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WAVE PROPAGATION IN A QUALITATIVE MODEL OF COMBUSTION UNDER EQUILIBRIUM CONDITIONS

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Abstract. We study various aspects of wave motion within the context of the Fickett-Majda qualitative model of combustion, under the assumption that the waves are propagating into an equilibrium state of a material governed by a two-way, model chemical reaction. In particular, we examine the hydrodynamic stability of an equilibrium state and the properties of a wavefront propagating into the state. We also investigate the signalling problem and use asymptotic methods and steepest descent to determine the long time behavior of the solution. Comparisons are made to the real physical model.

1. Introduction. In this paper we examine some mathematical problems of wave propagation originating in the Fickett-Majda qualitative model of detonation. Here we focus on waves propagating into a state of dynamic chemical equilibrium where the chemistry is governed by a model two-way or reversible reaction. In particular we analyze, within the constraints of the model, the stability of an equilibrium state and we compare the results for the model to the recent results of Logan and Kapila [10] for the physical system. Second, we examine how a signal propagates into an equilibrium state along a wavefront and again make comparisons to the real physical model. Finally, we consider the signalling problem and obtain, using Laplace transforms and applying the saddle point method, the asymptotic behavior of solutions of the model equations for long times.

The detonation analog of Fickett and Majda is a simplified qualitative model for studying shock-wave chemistry interactions in combustion theory where the strongly nonlinear waves of gas dynamics and the chemical kinetics interact substantially. The model bears the analogous relationship to reacting flows as Burger's equation does to ordinary compressible fluid flow. It was developed independently by Fickett [3] and Majda [11], and several works by both authors on various aspects of the model have followed. See, for example, Fickett [4–8] and Majda [12]. In this work we shall follow the formulation of Fickett and refer the reader to Fickett [3] or Majda [11] for the motivation. The interest in this paper is the acoustic-chemical interaction rather than shockwave-chemistry interaction.

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The simplified detonation model is defined by the system of equations

$$\rho_t + p_x = 0, \tag{1.1}$$

$$\lambda_t = r(\rho, \lambda), \tag{1.2}$$

$$p = f(\rho, \lambda) \tag{1.3}$$

for $\lambda = \lambda(x, t)$ and $\rho = \rho(x, t)$. The independent variables x and t represent space and time, ρ and p represent two state variables that are characteristic of the flow, and λ represents a dimensionless chemical reaction progress variable which measures the mass fraction of the product species B in a reversible chemical reaction

$$A \leftrightharpoons B.$$

Equation (1.1) is a kinematic wave equation (see, e.g., Whitham [14] or Logan [9]) relating ρ and p, and (1.3) is a given constitutive relation, or equation of state, relating p, ρ, and λ. Throughout we assume well-behaved equations of state (1.3) satisfying $f \in C^2$ with

$$f_\rho > 0, \quad f_{\rho\rho} > 0, \quad f_\lambda > 0. \tag{1.4}$$

Equation (1.2) is interpreted as a species equation governing the evolution of the chemical reaction, and the function of state r is the chemical reaction rate.

2. Reversible kinetics and sound speeds. We consider a model fluid in one dimension undergoing a two-way chemical reaction

$$A \underset{k_f}{\overset{k_b}{\leftrightharpoons}} B,$$

where $k_f = k_f(\rho)$ and $k_b = k_b(\rho)$ are the forward and backward going rate factors, given as functions of the state variable ρ. We assume k_f and k_b are positive, differentiable functions. By the law of mass action, the reaction rate is given by

$$r(\rho, \lambda) = (1 - \lambda)k_f(\rho) - \lambda k_b(\rho). \tag{2.1}$$

Equilibrium states $(\bar{\rho}, \bar{\lambda})$ are defined by the relation $r(\bar{\rho}, \bar{\lambda}) = 0$ or, from (2.1),

$$\frac{\bar{\lambda}}{1 - \bar{\lambda}} = \frac{k_f(\bar{\rho})}{k_b(\bar{\rho})}. \tag{2.2}$$

We define the equilibrium factor ("constant") by

$$K(\bar{\rho}) \equiv \frac{k_f(\bar{\rho})}{k_b(\bar{\rho})}. \tag{2.3}$$

In the same manner as in physical chemical kinetics (e.g., see Vincenti and Kruger [13, p. 84], we postulate an analog of *van't Hoff's equation*, viz.,

$$\frac{d}{d\rho} \ln K(\rho) = -\frac{q}{\rho^2} \quad \text{at } \rho = \bar{\rho}. \tag{2.4}$$

We assume $q > 0$ so that the forward reaction is exothermic. Then it is straightforward to show, using (2.1)–(2.4), that

$$r_\lambda(\bar{\rho}, \bar{\lambda}) < 0, \qquad r_\rho(\bar{\rho}, \bar{\lambda}) < 0, \tag{2.5}$$

and

$$g'(\bar{\rho}) = -\frac{r_\rho(\bar{\rho}, \bar{\lambda})}{r_\lambda(\bar{\rho}, \bar{\lambda})}, \tag{2.6}$$

where $r(\bar{\rho}, g(\bar{\rho})) = 0$.

