

COMBUSTION WAVES WITH REACTANT DEPLETION

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Abstract

A simple model for the propagation of a combustion wave is proposed and the speed of propagation is predicted. It is assumed that the reactant ignites at a specified temperature and then burns until depleted with reaction rate dependent on temperature and reactant concentration. The exact solution and linear stability are determined in the case of constant heat generation and a numerical scheme is developed to generate traveling wave solutions in the more general case. This numerical method is applied to the case where the temperature dependence of the reaction rate is modeled by the Arrhenius function.

1. Introduction

Combustion waves are of both theoretical and practical interest as they represent the spread of a reaction through a material. In the combustion literature such waves are often approximated by one dimensional models in which spatial variation in only one direction is considered—see for example Williams [11] and Frank-Kamenetskii [3]. The approximation is usually justified by considering spatial averages of the temperature and reactant distribution across the burning layer. Recently Mercer and Weber [7] published a numerical study of the validity of this simplification in a simple case and found good agreement in the cases of small heat loss to the environment or large layer thickness.

Previous work provides estimates of propagation speeds for one dimensional traveling waves with heat loss to the surrounding environment ignoring the effects of reactant consumption. Gray and Kordylewski [4] discuss monostable reaction functions in which two spatially homogeneous equilibrium solutions exist, only one of which is stable. Traveling wave solutions effect a transition from the unstable to the

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stable state. These same authors in [5] analyzed the more complicated bistable case in which combustion waves can take the system from one stable state to another (in either direction) or from an unstable state to either of two stable states. More recent papers by Mercer and Weber [6] and Weber and Watt [10] extended this work to a more complete range of parameter values.

The methods used in the above analyses fail when reactant consumption is included in the model because the equilibrium points (cold unburned fuel and cold burned fuel) have the same temperature. If reactant consumption is modeled with external heat loss ignored then traveling waves can be found which effect transitions from cold (unburned) material to hot (in which the reactant has been consumed) material. Bush and Fendell [2] and Weber *et al.* [9] have determined asymptotic approximations of traveling waves in this case.

When both reactant consumption and heat loss are allowed, traveling waves of the type discussed above no longer exist. Mercer *et al.* [8] investigate the existence of pseudo-waves which propagate with slowly changing form, but eventually such waves are extinguished. In this paper we propose a modified model for the propagation of a reaction through a solid fuel (such as a forest fire). The reactant is modeled as a homogeneous combustible slab and the reaction is assumed to propagate as a plane wave. Both heat loss to the environment and reactant concentration are included in the model. A combustion wave solution propagates as heat is generated in the reaction and carried forward by diffusion to the fresh fuel.

Traveling wave solutions only exist when the fuel far ahead of the flame does not react. This is known in combustion theory as the “cold boundary difficulty” (see Williams [11]) and is circumvented by introducing an ignition temperature in the reaction rate function. We assume the reactant does not burn until a specified ignition temperature is attained, and then the reaction proceeds with general temperature dependence until the reactant is completely consumed. Special cases of constant reaction rate and Arrhenius function dependence on temperature are treated explicitly. Our treatment of the cold boundary difficulty differs slightly from the approach mentioned by Williams [11, p. 146] inasmuch as we allow the reaction to proceed even after the temperature has dropped below the ignition temperature. Physically this is reasonable if the ignition inhibiting process is changed by the fire, for example drying of fuel, or creation of catalysts.

In Section 2, we present the mathematical model and in Section 3 we describe basic properties of traveling wave solutions. Sections 4 and 5 consider existence and stability of solutions respectively for the special case of constant reaction rate. Existence of solutions for general reaction rate dependence is discussed in Section 6 while extended results and numerical calculations for the special case of the Arrhenius reaction function are presented in Section 7.

2. The model

In this section, we present a model of one-dimensional combustion wave propagation in a solid fuel (wood for example) including the effects of reactant consumption and heat loss to the environment. Writing x for the coordinate in the direction of propagation of the wave and t for time, the temperature T (as measured from ambient) and reactant (unburned wood) concentration V , are supposed to satisfy the nondimensionalized equations (see Aris [1])

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} - hT + \delta R(V, T), \quad (2.1)$$

$$\frac{\partial V}{\partial t} = -\beta \delta R(V, T). \quad (2.2)$$

Here h and β are positive constants measuring the rate of heat loss to the atmosphere and the rate at which the fire consumes wood respectively and the Frank–Kamenetskii parameter $\delta > 0$ measures the rate at which the reaction produces heat. Because the wood is stationary, (2.2) has no diffusion term, and oxygen is supposed to be replenished sufficiently rapidly that its concentration is constant. First order reaction dependence on the reactant concentration is imposed, although generalizations to p^{th} order are described where relevant.

The reaction rate $R(V, T)$ is assumed to be zero when $T < T_0$ and $V = 1$ —the temperature has not yet climbed sufficiently high to ignite the reactant and there is no heat production. Otherwise, it takes the form

$$R(V, T) = Vf(T) \quad (2.3)$$

where we assume only that f is continuously differentiable and positive. Our primary interest is however in the cases of constant f and the classical Arrhenius forcing function

$$f(T) = \exp\left(\frac{T}{1 + \epsilon T}\right), \quad T \geq 0, \quad (2.4)$$

in which the parameter ϵ is inversely related to the (typically large) activation energy of the reaction.

