\} \frac{d\eta^+}{dt} \\ &+ \left\{ \left(\tau - \frac{1}{2}\right)[p_{\mathbf{a}}] + \frac{3}{2}(p_{\mathbf{a}}^- + p_{\mathbf{a}}^+) - 3\frac{[\boldsymbol{\sigma}]}{[v]} \right\} \cdot \frac{d\mathbf{a}}{dt} \Bigg\} \\ &- \frac{1}{p_v^- U(1-\mu)} \left\{ U[p_v]v_X^+ + U[p_\eta]\eta_X^+ + \frac{p_\eta^-[\theta]}{\theta^-\theta^+} \boldsymbol{\sigma}^+ \cdot \mathbf{h}^+ + U[p_{\mathbf{a}} \cdot \mathbf{a}_X] - \frac{p_\eta^-[\boldsymbol{\sigma} \cdot \mathbf{h}]}{\theta^-} \right\}. \end{aligned} \tag{3.7}$$

Equation (3.6) is the governing differential equation of the amplitude of the shock; it is of the same form as those which arise in other theories. In particular, we observe that if at any instant $\lambda = [v_X]$, then $d[v]/dt = 0$, i.e., at that instant the shock amplitude neither grows or decays. In general, however, we expect that $\lambda \neq [v_X]$, and hence the amplitude may either grow or decay. Before we can infer any results from (3.6) regarding the behavior of the shock we need to recall certain preliminary results.

Consider a particular instant of time. Hence v^+, η^+ and $\mathbf{a}$ are fixed. If we assume that (3.2) can be solved to express η^- as a function of v^-, and, as is customary, that

$$p_v < 0, \quad p_{vv} > 0, \quad p_\eta > 0 \tag{3.8}$$

then (i) the shock is compressive, (ii) the shock speed is subsonic with respect to the material behind the wave, and (iii) the entropy η^- increases with decreasing specific volume ε^-.

([5]) The relation includes as special cases those given by CHEN and GURTIN [1] and CHEN [2].

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With these results, we can show that μ and τ, defined by (3.4), obey the inequalities [6]

$$0 < \mu < 1, \quad \tau > \frac{1}{2}. \tag{3.9}$$

By (3.6) and (3.9), it is a simple matter to establish the following results on the local behavior of the shock:

At any instant

$$[v_X] > \lambda \Leftrightarrow \frac{d|[v]|}{dt} > 0, \tag{3.10}$$

$$[v_X] < \lambda \Leftrightarrow \frac{d|[v]|}{dt} < 0. \tag{3.11}$$

Equation (3.10) and (3.11) states that the magnitude of the shock either grows or decays according as $[v_X]$ is greater or less than λ. In other words, the shape of the pulse behind the shock has a definite effect on its behavior.

A most interesting application of our results is when the fluid ahead of the wave is well stirred, in the sense that each reaction is proceeding at the same rate at every point prior to the passage of the wave. Hence, the field quantities ahead of the wave are independent of position. In this instance (3.6) reduces to

$$\frac{d[v]}{dt} = \frac{U(2\tau-1)(1-\mu)}{(3\mu+1)\tau-(3\mu-1)}\{\mathring{\lambda}-v_X^-\}, \tag{3.12}$$

where

$$\mathring{\lambda} = -\frac{1}{p_v^-(2\tau-1)U(1-\mu)}\Bigg\{\{3p_v^-(1-\mu)+(\tau-2)[p_v]\}\dot{v}^+ + \left\{\left(\tau-\frac{1}{2}\right)[p_\eta]+\frac{3}{2}(p_\eta^-+p_\eta^+)+\frac{3[\theta]}{[v]}+\frac{p_\eta^-(2\tau-1)[\theta]}{\theta^-}\right\}\frac{\boldsymbol{\sigma}^+\cdot\mathbf{h}^+}{\theta^+} + \left\{\left(\tau-\frac{1}{2}\right)[p_\mathbf{a}]+\frac{3}{2}(p_\mathbf{a}^-+p_\mathbf{a}^+)-3\frac{[\boldsymbol{\sigma}]}{[v]}\right\}\cdot\mathbf{h}^+\Bigg\} + \frac{1}{p_v^-U(1-\mu)}\left\{p_\mathbf{a}^-\cdot[\mathbf{h}]+\frac{p_\eta^-[\boldsymbol{\sigma}\cdot\mathbf{h}]}{\theta^-}\right\}. \tag{3.13}$$