There are two sound speeds that play an important role in the sequel, the frozen sound speed c_f and the equilibrium sound speed c_e. In general, we define the *sound speed* $c = c(\rho, \lambda)$ by $c \equiv f_\rho(\rho, \lambda) > 0$, where f defines the equation of state (1.3). The *frozen sound speed* in the equilibrium state is then defined by

$$c_f \equiv f_\rho(\bar{\rho}, \bar{\lambda}). \tag{2.7}$$

On the other hand, the equilibrium state defines $\bar{\lambda}$ as a function of $\bar{\rho}$ through $\bar{\lambda} = g(\bar{\rho})$. Then $f(\bar{\rho}, g(\bar{\rho}))$ is a function of $\bar{\rho}$. We define the *equilibrium sound speed* c_e by

$$c_e \equiv \frac{d}{d\bar{\rho}} f(\bar{\rho}, g(\bar{\rho})). \tag{2.8}$$

If we define the *thermicity* $\sigma \equiv \sigma(\rho, \lambda)$ by

$$\sigma \equiv f_\lambda(\rho, \lambda), \tag{2.9}$$

then it follows that

$$c_e = c_f - \sigma(\bar{\rho}, \bar{\lambda})\frac{r_\rho(\bar{\rho}, \bar{\lambda})}{r_\lambda(\bar{\rho}, \bar{\lambda})}, \tag{2.10}$$

where $\bar{\lambda} = g(\bar{\rho})$ on the right side of (2.10). The proof of (2.10) follows by carrying out the chain rule differentiation on the right side of (2.8) and then using (2.6) and the definitions (2.7) and (2.9).

We remark that $c_e > 0$, $c_f > 0$, and since $\sigma r_\rho / r_\lambda > 0$, it follows that

$$c_e < c_f. \tag{2.11}$$

3. Stability of the equilibrium state. In this section we examine the hydrodynamic stability of an equilibrium state to small perturbations. We show that such perturbations decay in time, and no neutrally stable modes are present, as in the real physical model (see Logan and Kapila [10]).

Upon substitution of (1.3) into (1.1) we obtain the system

$$\rho_t + c\rho_x + \sigma\lambda_x = 0, \tag{3.1}$$

$$\lambda_t = r(\rho, \lambda), \tag{3.2}$$

where c and σ are the sound speed and thermicity, respectively. At time $t = 0$ we assume the fluid is in a state $(\bar{\rho}, \bar{\lambda})$ of chemical equilibrium, and we impose at that instant a small spatial perturbation. We inquire into the temporal and spatial evolution of that perturbation for $t > 0$. To this end, let

$$\rho = \bar{\rho} + \tilde{\rho}(x, t), \qquad \lambda = \bar{\lambda} + \tilde{\lambda}(x, t). \tag{3.3}$$

Substituting (3.3) into (3.1) and (3.2) and discarding the small nonlinear terms, while noting that $r(\rho, \lambda) = r_\rho(\bar{\rho}, \bar{\lambda})\tilde{\rho} + r_\lambda(\bar{\rho}, \bar{\lambda})\tilde{\lambda} + \cdots$ (and similarly for $\sigma(\rho, \lambda)$ and

$c(\rho, \lambda))$, we obtain the linearized equations for the perturbations:

$$\begin{aligned} \tilde{\rho}_t + c_f \tilde{\rho}_x + \sigma \tilde{\lambda}_x &= 0, \\ \tilde{\lambda}_t - r_\rho \tilde{\rho} - r_\lambda \tilde{\lambda} &= 0, \end{aligned} \tag{3.4}$$

where σ, r_ρ, and r_λ are evaluated at $(\bar{\rho}, \bar{\lambda})$. Proceeding with a normal mode analysis, we assume

$$\tilde{\rho} = R(t)e^{ikx}, \qquad \tilde{\lambda} = \Lambda(t)e^{ikx},$$

where k is a wave number. Substituting into (3.4) gives

$$\frac{d}{dt}\begin{pmatrix} R \\ \Lambda \end{pmatrix} = \begin{pmatrix} -ic_f k & -i\sigma k \\ r_\rho & r_\lambda \end{pmatrix}\begin{pmatrix} R \\ \Lambda \end{pmatrix}.$$

The eigenvalues of the coefficient matrix are determined from the characteristic equation, which in this case is

$$\xi^2 + (ic_f k - r_\lambda)\xi - ikc_e r_\lambda = 0, \tag{3.5}$$

where c_e is the equilibrium sound speed.

It is easier to study the roots of (3.5) using some elementary asymptotics rather than a direct approach. First, it is straightforward to see that (3.5) has no purely imaginary root for any wave number k.

For $k \ll 1$ we assume a regular expansion of the form

$$\xi \sim a_0 + a_1 k + a_2 k^2 + \cdots .$$

Substituting into (3.5) and collecting the $O(1)$, $O(k)$, etc. terms gives the roots

$$\begin{aligned} \xi &\sim r_\lambda + i(c_e - c_f)k + O(k^2), \\ \xi &\sim -ic_e k + \frac{c_e(c_f - c_e)}{r_\lambda}k^2 + O(k^3). \end{aligned} \tag{3.6}$$

Thus, to leading order, both roots have negative real part (see (2.5) and (2.11)) for small k.