The goal for our analysis is to give conditions under which traveling wave solutions exist and to determine the speed c of propagation of the combustion wave as a function of the ignition temperature T_0 for various values of the Frank-Kamenetskii parameter δ , the heat loss parameter h , and the consumption rate β .

3. Traveling waves

We seek traveling wave solutions of (2.1) and (2.2) which propagate with speed $c > 0$ to the left. Substituting

$$T(x, t) = \theta(x + ct) \quad \text{and} \quad V(x, t) = v(x + ct) \quad (3.1)$$

into (2.1), (2.2) we obtain two coupled ordinary differential equations in terms of $z = x + ct$,

$$\theta'' - c\theta' - h\theta + \delta R(v, \theta) = 0, \quad (3.2)$$

$$cv' = -\beta\delta R(v, \theta), \quad (3.3)$$

where ' is d/dz . Ahead of the ignition point ($z < 0$), the wood is not burning so $v(z) = 1$ and $R = 0$. The rise in temperature in this region is due only to diffusion of heat from the approaching fire. Assuming an ignition temperature $T_0 > 0$ at which the reaction begins, we find that for $z < 0$

$$\theta'' - c\theta' - h\theta = 0, \quad \theta(0) = T_0, \quad \theta(z) \rightarrow 0 \quad \text{as } z \rightarrow -\infty. \quad (3.4)$$

The solution of this equation is found to be

$$\theta(z) = T_0 e^{m_+ z}, \quad z \leq 0, \quad (3.5)$$

with

$$m_+ = \frac{1}{2} \left(\sqrt{c^2 + 4h} + c \right). \quad (3.6)$$

We impose continuity of v , θ , θ' at the ignition point $z = 0$. This is justified by integration across an infinitesimal interval containing $z = 0$. Behind the wave ($z > 0$), the temperature θ and reactant concentration v satisfy (3.2), (3.3) subject to

$$\theta(0) = T_0, \quad \theta'(0) = m_+ T_0, \quad v(0) = 1. \quad (3.7)$$

The first two conditions ensure continuity of θ and its derivative across the interface. The third condition ensures continuity of reactant concentration. Since f is a differentiable function it follows easily that the initial value problem (3.2), (3.3), (3.7) has a unique solution (which may or may not exist for all $z > 0$).

DEFINITION. A solution θ of (3.2), (3.3), (3.7) is a *traveling wave* if $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$.

We proceed to identify conditions under which traveling waves exist by reformulating the problem in terms of θ alone. A straightforward integration of (3.3) together with the initial condition in (3.7) shows that

$$v(z) = \Phi_\theta(z) \equiv \exp\left(-\frac{\beta\delta}{c} \int_0^z f(\theta(\xi)) d\xi\right), \tag{3.8}$$

and since f is positive it follows immediately that Φ_θ is strictly decreasing and $0 \leq \Phi_\theta(z) \leq 1$ on its domain. Moreover, if θ is bounded then $\Phi_\theta(z) \rightarrow 0$ as $z \rightarrow \infty$.

REMARK. For a reaction of order $0 < p \neq 1$, (3.3) is replaced by $cv' = -\beta\delta v^p f(\theta)$ and (3.8) becomes

$$\Phi_\theta(z) = \left(1 - \frac{(1-p)\beta\delta}{c} \int_0^z f(\theta(\xi)) d\xi\right)^{1/(1-p)}. \tag{3.9}$$

This has little effect and indeed the results of the following sections remain valid as stated. Note that if $p < 1$ then Φ_θ may vanish in finite time, in which case it remains zero thereafter.

Equations (3.2), (3.3), (3.7) can be reformulated as a single initial value problem for $z > 0$ of nonlocal type

$$\theta'' - c\theta' - h\theta + \Phi_\theta f(\theta) = 0, \quad \theta(0) = T_0, \quad \theta'(0) = m_+ T_0. \tag{3.10}$$

We now proceed to consider existence and stability of solutions for the special case when $f(\theta) = 1$. Further treatment of general $f(\theta)$ appears in Section 6.

4. Constant heat generation

Suppose the forcing function f is constant, $f(\theta) = 1$. Then (3.8) reduces to

$$\Phi_\theta(z) = e^{-\alpha z} \quad \text{with} \quad \alpha = \beta\delta/c \tag{4.1}$$

and the general solution of (3.10) which decays at infinity is easily found to be

$$\theta(z) = A e^{-m_- z} + \frac{\delta}{h - c\alpha - \alpha^2} e^{-\alpha z}, \tag{4.2}$$

