Readers' Forum

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Evolution of Weak Discontinuities in the Unsteady Flow of Thermally Conducting Dissociating Gases

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CONSIDER the discontinuity λ of the velocity gradient in the unsteady flow of a thermally conducting dissociating gas. Recently, Verma and Kumar[1] have attempted to derive a growth equation for λ, a "solution" to the growth equation, and a critical time t_c for the shock formation. Unfortunately, their analysis is very misleading and replete with errors and contradictions, a few of which are as follows (superscript 1 designates the equations of Ref. 1):

1) The set of their basic equations is incorrect because they have not been able to distinguish between the thermodynamic states of equilibrium and nonequilibrium. Thus, Eq. (6)[1] represents the rate equation for a *nonequilibrium* flow, whereas Eq. (5)[1] is the entropy equation for an *equilibrium* flow derived by Lighthill.[2] Moreover, the energy equation [Eq. (3)[1]] is incorrect because it does not include the entropy production term due to nonequilibrium dissociation.

2) During the analysis, they have assumed the constancy of several flow and field parameters, e.g., that of σ and C when deriving Eq. (16)[1] from Eq. (15)[1] and that of A and B thereafter. Note that, since the flow is unsteady, it is absurd to require that the parameters be constant.

3) Their growth equation [Eq. (16)[1]] is peculiar, to say the least. It is well known[3-5] that the behavior of the weak discontinuity in the solution of any quasilinear hyperbolic system is governed by a Bernoulli-type equation $\mathrm{d}\lambda/\mathrm{d}t = -\alpha\lambda+\beta\lambda^2$, where α and β depend upon the state of the gas ahead of the discontinuity surface. Equation (16)[1] however reads $\mathrm{d}\lambda/\mathrm{d}t=\lambda^2-A\lambda-B$.

4) Their primary result [Eq. (17)[1]], which purports to be the "solution" of Eq. (16)[1], is still more peculiar: it is derived by treating A and B as constants and it expresses the independent variable t as a function of λ. A similar comment applies to the derivation of the strange criterion in Eq. (18)[1].

The purpose of this Note is to set up the proper basic equations and to derive the correct growth equation for λ, from which the solution and the criterion for blowup are easily obtained. Our analysis is applicable not only to dissociating gases, but also to chemically reacting, vibrationally relaxing, or ionizing gases. The notation is as follows: t is the time, T the temperature, K the coefficient of thermal conductivity, q the degree of dissociation, σ the gas density, p the pressure, ϵ the total energy of the gas per unit mass, $h=\epsilon+(p/\sigma)$ the specific enthalpy, and u_i $(i=1,2,3)$ the gas velocity components. As usual, $\mathrm{d}/\mathrm{d}t=\partial/\partial t+u_i\,\partial/\partial x_i$ is the material time derivative, and a comma followed by an index i denotes the partial derivative with respect to the space coordinate x_i.

The equations of continuity and momentum are as in Ref. 1. The equation of energy for a thermally conducting gas is,[6]

$$\partial_t[\sigma(\epsilon+\tfrac{1}{2}u^2)]+[\sigma u_i(\epsilon+\tfrac{1}{2}u^2)]_{,i}=-(pu_i)_{,i}+(KT_{,i})_{,i}$$

where $\partial_t=\partial/\partial t$. Using the equations of continuity and momentum, the above equation can be written as

$$\sigma(\mathrm{d}h/\mathrm{d}t)-(\mathrm{d}p/\mathrm{d}t)=KT_{,ii} \tag{1}$$

Note that for a nonequilibrium flow of a dissociating gas, h and ϵ are known functions of the state variables p, T, and q (Ref. 7, pp. 247-251, 290) and the change in entropy S is obtained from the Gibbs relation[7,8] (Ref. 7, p. 250),

$$T\mathrm{d}S=\mathrm{d}h-\sigma^{-1}\mathrm{d}p+\Lambda\mathrm{d}q \tag{2}$$

where Λ is the affinity of internal transformation characterized by the variable q. Since S is a function of p, T, and q,

$$S=S(p,T,q) \tag{3}$$

from Eq. (2) we may regard σ, Λ as known functions,

$$\sigma=\sigma(p,T,q);\quad \Lambda=\Lambda(p,T,q) \tag{4}$$

Applying Eq. (2) to the changes to a fluid element, we obtain in view of Eq. (1),

$$\sigma T(\mathrm{d}S/\mathrm{d}T)=KT_{,ii}+\sigma\Lambda(\mathrm{d}q/\mathrm{d}t) \tag{5}$$

which is the correct form of the energy equation [cf. Eq. (3)[1]]. The reaction rate equation for the flow is the same as in Ref. 1,

$$\mathrm{d}q/\mathrm{d}t=W \tag{6}$$

where W is a known function of p, T, and q.