For $k \gg 1$, Eq. (3.5) is singular. One dominant balance is clearly $ic_f k\xi \sim ikc_e r_\lambda$, which gives the root

$$\xi \sim \frac{c_e r_\lambda}{c_f} + O(k^{-1}). \tag{3.7}$$

The other dominant balance is $\xi^2 \sim -ic_f k\xi$ or $\xi \sim -ic_f k$. Therefore, assuming the expansion $\xi \sim -ic_f k + a_0 + a_1 k^{-1} + \cdots$ we substitute into (3.5) to obtain

$$\xi \sim -ic_f k + r_\lambda + O(k^{-1}). \tag{3.8}$$

Therefore, both roots (3.7) and (3.8) for large k have negative real part.

In summary, for large and small values of k the roots of (3.5) lie in the left half of the complex plane, and since by our earlier remark k cannot have a purely imaginary root, the roots cannot pass into the right half-plane as k increases from zero to infinity. Consequently, the eigenvalues of the coefficient matrix have negative real part and so both modes decay. We have proved:

THEOREM 1. An equilibrium state in the qualitative model of detonation governed by (3.1) and (3.2) is asymptotically stable.

Qualitatively, the theorem states that if an equilibrium is disturbed, then the system returns to that state in long time.

4. Wavefront expansion for the analog. It is easy to see that the system (3.1)–(3.2) is hyperbolic and so information is carried into the region of interest from boundary and/or initial data. Generally, any abrupt changes in the data along a boundary will be propagated along the characteristics that pass through those boundary points. Here we consider the problem of a signal at $t = 0$ that is propagating into an equilibrium state $\bar{\rho}$, $\bar{\lambda}$ (constant) for $x > 0$ such that the derivatives in ρ_x and λ_x suffer discontinuities at $x = 0$, but ρ and λ are continuous. A schematic spacetime diagram is shown in Fig. 1. The signal (jump discontinuities ρ_x and λ_x at $t = 0$, $x = 0$) is propagated into $x > 0$, $t > 0$ along a wavefront $x = X(t)$. We determine the wavefront and how those discontinuities propagate along it.

The argument given is analogous to that presented in Whitham [14, pp. 127–134], where the method is applied to flood waves. We let $\xi \equiv x - X(t)$ and expand ρ and λ as functions of ξ and t near the wavefront. Thus we assume $\rho = \bar{\rho}$ and $\lambda = \bar{\lambda}$ for $\xi > 0$, and

$$\rho = \bar{\rho} + \rho_1\xi + \tfrac{1}{2}\rho_2\xi^2 + \cdots ,$$
$$\lambda = \bar{\lambda} + \lambda_1\xi + \tfrac{1}{2}\lambda_2\xi^2 + \cdots , \qquad \xi < 0,$$

where the ρ_i and λ_i are functions of t and $\xi = \xi(x, t) = x - X(t)$. Then for $\xi < 0$,

$$\begin{aligned} \rho_t &= -\rho_1\dot{X} + (\dot{\rho}_1 - \rho_2\dot{X})\xi + \cdots , \\ \rho_x &= \rho_1 + \rho_2\xi + \cdots , \end{aligned} \tag{4.1}$$

and similarly for λ_t and λ_x, where the overdot denotes d/dt. Substituting these expansions into the partial differential equations (3.1) and (3.2) and collecting $O(1)$ terms gives:

$$O(1): \begin{pmatrix} c_f - \dot{X} & \sigma \\ 0 & \dot{X} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \lambda_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{4.2}$$

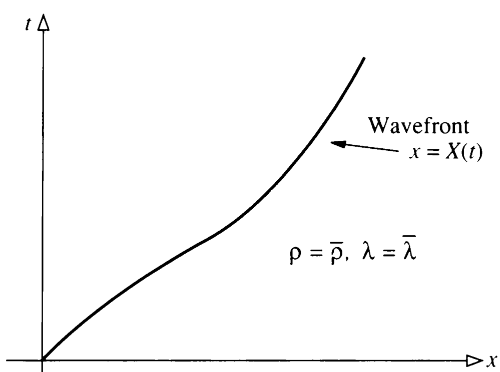

FIG. 1

This system has a nontrivial solution ρ_1, λ_1 provided the determinant of the coefficient matrix vanishes, i.e.,

$$\dot{X} = c_f \quad \text{or} \quad \dot{X} = 0. \tag{4.3}$$

We take $\dot{X} = c_f$ or $X(t) = c_f t$, which determines the wavefront. The $O(\xi)$ equations are:

$$O(\xi) : \dot{\rho}_1 + c_\rho \rho_1^2 + c_\lambda \lambda_1 \rho_1 + \sigma \lambda_2 + \sigma_\rho \rho_1 \lambda_1 + \sigma_\lambda \lambda_1^2 = 0,$$
$$\dot{\lambda}_1 - c_f \lambda_2 - r_\rho \rho_1 - r_\lambda \rho_1 = 0,$$

where c_ρ, c_λ, σ, σ_ρ, σ_λ, r_ρ, and r_λ are all evaluated at $(\bar{\rho}, \bar{\lambda})$. Adding c_f times the first equation to σ times the second gives

$$c_f \dot{\rho}_1 + \sigma \dot{\lambda}_1 + c_f c_\rho \rho_1^2 + c_f \sigma_\lambda \lambda_1^2 + c_f (c_\lambda + \sigma_\rho) \rho_1 \lambda_1 - \sigma (r_\rho \rho_1 + r_\lambda \lambda_1) = 0. \tag{4.4}$$

Now, a nontrivial solution to the $O(1)$ equations (4.2) is $\rho_1 = 1$, $\lambda_1 = 0$. Therefore all solutions to (4.2) can be represented by $\eta(t)[1, 0]^T$ for some function η. Substituting into (4.4) gives

$$\dot{\eta} + c_\rho \eta^2 - \frac{\sigma r_\rho}{c_f} \eta = 0, \tag{4.5}$$

which is a Riccati equation for η. By (1.4) we have $c_\rho > 0$, and also $\sigma r_\rho / c_f < 0$. Multiplying by η^{-2} transforms (4.5) into a linear equation whose solution is found to be

$$\eta = \frac{\eta_0 b}{(b - \eta_0) e^{at} + \eta_0}, \tag{4.6}$$

where $a \equiv -\sigma r_\rho / c_f > 0$, $b \equiv \sigma r_\rho / c_f c_\rho < 0$, and $\eta_0 = \eta(0)$.