where

$$m_- = \frac{1}{2} \left(\sqrt{c^2 + 4h} - c\right). \tag{4.3}$$

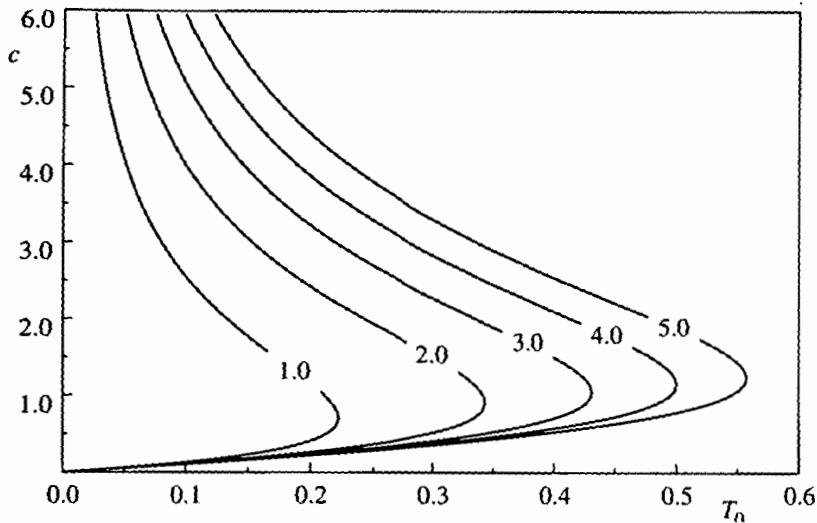


FIGURE 1. Wave speed c versus ignition temperature T_0 ($f \equiv 1$, $\beta = 0.5$, $h = 1.0$, δ shown on graph).

The initial condition $\theta(0) = T_0$ determines A which gives

$$\theta(z) = \left(T_0 - \frac{\delta}{h - c\alpha - \alpha^2} \right) e^{-m_-z} + \frac{\delta}{h - c\alpha - \alpha^2} e^{-\alpha z}, \quad z \geq 0, \quad (4.4)$$

and to satisfy the second initial condition $\theta'(0) = m_+ T_0$ requires

$$T_0 = \frac{\delta}{\sqrt{c^2 + 4h}} \frac{m_- - \alpha}{h - c\alpha - \alpha^2} = \frac{2\delta c}{\sqrt{c^2 + 4h} (c\sqrt{c^2 + 4h} + c^2 + 2\beta\delta)}. \quad (4.5)$$

REMARK. In the resonant case $m_- = \alpha$ the above exponentials are equal and the solution θ contains a factor linear in z but is unchanged in character. In this case it is straightforward to verify that also $h - c\alpha - \alpha^2 = 0$ and the final expression in (4.5) shows that the singularity is removable. Thus (4.5) defines T_0 as a smooth function of c .

For large and small c it follows immediately from (4.5) that

$$T_0 \sim c/2\beta\sqrt{h} \quad \text{as } c \rightarrow 0^+, \quad (4.6)$$

and

$$T_0 \sim \delta/c^2 \quad \text{as } c \rightarrow \infty. \quad (4.7)$$

Figure 1 shows graphs of (4.5) for various values of δ .

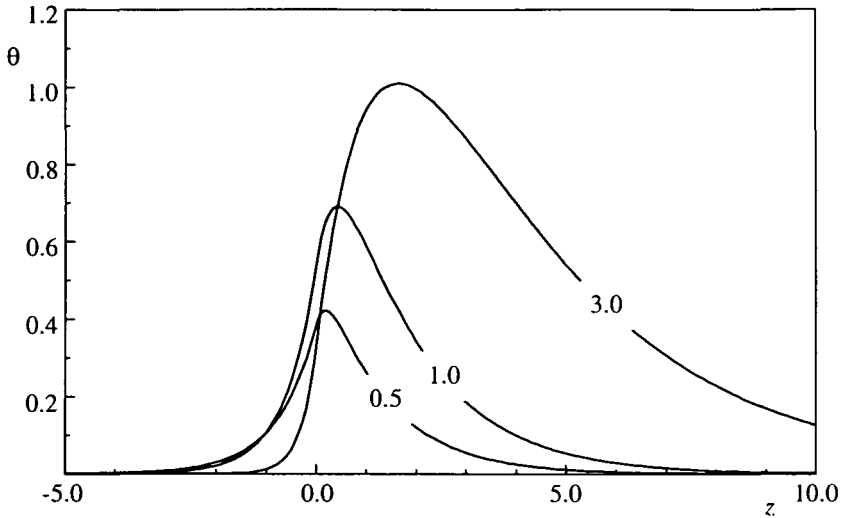


FIGURE 2. Temperature profile for traveling waves ($f \equiv 1, \beta = 0.5, h = 1.0, \delta = 5.0, c$ shown on graph).

There exists a *critical value* of the ignition temperature $T_{0,cr}$ with the property that there are two traveling waves (of differing speeds) for $T_0 < T_{0,cr}$ and none for $T_0 > T_{0,cr}$. With $\delta = 5.0$ and for each of the values $c = 0.5, 1.0,$ and $3.0,$ (4.5) gives the corresponding values of T_0 as $0.386, 0.543, 0.335.$ This gives all the information required to plot the corresponding traveling waves in Figure 2. The label on the curves indicates the speed of propagation of the wave.

A formula can be derived for the wave speed c corresponding to the critical ignition temperature T_0 . To obtain this relation, we treat T_0 as a function of c in (4.5) and differentiate logarithmically to obtain

$$\frac{T'_0}{T_0} = 2 \frac{4\beta\delta h - c^3\sqrt{c^2 + 4h} - c^4 - 2c^2h}{c(c^2 + 4h)(c\sqrt{c^2 + 4h} + c^2 + 2\beta\delta)}. \tag{4.8}$$

The left-hand side is zero at the turning point of the solution curve so setting the right-hand side to zero yields an expression for c at the critical point. Implicitly we have

$$4\beta\delta h = c^3\sqrt{c^2 + 4h} + c^4 + 2c^2h. \tag{4.9}$$

Since the right-hand side of this equation increases monotonically with c it is clear that the critical initial temperature is unique.