Consider now the singular surface $\Sigma(t)$ moving into a region which is undergoing known deformations up to the time of the arrival of Σ. Denote by n_i a unit normal to Σ, pointing into the medium ahead. As in Ref. 1, we consider the case when Σ is moving with a nonzero finite speed U which leads to the relation $[q_{,i}]n_i=0$ [cf. Eq. (8c)[1]]. Equations (7-9)[1] will now be used to compute several quantities. If we differentiate Eq. (3) and the first relation in Eq. (4) w.r.t. x_i, multiply by n_i, and consider jumps across Σ, then using the first-order compatibility conditions of Thomas[9] and the relations $[q_{,i}]n_i=0$ and $[T_{,i}]n_i=0$ of Ref. 1, we obtain

$$a^2\zeta=\mu,\quad \theta=S_p\mu \tag{7}$$

where a is the isothermal speed of sound given by $a^2=(1/\sigma_p)$; $\theta=[S_{,i}]n_i$, μ, and ζ are the same as in Ref. 1; and the subscripts signify partial derivatives w.r.t. the indicated variable while holding the remaining ones in the set (p,T,q) fixed. In view of Eqs. (8a)[1], (8b)[7], and Eq. (7), it follows that $U=a$, i.e., the wave front propagates with the isothermal speed of sound.

Considering jumps across Σ in Eq. (5), and using the first-order compatibility conditions of Thomas[9] we obtain, in view

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of the above and Eq. (8b)[1],

$$[T_{,ii}] = -(TS_p\sigma^2 a^2/K)\lambda \tag{8}$$

Also, in view of Eq. (9)[1], the second-order compatibility condition of Thomas[9] yields

$$[T_{,ii}] = [T_{,ij}]_{n_i n_j} \tag{9}$$

Similarly, when we differentiate Eq. (6) w.r.t. x_j, multiply by n_j, consider jumps across Σ, and use the second-order compatibility conditon of Thomas[9] and the foregoing results, we have

$$[q_{,ij}]n_i n_j = a^{-1}[(q_{,i})_2 n_i - a\sigma W_p]\lambda \tag{10}$$

Finally, we differentiate the first relation in Eq. (4) w.r.t. x_i and x_j, multiply by $n_i n_j$, consider jumps across Σ, and use Eqs. (8-10) and the second-order compatibility condition of Thomas[9] to obtain

$$\begin{aligned}\bar{\mu} - a^2\bar{\zeta} = \lambda[&(TS_p\sigma_T\sigma^2 a^4/K) + a\sigma_q(a\sigma W_p \\ &- (q_{,i})_2 n_i) + 4\sigma a_p(p_{,i})_2 n_i - 2a^3\sigma(\sigma_{pT}(T_{,i})_2 n_i \\ &+ \sigma_{pq}(q_{,i})_2 n_i)] - 2a\sigma^2 a_p\lambda^2\end{aligned} \tag{11}$$

where $\bar{\mu} = [p_{,ij}]n_i n_j$ and $\bar{\zeta} = [\sigma_{,ij}]n_i n_j$.

Introducing the Eqs. (11)[1] and (12)[1] (which are nothing but the Eqs. (5) and (6) of Elcrat[5] in the relevant notation), following the reasoning of Elcrat,[5] and using Eq. (11) and the relation $a\zeta = \sigma\lambda$, we arrive at the desired growth equation of λ along the bicharacteristics,

$$(\mathrm{d}\lambda/\mathrm{d}t) = -\alpha\lambda + \beta\lambda^2 \tag{12}$$

where

$$\begin{aligned}\alpha = &\frac{\mathrm{d}}{\mathrm{d}t}\log\left(\frac{\sigma}{a}\right)^{1/2} + \frac{1}{2a}\left(\frac{\partial u_i}{\partial t} + u_j u_{i,j}\right)_2 n_i \\ &+ 2(u_{i,j})_2 n_i n_j - \sigma_{pT}a^3(T_{,i})_2 n_i + a(2\sigma)^{-1}(\sigma_{,i})_2 n_i - a\Omega \\ &- a(2\sigma)^{-1}(2\sigma_{pq}a^2 + \sigma_q)(q_{,i})_2 n_i + \tfrac{1}{2}a^2\sigma_q W_p \\ &+ (\sigma TS_p\sigma_T a^4/2K) + 2a_p(p_{,i})_2 n_i\end{aligned}$$

and

$$\beta = 1 + \sigma a a_p$$

Clearly α and β are, in general, functions of t. The solution of Eq. (12) is easily found to be

$$\lambda = \{\exp[-F(t)]\}\Big/\left\{\lambda_0^{-1} - \int_0^t \beta(\tau)\exp[-F(\tau)]\mathrm{d}\tau\right\} \tag{13}$$

where λ_0 is the value of λ at $t=0$, and

$$F(t) = \int_0^t \alpha(\tau)\mathrm{d}\tau$$

It remains to examine when the weak discontinuity damps out ($\lambda\to 0$), or grows into a shock wave ($|\lambda|\to\infty$). The theorems of Menon and Sharma[10] are adequate for this purpose (see also Shyam et al.[11] Menon et al.,[12] and Chen[13]). Suppose that either $\beta>0$ for all t or $\beta<0$ for all t. There cannot be a shock formation if λ_0 and β are of opposite signs. On the other hand, when $\mathrm{sgn}\lambda_0 = \mathrm{sgn}\beta$, define

$$\gamma = \left[\int_0^\infty |\beta(t)|\exp[-F(t)]\mathrm{d}t\right]^{-1}$$

If $|\lambda_0| > \gamma$, then the discontinuity grows into a shock in a finite time t_c given by the solution of

$$\int_0^{t_c} \beta(t)\exp[-F(t)]\mathrm{t}t = 1/\lambda_0$$

while if $|\lambda_0| < \gamma$, then there cannot be a shock formation; in particular, if

$$\int_0^\infty |\beta(t)|\exp[-F(t)]\mathrm{d}t = \infty$$

the discontinuity, no matter how small initially, always grows into a shock in a finite time t_c.

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