We may interpret this solution as follows. Since $\eta = \rho_1$, it follows from (4.1) that η represents the negative jump in the derivative in ρ_x, namely

$$[\![\rho_x]\!] = \rho_x^+ - \rho_x^- = -\eta.$$

Thus $\eta > 0$ is a rarefaction wave and $\eta < 0$ is a compression wave (see Fig. 2). Equation (4.5) describes the evolution of the jump discontinuity in ρ_x along the wave front $x = c_f t$.

If $\eta_0 > 0$ then (4.6) shows that η decays as $t \to \infty$. For an initial compression wave, where $\eta_0 < 0$, there are two possibilities. If $b < \eta_0 < 0$, it follows from (4.6) that η will decay to zero as $t \to \infty$. However, if $\eta_0 < b$, then η will blow up at a finite time given by

$$t_B = a^{-1} \ln \left(\frac{\eta_0}{\eta_0 - b} \right).$$

Therefore, compression waves, if they are strong enough initially, will strengthen into shocks; weak compressions will die out, as will rarefactions.

We remark again that the results of this section have been obtained in a different manner by Fickett [4].

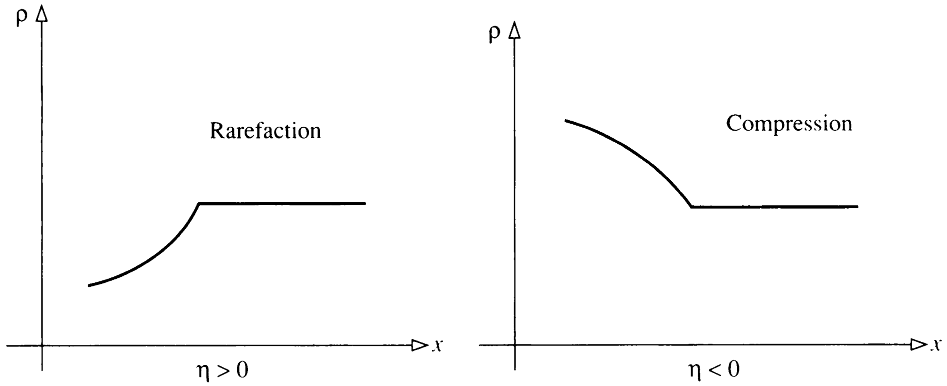

FIG. 2

5. Wavefront expansion—physical system. It is interesting to compare the results of the previous section to the results of a wavefront expansion done on the real physical model. In Eulerian coordinates, the one-dimensional governing equation for the inviscid, adiabatic flow of an ideal, reacting gas are (see, for example, Logan and Kapila [10]):

$$\frac{Dv}{Dt} - vu_x = 0, \tag{5.1}$$

$$v\frac{Du}{Dt} - RTv_x + RvT_x = 0, \tag{5.2}$$

$$\frac{DT}{Dt} + (\gamma - 1)Tu_x - \frac{q}{c_v}r(\lambda, T) = 0, \tag{5.3}$$

$$\frac{D\lambda}{Dt} = r(\lambda, T), \tag{5.4}$$

where u, v, T, and λ are the state variables (particle velocity, specific volume, temperature, and reaction progress variable), R, γ, q, and c_v are constants (gas constant, ratio of specific heats, heat of reaction, and specific heat at constant volume), and the function r is the reaction rate. Equations (5.1)–(5.3) are balance of mass, momentum, and energy, respectively, and (5.4) is the chemical species equation. The operator D/Dt denotes the material derivative $\partial/\partial t + u\partial/\partial x$.

As in Sec. 4 we consider initial jump discontinuities in u_x, v_x, T_x, and λ_x propagating into $x > 0$ along a yet unspecified wavefront $\xi(x, t) \equiv x - X(t) = 0$. Ahead of the wave we assume $u = \bar{u}$, $v = \bar{v}$, $T = \overline{T}$, $\lambda = \bar{\lambda}$, a constant equilibrium state. Near the wavefront $(\xi < 0)$ we assume

$$v = \bar{v} + v_1(t)\xi + \tfrac{1}{2}v_2(t)\xi^2 + \cdots$$

and similarly for u, T, and λ. Substituting the expansions into (5.1)–(5.4) we obtain at $O(1)$ the equations

$$O(1): \begin{pmatrix} \dot{X} & \bar{v} & 0 & 0 \\ R\overline{T} & \bar{v}\dot{X} & -R\bar{v} & 0 \\ 0 & (\gamma-1)\overline{T} & -\dot{X} & 0 \\ 0 & 0 & 0 & -\dot{X} \end{pmatrix} \begin{pmatrix} v_1 \\ u_1 \\ T_1 \\ \lambda_1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{5.5}$$

A nontrivial solution exists only if the determinant of the coefficient matrix vanishes, or

$$\dot{X}^2 = \gamma R\overline{T} \equiv c_f^2, \tag{5.6}$$

where c_f is the sound speed in the equilibrium state. Equation (5.6) is the eikonal equation which determines the wavefront

$$x = c_f t \tag{5.7}$$

propagating into $x > 0$. Thus a signal (jump discontinuity at $x = 0$, $t = 0$) propagates into the equilibrium mixture at the speed sound waves propagate in an ideal gas at temperature $\overline{T}$.