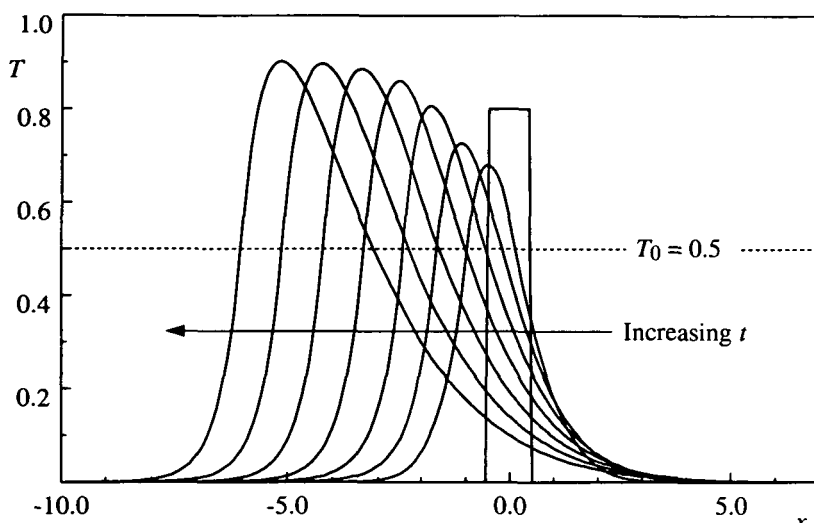


FIGURE 3. Stable wave temperature profiles: $t = 0, 0.5, 1.0, \dots$ ($f \equiv 1, \beta = 0.5, h = 1.0, \delta = 5.0, c = 1.88$).

5. Stability of the traveling wave

For a given ignition temperature, Figure 1 shows that there are two traveling waves of different speeds, one slow and one fast. This raises the question of stability of these waves, that is, for suitable initial conditions does the solution of (2.1), (2.2) tend to the traveling wave solution or does it die out (or do something else) as time increases? Linear stability analysis shows that the upper branch is stable and the lower unstable, and this is borne out by numerical experiments. Figures 3 and 4 show the evolution of the solution of (2.1), (2.2) for the two values $c = 0.785$ and 1.88 , one below and the other above the critical value of 1.24 (obtained by using a simple explicit forward difference formula to solve (2.1), (2.2) with $f = 1, \Delta x = 0.1$ and $\Delta t = \Delta x^2/6$). Both correspond to an ignition temperature of $T_0 = 0.5 < T_{0,cr} = 0.557$. In the first diagram a square wave initial temperature (initial reactant concentration is 1 for $x < 0, 0$ for $x > 0$) tends quickly to the traveling wave, while in the second an initial condition very close to the traveling wave solution (in both temperature and reactant) is quickly extinguished.

For linear stability, we consider the time dependent problem in the moving coordinate and perturb the steady solution found above, linearizing in the perturbations. There are two methods for perturbing the ignition point of the solution. We can either (1) allow the moving coordinate to vary in such a way that the ignition point always occurs at $z = 0$, or (2) we can hold the moving coordinate system at a fixed speed

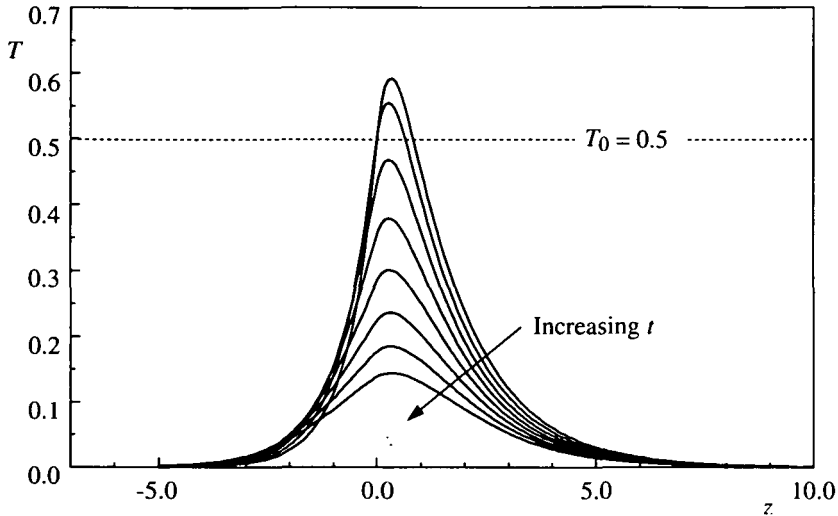


FIGURE 4. Unstable wave temperature profiles: $t = 0, 0.2, 0.4, \dots$ ($f \equiv 1, \beta = 0.5, h = 1.0, \delta = 5.0, c = 0.785$).

and allow the ignition point to be perturbed from zero. Both methods arrive at the same dispersion relation for the growth rate of the perturbations. Here we present the second method. The time dependent problem for $f(T) = 1$ can be written

$$\frac{\partial T}{\partial t} + hT + c \frac{\partial T}{\partial z} - \frac{\partial^2 T}{\partial z^2} = \begin{cases} 0 & z < Z, \\ \delta V & z > Z, \end{cases} \tag{5.1}$$

$$\frac{\partial V}{\partial t} + c \frac{\partial V}{\partial z} = \begin{cases} 0 & z < Z, \\ -\beta \delta V & z > Z, \end{cases} \tag{5.2}$$

$$[T]_{z=Z} = 0, \quad [T']_{z=Z} = 0, \quad [V]_{z=Z} = 0, \tag{5.3}$$

where $z = Z$ is the ignition point where $T = T_0$ and $[]_{z=Z}$ denotes the jump of the contained quantity at the point $z = Z$. Note that $Z = 0$ for the steady traveling wave solution.