As a further special case of (3.13), we can consider the situation where $\dot{v}^+$ and $\boldsymbol{\sigma}^+$ are zero. When $\boldsymbol{\sigma}^+$ is zero, it follows from the energy equation that $\dot{\eta}^+$ is also zero. In a state $(v^+, \eta^+, \mathbf{a}^+)$ such that $\boldsymbol{\sigma}^+ = \mathbf{0}$ the inequality (2.6) has the following implications [7]:

$$\boldsymbol{\sigma}_v(v^+, \eta^+, \mathbf{a}^+)\cdot\mathbf{h}(v^+, \eta^+, \mathbf{a}^+) = 0, \tag{3.14}$$

$$\boldsymbol{\sigma}_\eta(v^+, \eta^+, \mathbf{a}^+)\cdot\mathbf{h}(v^+, \eta^+, \mathbf{a}^+) = 0, \tag{3.15}$$

$$\boldsymbol{\sigma}_\mathbf{a}(v^+, \eta^+, \mathbf{a}^+)\,\mathbf{h}(v^+, \eta^+, \mathbf{a}^+) = \mathbf{0}. \tag{3.16}$$

Equations (3.14), (3.15) and (3.16) can be viewed as a system of $N+2$ equations with N unknowns $\mathbf{h}^+$. They place certain restrictions on the possible values of $\dot{\mathbf{a}}^+ = \mathbf{h}(v^+, \eta^+, \mathbf{a}^+)$.

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(6) See, for example, CHEN [2].

(7) BOWEN [5, Sec. 4].

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If the rank of the matrix of coefficients is N then $\dot{\mathbf{a}}^+ = \mathbf{0}$. In which case, our results would be the same as those given by CHEN and GURTIN [1]. However, if the rank of the matrix of coefficients is less than N, then $\dot{\mathbf{a}}^+ = \mathbf{h}^+$ need not vanish. Chemical reactions which occur with a zero chemical affinity are known to exist. They are called spinodal decompositions([8]). In this special case (3.13) with (2.8) and (3.14) reduces to

$$(3.17)\qquad \mathring{\lambda} = -\frac{1}{p_v^-(2\tau-1)\,U(1-\mu)}\left\{3\tau p_{\mathbf{a}}^- - 3\frac{\boldsymbol{\sigma}^-}{[v]}\right\}\cdot\mathbf{h}^+ + \frac{1}{(1-\mu)\,U\theta^- p_v^-}\{\theta^- p_{\mathbf{a}}^- + p_\eta^-\boldsymbol{\sigma}^-\}\cdot\mathbf{h}^-.$$

In closing, we wish to record the limiting form of (3.17) which is valid for weak shocks, i.e., in the limit as $[v]\to 0$. Following the procedure used by CHEN and GURTIN [1], (3.17) yields

$$(3.18)\qquad \mathring{\lambda}\to\frac{2\boldsymbol{\sigma}_v^+\cdot\mathbf{h}_v^+}{U_0 p_{vv}^+}\qquad\text{as}\qquad [v]\to 0.$$

where $\varrho_0^2 U_0^2 = -p_v^{\pm}$. Equation (3.18) is equivalent to that obtained by CHEN and GURTIN [1] under the different assumption that the region ahead of the wave is in a weak chemical equilibrium state([9]). In the case where both $\boldsymbol{\sigma}^+$ and $\mathbf{h}^+$ are zero, we can prove, as CHEN and GURTIN [1] proved, that $\mathring{\lambda}\geqslant 0$.

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([8]) See, for example, KUBASCHEWSKI, EVANS and ALCOCK [6], pp. 69–70.

([9]) Here, we should point out that our λ is $-1/\varrho_0^2$ times the λ given by CHEN and GURTIN [1], Eq. (48). Also, their Eq. (48) is also valid when $\boldsymbol{\sigma}^+\neq 0$ because (2.6) implies that $\boldsymbol{\sigma}^+\cdot\mathbf{h}^+ = 0$ in a weak chemical equilibrium state.

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