Since the coefficient matrix in (5.5) has rank 3, all solutions of (5.5) can be represented as some multiple $\eta(t)$ of any solution. In the present case, a solution of (5.5) is given by $v_1 = -\bar{v}$, $u_1 = c_f$, $T_1 = (\gamma-1)\overline{T}$, $\lambda_1 = 0$, so

$$\begin{pmatrix} v_1 \\ u_1 \\ T_1 \\ \lambda_1 \end{pmatrix} = \begin{pmatrix} -\bar{v} \\ c_f \\ (\gamma-1)\overline{T} \\ 0 \end{pmatrix} \eta(t), \tag{5.8}$$

where $\eta(t)$ is to be determined.

Now, the $O(\xi)$ equations are

$$-\dot{v}_1 + \dot{X}v_2 + \bar{v}u_2 = 0, \tag{5.9}$$

$$\bar{v}\dot{u}_1 - \bar{v}u_2\dot{X} - R\overline{T}v_2 + R\bar{v}T_2 - v_1u_1\dot{X} + \bar{v}u_1^2 = 0, \tag{5.10}$$

$$\dot{T}_1 - \dot{X}T_2 + \gamma T_1u_1 + (\gamma-1)\overline{T}u_2 - \frac{q}{c_v}r_T T_1 - \frac{q}{c_v}r_\lambda\lambda_1 = 0, \tag{5.11}$$

$$-\dot{X}\lambda_2 + u_1\lambda_1 - r_\lambda\lambda_1 - r_T T_1 = 0, \tag{5.12}$$

where r_T and r_λ are evaluated at $\bar{\lambda}$ and $\overline{T}$. The second-order perturbations v_2, u_2, T_2, λ_2 can be eliminated from these equations (generally) by multiplying by a left eigenvector of the coefficient matrix in (5.5). In the present case we may carry this out directly by multiplying (5.9) by $R\overline{T}$ and (5.10) by $\dot{X}$ and adding. The result is then added to $R\bar{v}$ times (5.11) to obtain

$$\begin{aligned} R\bar{v}\dot{T}_1 + R\bar{v}\gamma T_1u_1 - R\bar{v}\frac{q}{c_v}r_T T_1 - \frac{q}{c_v}R\bar{v}r_\lambda\lambda_1 \\ - R\overline{T}\dot{v}_1 + \dot{X}\bar{v}\dot{u}_1 - \gamma R\overline{T}v_1u_1 + \bar{v}\dot{X}u_1^2 = 0. \end{aligned} \tag{5.13}$$

Substituting (5.8) and using (5.6) gives a single Riccati equation for $\eta(t)$:

$$\dot{\eta} + \frac{\gamma+1}{2}\eta^2 - \frac{qr_T(\gamma-1)}{2\gamma c_v}\eta = 0, \tag{5.14}$$

where $r_T < 0$ (see Logan and Kapila [10] for a demonstration that $r_T < 0$).

Qualitatively, (5.14) has the same form as the analog (see (4.5)), and so the same conclusions can be drawn regarding the propagation of compression and rarefaction waves along the wavefront. The solution of (5.14) is

$$\eta(t) = \frac{2Q\eta_0}{\gamma+1} \frac{1}{(\eta_0 + \frac{2Q}{(\gamma+1)})e^{Qt} - \eta_0}, \tag{5.15}$$

where $\eta_0 = \eta(0)$ and $Q \equiv -qr_T(\gamma-1)/2\gamma c_v > 0$. As in Sec. 4, η is proportional to the derivative jumps along the wavefront.

It is interesting to note that (5.14) does not depend on r_λ, the variation of the reaction rate with λ. Therefore, if $r = r(\lambda)$ (for example, $r(\lambda) = (1-\lambda)k_f - \lambda k_b$, k_f, k_b constant), then $r_T = 0$ and (5.14) becomes

$$\dot{\eta} + \frac{\gamma+1}{2}\eta^2 = 0.$$

In this case $\eta = ((\gamma+1)t/2 + \eta_0)^{-1}$ and blow-up always occurs if $\eta_0 < 0$ (compression). If $\eta_0 > 0$ there is algebraic decay (rarefaction).

Finally, we note that blow-up occurs in (5.15) whenever $\eta_0 < 0$ and $\eta_0 < 2Q/(\gamma+1)$, i.e., if the compression wave is strong enough. In conclusion, we note that the Fickett-Majda qualitative model closely mirrors the behavior of the physical system in the present problem.