Perturbing the variables T, V and Z as follows:

$$T(z, t) = \theta(z) + \epsilon \tau(z) e^{\mu t}, \quad V(z, t) = v(z) + \epsilon \nu(z) e^{\mu t}, \quad Z = 0 + \epsilon \zeta e^{\mu t}, \tag{5.4}$$

we obtain, by linearizing in ϵ , equations for τ, ν, ζ and the growth rate μ ,

$$(h + \mu)\tau + c\tau' - \tau'' = \begin{cases} 0 & z < 0, \\ \delta\nu & z > 0, \end{cases} \tag{5.5}$$

$$(\mu + \delta\beta)v + cv' = 0, \tag{5.6}$$

$$[\tau] = 0, \quad [v] = -\zeta[v'] = \zeta\delta\beta/c, \tag{5.7}$$

$$[\tau'] = -\zeta[\theta''] = \zeta \left\{ (m_+^2 - m_-^2) T_0 + \frac{\delta}{h - c\alpha - \alpha^2} (m_-^2 - \alpha^2) \right\}. \tag{5.8}$$

Here [] denotes the jump of the contained quantity at $z = 0$. In addition, the definition of Z gives the relation $\tau(0) + \zeta\theta'(0) = 0$ or

$$\tau(0^-) = -\zeta m_+ T_0. \tag{5.9}$$

The solutions τ and v after forcing boundedness as $z \rightarrow \pm\infty$ are

$$v = \begin{cases} 0 & z < 0, \\ B e^{-(\alpha+\mu/c)z} & z > 0, \end{cases} \tag{5.10}$$

$$\tau = \begin{cases} A e^{r_+z} & z < 0, \\ C e^{-r_-z} + \frac{\delta B e^{-(\alpha+\mu/c)z}}{h - c\alpha - \alpha^2 - 2\alpha\mu/c - \mu^2/c^2} & z > 0, \end{cases} \tag{5.11}$$

where

$$r_{\pm} = \frac{1}{2} \left(\sqrt{c^2 + 4h + 4\mu \pm c} \right). \tag{5.12}$$

The constants A, B, C, ζ and μ are to be determined by the conditions (5.7), (5.8), (5.9). Using (5.7) and (5.9) we can write A, B and C in terms of ζ :

$$A = -\zeta m_+ T_0, \tag{5.13}$$

$$B = \zeta\alpha, \tag{5.14}$$

$$C = -\zeta \left\{ m_+ T_0 + \frac{\delta\alpha}{\bar{\alpha} - 2\alpha\mu/c - \mu^2/c^2} \right\}, \tag{5.15}$$

where $\bar{\alpha} = h - c\alpha - \alpha^2$. Using these we can eliminate A, B and C from (5.8) and obtain

$$\zeta \left[\frac{\delta\alpha \left(\alpha + \frac{\mu}{c} - r_- \right)}{\left(\bar{\alpha} - 2\frac{\alpha\mu}{c} - \frac{\mu^2}{c^2} \right)} + \left(T_0 (m_+^2 - m_-^2 - r_- m_+ - r_+ m_+) + \frac{\delta}{\bar{\alpha}} (m_-^2 - \alpha^2) \right) \right] = 0. \tag{5.16}$$

Nontrivial solutions ($\zeta \neq 0$) exist only if the square brackets are zero. This solvability condition gives the dispersion relation between the growth rate μ and the parameters of the problem.

We simplify the dispersion relation by substituting for T_0 using (4.5) rewritten here as

$$\frac{T_0}{\delta} = \frac{m_- - \alpha}{(m_- + m_+) \bar{\alpha}}. \tag{5.17}$$

Dividing (5.16) by $\zeta \delta$, using (5.17) and noting that $(m_+ + \alpha)(m_- - \alpha) = \bar{\alpha}$, we obtain the dispersion relation

$$\frac{m_+(\alpha - m_-)(r_+ + r_-)}{(m_+ + m_-)\bar{\alpha}} + 1 + \frac{\alpha(\alpha + \frac{\mu}{c} - r_-)}{(\bar{\alpha} - 2\frac{\alpha\mu}{c} - \frac{\mu^2}{c^2})} = 0. \tag{5.18}$$

Eliminating m_{\pm} and r_{\pm} , writing the square roots as $d_1 = \sqrt{c^2 + 4h + 4\mu}$ and $d = \sqrt{c^2 + 4h}$ and forming a common denominator yields

$$\frac{\{(c + d)(c - d + 2\alpha)d_1 + 4d\bar{\alpha}\}(\bar{\alpha} - 2\frac{\alpha\mu}{c} - \frac{\mu^2}{c^2}) + 4d\bar{\alpha}\alpha(\alpha + \frac{\mu}{c} + \frac{c-d_1}{2})}{4d\bar{\alpha}(\bar{\alpha} - 2\frac{\alpha\mu}{c} - \frac{\mu^2}{c^2})} = 0. \tag{5.19}$$