6. The signalling problem. The equations for near-equilibrium flow are given by (3.4). We may obtain a single equation for $\tilde{\rho}$ by taking $\partial/\partial t$ of the first equation in (3.4) while taking $\partial/\partial x$ of the second, and then eliminating $\tilde{\lambda}$. The result is (dropping the tilde)

$$\frac{\partial}{\partial t}(\rho_t + c_f\rho_x) - r_\lambda(\rho_t + c_e\rho_x) = 0. \tag{6.1}$$

Equation (6.1) is a linear wave equation with operators $\partial/\partial t$, $\partial/\partial t + c_f\partial/\partial x$, and $\partial/\partial t + c_e\partial/\partial x$. We may expect waves of speeds zero, c_f, and c_e to play an important role in the analysis. General equations of this type are discussed in detail in Whitham [14, Chapter 10]. A heuristic argument is given in Fickett [4, p. 63] for the behavior of solutions of (6.1). It is our intent in this section to present a careful mathematical analysis of (6.1) by studying the boundary value problem consisting of (6.1) on the domain $x > 0$, $t > 0$, and the following initial and boundary data:

$$\rho(x, 0) = 0, \quad \rho_t(x, 0) = 0, \qquad x > 0, \tag{6.2}$$

$$\rho(0, t) = f(t), \qquad t > 0. \tag{6.3}$$

We shall assume that $f(t)$ is integrable on $[0, \infty)$. Since the problem is linear, without loss of generality we may take $\rho(x, 0) = \bar{\rho} = 0$. Physically, we are thinking of a system $x > 0$ in chemical equilibrium $\rho = \bar{\rho}$ for times $t \leq 0$. At $t = 0$ a piston at $x = 0$ is given a small impulse causing ρ to take the value $f(t)$ for $t > 0$ at $x = 0$. (For an analysis of the signalling problem for the real physical system, see Chu [2] or Williams [15, pp. 121–127].)

The above boundary value problem can be solved by the Laplace transform method and the solution can be analyzed by the method of steepest descent. Let $R(x, s)$ denote the Laplace transform (on t) of $\rho(x, t)$. That is,

$$L(\rho) \equiv R(x, s) \equiv \int_0^\infty \rho(x, t)e^{-st}\, dt. \tag{6.4}$$

Using (6.2) and the properties of the Laplace transform, it easily follows that

$$L(\rho_t) = sR, \quad L(\rho_{tt}) = s^2R, \quad L(\rho_{xt}) = sR_x, \quad L(\rho_x) = R_x.$$

Therefore, upon taking the Laplace transform of (6.1) we obtain

$$(c_f s + ac_e)R_x + (s^2 + as)R = 0, \tag{6.5}$$

where $a \equiv -r_\lambda > 0$. Solving (6.5) and using (6.3) gives

$$R(x, s) = F(s)\exp\left\{\frac{-x}{c_f}\left[\frac{s^2 + as}{s + a\mu}\right]\right\}, \tag{6.6}$$

where $F(s) = L(f)$ and $\mu \equiv c_e/c_f < 1$. By the inversion theorem

$$\rho(x, t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} F(z)\exp\left(t\left\{z - \frac{x}{c_f t}\frac{z^2 + az}{z + a\mu}\right\}\right) dz, \tag{6.7}$$

where the path of integration $\operatorname{Re} z = \gamma$ lies to the right of any singularities of $F(z)$ and the essential singularity $z = -a\mu < 0$. Since $f(t)$ is integrable on $0 \le t < \infty$, there are no singularities of F in the half-plane $\operatorname{Re} z \ge 0$. Thus we may take $\gamma > 0$.

We can now prove the following theorem.

THEOREM 2. If f is integrable on $[0, \infty)$ and if $x > c_f t$, then $\rho(x, t) \equiv 0$.

The conclusion of this theorem confirms the results of Sec. 4, namely that the leading signal into the medium travels with the frozen sound speed c_f. Exactly the same result will hold for any type of applied source $f(t)$ since the exponential function in (6.7) depends only on the properties of the fluid and not on the properties of the input signal.

The proof of Theorem 2 is carried out by direct calculation. We close the contour $[\gamma - i\delta, \gamma + i\delta]$ to the right with a contour Γ_δ which may be taken to be an arc of a circle $z = R\exp(i\theta)$, $R^2 = \gamma^2 + \delta^2$, $-\theta_0 \le \theta \le \theta_0$, with $\theta_0 = \arctan(\delta/\gamma)$. By the residue theorem, the integral over the closed path is zero. It remains to show that

$$\lim_{\delta \to \infty}\int_{\Gamma_\delta} F(z)\exp\left(t\left\{z - \frac{x}{c_f t}\frac{z^2 + az}{z + a\mu}\right\}\right) dz = 0. \tag{6.8}$$

The integral may be written

$$I \equiv i\int_{-\theta_0}^{\theta_0} \mathrm{Re}^{i\theta} F(\mathrm{Re}^{i\theta})\exp\{t\operatorname{Re} h(\mathrm{Re}^{i\theta})\}\exp\{it\operatorname{Im} h(\mathrm{Re}^{i\theta})\}\, d\theta,$$

where

$$h(z) \equiv z - \frac{x}{c_f t}\frac{z^2 + az}{z + a\mu}.$$

Then

$$|I| \leq \int_{-\pi/2}^{\pi/2} R|F(\mathrm{Re}^{i\theta})| e^{t \operatorname{Re} h(\mathrm{Re}^{i\theta})} \, d\theta. \tag{6.9}$$

But

$$\operatorname{Re} h(\xi + i\eta) = \xi \left(1 - \frac{x}{c_f t}\right) - \frac{ax}{c_f t}(1 - \mu) \frac{\xi^2 + \eta^2 + a\mu\xi}{(\xi + a\mu)^2 + \eta^2}$$

and therefore

$$\begin{aligned} e^{t \operatorname{Re} h(\mathrm{Re}^{i\theta})} &= \exp\left\{ tR \left(1 - \frac{x}{c_f t}\right) \cos\theta \right\} \\ &\quad \times \exp\left\{ -\frac{ax}{c_f t}(1 - \mu) \frac{R^2 + a\mu R \cos\theta}{R^2 + a^2\mu^2 + 2a\mu R \cos\theta} \right\}. \end{aligned}$$

For large R the second exponential on the right side is bounded by unity. The first exponential has a negative argument since $x > c_f t$. Since $F(\mathrm{Re}^{i\theta}) \to 0$ as $R \to \infty$ we may apply Jordan's Lemma (see Carrier, Krook, and Pearson [1, p. 81]) to show that the right side of (6.9) tends to zero as $R \to \infty$, and so (6.8) holds. This completes the proof of Theorem 2.

When $x < c_f t$, then the contour $[\gamma - i\delta, \gamma + i\delta]$ may be closed to the left with a path Γ_δ which encloses the singularities of F and essential singular point at $-a\mu$. In this case the residues at the singular points will give a nonzero contribution to the integral in (6.7). The method of steepest descent, or saddle point method, can be applied to find the asymptotic behavior of (6.7) for large t, provided x/t is constant. Thus we have the integral

$$\rho(x, t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} F(z) e^{th(z)} \, dz, \qquad t \gg 1, \ \gamma > 0, \tag{6.10}$$

where

$$h(z) = z - \frac{x}{c_f t} \frac{z^2 + az}{z + a\mu}, \qquad a = -r_\lambda, \ \mu = c_e/c_f.$$

The saddle points are at $h'(z) = 0$ or, after some algebra,

$$z_\pm = -a\mu \pm \frac{a}{1 - m} \sqrt{m(1 - m)\mu(1 - \mu)}, \tag{6.11}$$

where we have denoted $m \equiv x/c_f t$. We note that the saddle points $z_\pm$ are both real.

The path of steepest descent passing through z_+, the saddle point with the largest real part, is $\operatorname{Im} h(z) = \operatorname{Im} h(z_+)$. If $z = \xi + i\eta$, then

$$\operatorname{Im} h(z) = \eta \left\{ 1 - m \left(1 + \frac{a^2\mu(1 - \mu)}{(\xi + a\mu)^2 + \eta^2} \right) \right\}.$$

Setting $\xi = z_+$ and $\eta = 0$, we obtain

$$\eta \left\{ 1 - m \left(1 + \frac{a^2\mu(1 - \mu)}{(\xi + a\mu)^2 + \eta^2} \right) \right\} = 0.$$

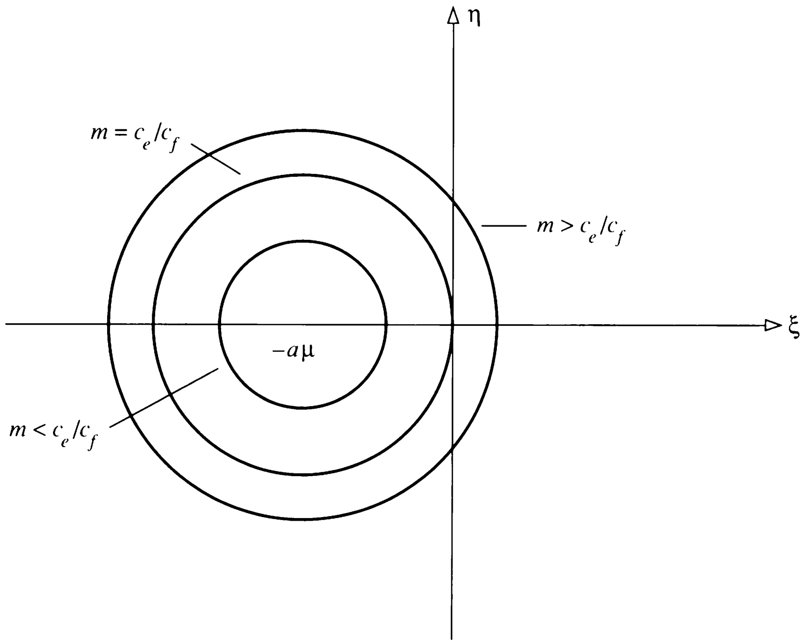

FIG. 3

Thus $\eta = 0$ or

$$(\xi + a\mu)^2 + \eta^2 = \frac{a^2\mu(1-\mu)m}{1-m}.$$

In the $\xi\eta$-plane this is a circle centered at $(-a\mu, 0)$ of radius

$$r_m \equiv \frac{a}{1-m}\sqrt{m(1-m)\mu(1-\mu)}.$$

Therefore the path of steepest descent is a circle that passes through both saddle points (compare (6.11)). We summarize the conclusions in the following remark.

REMARK. Let $m \equiv x/c_f t$. Then $0 < m < 1$ and
(i) $z_+ \to +\infty$ as $m \to 1^-$.
(ii) For $c_e/c_f < m < 1$ we have $r_m > a\mu$ and so $z^+ > 0$.
(iii) For $m = c_e/c_f$ we have $z^- = -2\mu a$, $z^+ = 0$.
(iv) For $0 < m < c_e/c_f$ we have $r_m < a\mu$ so that $z^+ < 0$.
Fig. 3 shows the paths of steepest descent for various values of m. Clearly $r_m \to 0$ as $m \to 0$.