Traveling wave solutions are invariant to translations. This symmetry implies that there will always be perturbation solutions corresponding to zero growth rate. (Here the solution is $\tau = 0, \nu = 0, \zeta = 1, \mu = 0$.) We do not wish to consider those perturbations when discussing stability so we factor μ from the dispersion relation. Setting the numerator to zero and collecting terms with μ we obtain

$$\bar{\alpha}(d - d_1)(4h - 2\alpha c) = \bar{\alpha}\mu \left\{ \frac{4d\alpha}{c} + \frac{4d\mu}{c^2} + d_1(-4h + 2\alpha(c + d)) \left(\frac{2\alpha}{c\bar{\alpha}} + \frac{\mu}{c^2\bar{\alpha}} \right) \right\}. \tag{5.20}$$

Multiplying both sides by $d^2 + dd_1$, dividing by μ and retaining the denominator from (5.19) yields

$$\frac{4h - 2\alpha c + (d^2 + dd_1) \left\{ \frac{\alpha}{c} + \frac{\mu}{c^2} + \frac{d_1}{d\bar{\alpha}} \left(-h + \frac{\alpha}{2}(c + d) \right) \left(\frac{2\alpha}{c} + \frac{\mu}{c^2} \right) \right\}}{\bar{\alpha} - 2\frac{\alpha\mu}{c} - \frac{\mu^2}{c^2}} = 0. \tag{5.21}$$

Equation (5.21) is the dispersion relation we study to investigate the stability of the traveling wave solutions. To facilitate the exposition, we identify parameter groups which simplify the relation. Introducing the quantities

$$\begin{aligned} \Omega &= \mu/c^2; & H &= h/c^2; & \gamma &= \alpha/c = \beta\delta/c^2; & D &= d/c; \\ D_1 &= d_1/c; & \bar{\gamma} &= H - \gamma - \gamma^2 = \bar{\alpha}/c^2; \end{aligned} \tag{5.22}$$

the relation (5.21) becomes

$$\frac{4H - 2\gamma + (D^2 + DD_1) \left\{ \gamma + \Omega + \frac{D_1}{D\bar{\gamma}} \left(\frac{\gamma(1+D)}{2} - H \right) (2\gamma + \Omega) \right\}}{\bar{\gamma} - 2\gamma\Omega - \Omega^2} = 0. \tag{5.23}$$

The stability result of primary interest is that the turning point of the solution curve in Figure 1 is a stability boundary with stable solutions for larger values of c and unstable solutions for lower values of c .

To show this, we use (4.9) for the turning point of the curve and show that solutions of this equation satisfy the dispersion relation with $\Omega = 0$. Rewriting (4.9) in the scaled variables and using the fact that $4H = (D + 1)(D - 1)$, we have

$$\gamma = \frac{D + 1 + 2H}{4H} = \frac{D + 1}{2(D - 1)}. \tag{5.24}$$

Setting $\Omega = 0$ and thus $D_1 = D$ in (5.23) yields

$$\frac{4H(1 + 2\gamma)(\gamma^2 + \gamma - H) + 4\gamma D^2 \left(H - \frac{\gamma}{2}(1 + D) \right)}{(H - \gamma - \gamma^2)^2} = 0, \tag{5.25}$$

which can be rewritten by factoring the top and bottom and writing H in terms of D as $4H = (D + 1)(D - 1)$,

$$\frac{2(D + 1)(D - 1) \left(\gamma - \frac{D-1}{2} \right)^2 \left(\gamma - \frac{D+1}{2(D-1)} \right)}{\left(\gamma - \frac{D-1}{2} \right)^2 \left(\gamma + \frac{1+D}{2} \right)^2} = 0. \tag{5.26}$$

The common factor $\gamma - (D - 1)/2$ in numerator and denominator corresponds to the resonant case in (5.5) where $\bar{\alpha} = 0$, and does not affect stability. The only other factor that can be zero for positive parameter values is the last which is zero precisely at the turning point given by (5.24). We have shown that the turning point is a stability boundary. By solving the dispersion relation numerically on either side of this point, we show that low values of c correspond to unstable solutions.

As a result of the linear stability analysis, we conclude that for given values of the parameters there is a minimum propagation speed of the traveling wave which occurs at the maximum possible ignition temperature $T_{0,cr}$. As this ignition temperature falls (due to drying of the wood for example) the propagation speed increases. Figure 5 shows the critical speed and ignition temperatures as a function of the Frank–Kamenetskii parameter δ .

6. Existence of traveling waves—the general case

We return to the case of general f . Suppose henceforth that θ solves (3.10). We begin with the main result of this section.

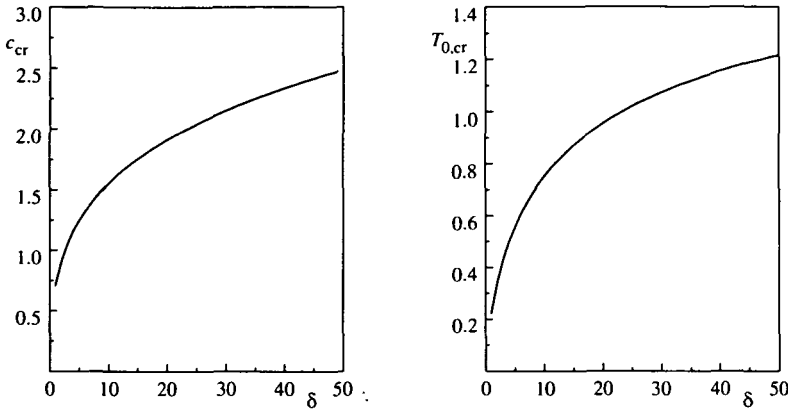


FIGURE 5. Critical c and T_0 values versus δ ($f \equiv 1, \beta = 0.5, h = 1.0$).