For m close to unity, i.e., near the wavefront, the dominant contribution to (6.10) comes from a neighborhood of z_+, where z_+ is large. Therefore we can determine the asymptotic behavior for $t \gg 1$ of $\rho(x, t)$ near the wavefront by expanding the integrand in (6.10) for large z. We have

$$th(z) = tz\left(1 - \frac{x}{c_f t}\right) - \frac{ax}{c_f}(1-\mu) + tO\left(\frac{1}{z}\right) \qquad (|z| \text{ large}).$$

Therefore from (6.10)

$$\rho(x, t) \sim \frac{1}{2\pi i} e^{-ax(1-\mu)/c_f} \int_{\gamma-i\infty}^{\gamma+i\infty} F(z) e^{t(1-x/c_f t)z} \, dz,$$

where $\gamma \gg 1$. But by the shift theorem for Laplace transforms,

$$\frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} F(z) e^{(t-x/c_f)z} \, dz = f(t - x/c_f).$$

Therefore we have shown the following result.

THEOREM 3. Let f be integrable on $[0, \infty)$. Then near the wavefront $x = c_f t$ the solution ρ is given by

$$\rho(x, t) \sim f(t - x/c_f) \exp\{-ax(1-\mu)/c_f\} \quad \text{as } t \to \infty.$$

This result shows that near the wavefront the first disturbance is a travelling wave propagating with the frozen sound speed c_f. However, this disturbance is damped out exponentially and is negligible at distances on the order c_f/a, where $a \equiv -r_\lambda > 0$. As r_λ gets large, i.e., as the sensitivity of the reaction rate with the chemical progress variable increases, the disturbance near the wavefront becomes negligible for all $x > 0$.

Now we determine the behavior of $\rho(x, t)$ on the rays $x/c_f t = m < 1$. By the method of steepest descent the dominant contribution to (6.10) comes from a neighborhood of the saddle z_+, where now z_+ is finite. Expanding $h(z)$ in a neighborhood of z_+ gives

$$h(z) = h(z_+) + \tfrac{1}{2} h''(z_+)(z - z_+)^2 + \cdots.$$

Then (6.10) gives

$$\rho(x, t) \sim \frac{1}{2\pi i} e^{th(z_+)} \int_{c_m} F(z_+) e^{th''(z_+)(z-z_+)^2/2} \, dz \quad \text{as } t \to \infty,$$

where c_m is the path of steepest descent, the circle centered at $(-\mu a, 0)$ of radius r_m. The asymptotic expression above is dominated by the $\exp(th(z_+))$ factor in front of the integral; the integral itself will contribute only an algebraic factor $t^{-1/2}$ (see, for example, Carrier, Krook, and Pearson [1, pp. 257ff]). Therefore we examine the exponential term and determine where the exponent is maximum. To this end we write

$$h = h(z_+, x, t) \equiv z_+ - \frac{x}{c_f t} \frac{z_+^2 + az_+}{z_+ + a\mu}.$$

Then regarding $z_+ = z_+(x, t)$ through the relation $h_z(z_+, x, t) = 0$ which defines z_+, we set

$$\frac{\partial h}{\partial x}(z_+, x, t) = \frac{\partial h}{\partial z_+} \frac{\partial z_+}{\partial x} + \frac{\partial h}{\partial x} = 0$$

or

$$\frac{\partial h}{\partial x} = -\frac{1}{c_f t} \frac{z_+^2 + az_+}{z_+ + a\mu} = 0.$$

Hence $z_+ = 0$ or $z_+ = -a$. Clearly $z_+ = 0$ makes $h(z_+)$ maximum (zero) and so the exponential $\exp(th(z_+))$ has a maximum value of unity when $z_+(x, t) = 0$ or, from (6.11), when $m = \mu$ or $x = c_e t$. Therefore, the main disturbance travels with the equilibrium sound speed c_e; for t large, the disturbance is exponentially small except near the ray $x = c_e t$. To obtain more quantitative information we can expand $h(z)$ in the integral in (6.10) about $z_+ = 0$. This expansion is

$$th(z) = z\left(t - \frac{x}{c_e}\right) + \frac{x}{c_f}\frac{1-\mu}{a\mu^2}z^2 + O(z^3).$$

Then, to first order, again using the shift theorem for Laplace transforms,

$$\frac{1}{2\pi i}\int_{c_m} F(z)e^{z(t-x/c_e)}\,dz \sim f(t - x/c_e) \quad \text{as } t \to \infty,$$

where c_m is the circle of radius μa, centered at $(-\mu a, 0)$. We formally record the result.

THEOREM 4. Let f be integrable on $[0, \infty)$. Then near the ray $x = c_e t$ the solution ρ is given by

$$\rho(x, t) \sim f(t - x/c_e) \quad \text{as } t \to \infty.$$

In summary, acoustic signals governed by (6.1)–(6.3) propagate into the medium $x > 0$ with the leading signal travelling at the frozen sound speed c_f. Along this precursor the signal strength decays exponentially. Behind the precursor is the main body of the signal travelling at the equilibrium sound speed c_e.

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