THEOREM 1. *Suppose θ is bounded. Then $0 < \theta(z) < 1/\beta$ for all z and $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$, that is, θ is a traveling wave.*

PROOF. First, suppose $\theta \leq 0$ somewhere and let $z_0 \geq 0$ be the first point at which this happens. Then $\theta'(z) < 0$ for all $z \geq z_0$ for if θ' were to vanish then at this point $\theta'' \geq 0$ and the left side of (3.10) would be positive. Rearranging (3.10) as

$$(\theta' - c\theta)' = h\theta - \delta\Phi_\theta f(\theta) \tag{6.1}$$

it becomes clear that the right side of this is negative for $z > z_0$ and therefore $\theta' - c\theta$ is decreasing there. Since θ is decreasing, it follows that θ' is also, and hence $\theta(z) \rightarrow -\infty$ as $z \rightarrow \infty$, contradicting boundedness of θ . It follows that $\theta(z) > 0$.

Now consider the case $\theta > 0$. If θ is not eventually monotone then it must have a sequence $z_n \rightarrow \infty$ as $n \rightarrow \infty$ of maximum points. At each of these points $\theta' = 0$ and $\theta'' \leq 0$ so using (3.10) and the remark following (3.8) $0 < h\theta(z_n) \leq \delta\Phi_\theta(z_n)f(\theta(z_n)) \rightarrow 0$ as $z \rightarrow \infty$ so that $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$. On the other hand if θ is eventually monotone and $\theta(z) \rightarrow L > 0$ then again from (3.10) it follows that $\theta''(z) - c\theta'(z) > hL/2$ for all $z > \text{some } z_1$. Integrating this inequality over (z_1, z) shows that $\theta'(z) \rightarrow \infty$ as $z \rightarrow \infty$ and this contradicts the boundedness assumption. Hence $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$.

There remains only to establish the bound $\theta(z) < 1/\beta$. Since $\theta'(0) > 0$ and we now know $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$, θ must have a maximum point at some $z_m > 0$. Dividing (3.3) by β and adding to (3.2) gives $\frac{d}{dz}(\theta' - c\theta - cv/\beta) = h\theta$. Integrating gives

$$\theta'(z) - c\theta(z) - \frac{c}{\beta}v(z) = (m_+ - c)T_0 - \frac{c}{\beta} + h \int_0^z \theta(z) dz \tag{6.2}$$

and at z_m this reduces to

$$\theta(z_m) = \frac{1}{\beta} - \left[\frac{1}{\beta} v(z_m) + \frac{m_-}{c} T_0 + \frac{h}{c} \int_0^{z_m} \theta(z) dz \right]. \tag{6.3}$$

Since the quantity in square brackets is positive, the result follows and the proof is completed.

REMARK. No traveling wave can exist if the ignition temperature $T_0 \geq 1/\beta$. Physically this means that high temperatures can be attained only if the reactant is not consumed too fast.

COROLLARY. For fixed values of all the other parameters there exists a value of $T_0 \in (0, 1/\beta)$ for which θ is a traveling wave.

PROOF. This follows from the continuous dependence of the solution of (3.2), (3.3), (3.7) on the initial values, the fact that the solutions corresponding to $T_0 \leq 0$ or $T_0 \geq 1/\beta$ tend respectively to $-\infty$ or $+\infty$, and the result of the theorem that θ need only be bounded to be a traveling wave.

REMARK. It would be nice to show that this value of T_0 is uniquely defined. This is certainly the case in the previous section and all the numerical experiments performed on the system (3.2), (3.3), (3.7) support this conclusion, but a proof seems elusive. We do however have the following special case.

THEOREM 2. If $0 \leq f'(\theta) \leq h/\delta$ for $0 < \theta < 1/\beta$ then a traveling wave exists for only one value of T_0 .

PROOF. Suppose to the contrary that θ_1 and θ_2 are traveling wave solutions of (3.10) with different initial temperatures but the same values of the remaining parameters. We may assume $\theta_1(0) < \theta_2(0)$ and it follows from (3.10) that also $\theta_1'(0) < \theta_2'(0)$. Since both $\theta_1(z)$ and $\theta_2(z) \rightarrow 0$ as $z \rightarrow \infty$ it follows that $\theta_2 - \theta_1$ has a positive maximum point. Let $z_m > 0$ be the first such point. Since $\theta_1(z) < \theta_2(z)$ for $0 \leq z \leq z_m$, (3.8) shows that $\Phi_{\theta_1}(z) > \Phi_{\theta_2}(z)$ on this same interval. Now use (3.10) with θ_1 and θ_2 and subtract to obtain

$$\begin{aligned} (\theta_2 - \theta_1)'' - c(\theta_2 - \theta_1)' - h(\theta_2 - \theta_1) \\ + \delta\Phi_{\theta_2}(f(\theta_2) - f(\theta_1)) + \delta f(\theta_1)(\Phi_{\theta_2} - \Phi_{\theta_1}) = 0. \end{aligned} \tag{6.4}$$

At z_m the first term here is not positive, the second vanishes and the last is negative. It follows that

$$h(\theta_2 - \theta_1) < \delta\Phi_{\theta_2}(f(\theta_2) - f(\theta_1)) < \delta(f(\theta_2) - f(\theta_1)), \tag{6.5}$$

the last inequality following from $0 \leq \Phi_{\theta_2} < 1$ and the monotonicity of f . Therefore

$$\frac{f(\theta_2) - f(\theta_1)}{\theta_2 - \theta_1} > \frac{h}{\delta} \tag{6.6}$$

and the mean value theorem then contradicts the assumption $f'(\theta) \leq h/\delta$.

REMARK. In the case of constant f the conditions of Theorem 2 are clearly satisfied and the conclusion is supported by the previous section. For the Arrhenius function, $f'(\theta) = (1/(1 + \epsilon\theta)^2) \exp(\theta/(1 + \epsilon\theta)) < e^{1/\epsilon}$ for $\theta \geq 0$ so uniqueness of traveling waves is guaranteed for $e^{1/\epsilon} < h/\delta$.

7. Numerical experiments

In the case of general f the analytic solution of (3.10) is no longer obtainable and a numerical approach must be found. For fixed values of δ , β and h (and ϵ in the case of the Arrhenius function) the value of the ignition temperature T_0 of the traveling wave for given c can be determined by solving (3.2), (3.3), (3.7) using a numerical scheme for initial value problems and shooting for the limiting condition $\theta(z) \rightarrow 0$ as $z \rightarrow \infty$. As soon as the solution leaves the interval $0 < \theta < 1/\beta$ the shooting variable T_0 can be updated and the required value found by bisection. In this way Figure 6 was computed for several values of δ using the standard fourth-order Runge-Kutta algorithm with a step length of 5×10^{-3} .

As in Section 4 it appears that traveling waves corresponding to low ignition temperature must travel very slowly or very fast. This is proved in general as follows.

THEOREM 3. $T_0 \rightarrow 0$ as $c \rightarrow 0^+$ or $c \rightarrow \infty$.

PROOF. Write (6.3) in the form

$$\frac{1}{\beta} - \left(\frac{m_+}{c} - 1\right) T_0 = \theta(z_m) + \frac{1}{\beta} v(z_m) + \frac{h}{c} \int_0^{z_m} \theta(z) dz > 0 \tag{7.1}$$

$$\Rightarrow T_0 < \frac{c}{\beta m_-} \rightarrow 0 \text{ as } c \rightarrow 0^+. \tag{7.2}$$

For the second result, let $\delta f(\theta) - h\theta \leq K$ for $0 < \theta < 1/\beta$. Clearly $K > 0$ depends only on h , δ and f and not on either c or T_0 . From (3.2),

$$\frac{d}{dz} (\theta' - c\theta) \geq -K \tag{7.3}$$

and integrating gives $\theta'(z) - c\theta \geq (m_+ - c)T_0 - Kz$. Rewrite this as

$$\frac{d}{dz} (e^{-cz}\theta(z)) \geq ((m_+ - c)T_0 - Kz) e^{-cz} \tag{7.4}$$

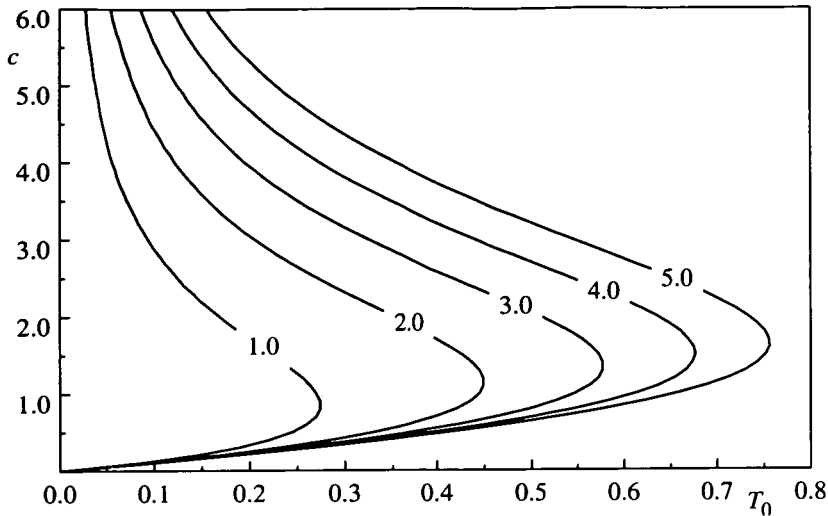


FIGURE 6. Wave speed c versus ignition temperature T_0 ($\epsilon = 0.3$, $\beta = 0.5$, $h = 1.0$, δ shown on graph).

and integrate again, this time over all $z > 0$, to obtain

$$-T_0 \geq \frac{1}{c} (m_+ - c) T_0 - \frac{K}{c^2} \Leftrightarrow T_0 \leq \frac{K}{cm_+} \quad (7.5)$$

and the second result is proved.

REMARK. The expression occurring in (7.5) has the same asymptotics as (4.5) using $K = \delta$. For (7.2) this is not true because of the crude inequality $\int_0^{z_m} \theta dz > 0$ (in fact it differs by a factor of 2).

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