ANZIAM J. 46(2004), 1–16

NON-ADIABATIC COMBUSTION WAVES FOR GENERAL LEWIS NUMBERS: WAVE SPEED AND EXTINCTION CONDITIONS

A. C. MCINTOSH[1], R. O. WEBER[2] and G. N. MERCER[2]

(Received 14 August, 2002)

Abstract

This paper addresses the effect of general Lewis number and heat losses on the calculation of combustion wave speeds using an asymptotic technique based on the ratio of activation energy to heat release being considered large. As heat loss is increased twin flame speeds emerge (as in the classical large activation energy analysis) with an extinction heat loss. Formulae for the non-adiabatic wave speed and extinction heat loss are found which apply over a wider range of activation energies (because of the nature of the asymptotics) and these are explored for moderate and large Lewis number cases—the latter representing the combustion wave progress in a solid. Some of the oscillatory instabilities are investigated numerically for the case of a reactive solid.

1. Introduction

Earlier work [8, 12] has explored the classical combustion wave (premixed flame propagation) problem using a different grouping of parameters to that used in the past. In particular, instead of using asymptotic analysis based on activation energy being large, the same equations have been recast in terms of the ratio of activation energy to heat release. This theory is distinct from the traditional large activation energy approach, since there is no one to one mapping between the two approaches. Nevertheless there is a good correspondence between the two theories, and arguably the new approach has the distinct advantage of still being valid for quite low activation energies (see [12, Figure 3]).

The present approach has more readily shown the bifurcation behaviour that can occur at moderate values of the ratio (β) of activation energy to heat release. Such instabilities have been well known in the work of Bayliss and co-authors [2, 5]. The

[1]Fuel and Energy Department, University of Leeds, Leeds, LS2 9JT, U.K.
[2]School of Mathematics and Statistics, University College of New South Wales, ADFA, Canberra, ACT 2600, Australia; e-mail: row@adfa.edu.au.

later work of Metcalf *et al.* [10] and Balmforth *et al.* [1] has also shown that this is a general phenomenon that can occur at general Lewis numbers and with different reaction terms. For Arrhenius kinetics with infinite Lewis number (that is, solid fuels) there are indications (known experimentally [11] and confirmed numerically [4, 6] that there is a possible period-doubling route to chaos. The paper by Weber *et al.* [12] was able to confirm this with an accurate value determined for the minimum wave speed.

It is known from classical large activation energy analysis that heat losses have a great effect on the stability of combustion fronts, and with the new scheme for the grouping of the parameters, Mercer *et al.* [9] have shown numerically that oscillatory instabilities occur for non-adiabatic systems with again a period-doubling route to chaos. This present paper concentrates on the influence of global heat loss on the propagation speeds of combustion fronts for general Lewis numbers. In particular we derive modified analytical expressions for the wave speed using *large β asymptotic analysis* (rather than large activation energy asymptotics). As mentioned earlier, β is the ratio of activation energy to heat release.

There is a wide range of reaction possibilities. Normally for the common hydrocarbon reactions the heat release is large but generally the activation energy is larger still, so that β is then large. Only if the activation energy is low with high heat release, would the analysis here not be valid, and this is not usually found in practice. The remaining case of low heat release with moderate activation energy is feasible since then the wave propagates with a thicker reaction region (since the activation temperature is low) but with a low temperature rise. Though the kinetics can certainly not be described accurately by one-step chemistry as used here, qualitatively an example of low heat release with moderate activation energy is the 'cool flames' phenomena ([7, pp. 200–204]). Thus there can be practical cases of burning where heat release is small and activation energy is not great, and consequently this theory has the advantage of being able to widen the applicability of asymptotic analysis to similar cases in gases and solids where a relatively low activation energy value pertains.

Using this approach, extinction values of heat loss for these fronts are derived and we further show some numerical results concerning the solid fuel oscillatory instability.

2. Mathematical model

The derivation of the governing equations is well known from earlier papers (see, in particular, [12]). For the case of global heat loss, the non-dimensional forms of the differential equations are

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} + ye^{-1/u} - \ell(u - u_a) = 0, \tag{2.1}$$

https://doi.org/10.1017/S1446181100013638 Published online by Cambridge University Press

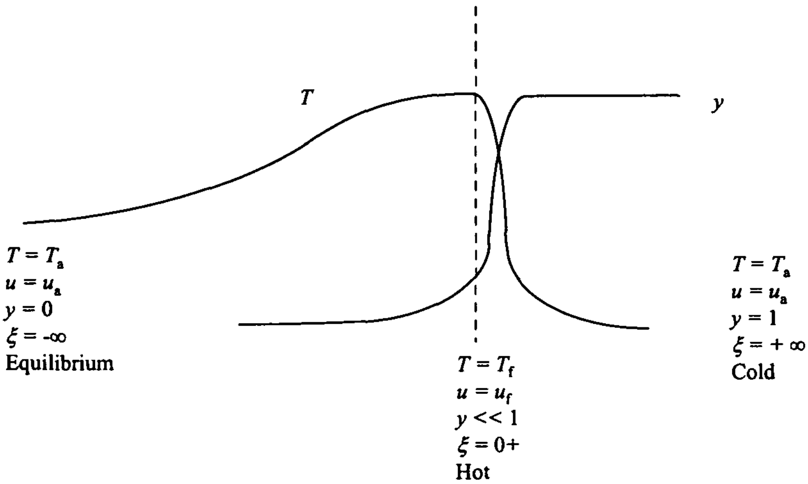

FIGURE 1. Schematic of combustion wave with heat loss.

$$\frac{1}{L}\frac{d^2y}{d\xi^2} + \frac{dy}{d\xi} - \beta y e^{-1/u} = 0, \tag{2.2}$$

where it should be recognised that $\xi = x - ct$ is a coordinate following the combustion wave travelling with speed c and time t is non-dimensionalised with respect to a characteristic time $t_0 \equiv c_p(E/R)/QA$, with distance x non-dimensionalised with respect to a characteristic length $d_0 \equiv \sqrt{(k/\rho)(E/R)/QA}$. The parameter groupings are as follows: Lewis number $L \equiv k/(\rho D c_p)$, heat loss $\ell \equiv hSE/(V\rho QAR)$, ratio of activation energy to heat release $\beta \equiv Ec_p/RQ$, temperature $u \equiv RT/E$, where $k/\rho c_p$ is thermal thermal diffusivity ($\mathrm{m^2s^{-1}}$) (k, ρ and c_p are thermal conductivity ($\mathrm{W\,m^{-1}K^{-1}}$), density ($\mathrm{kg\,m^{-3}}$) and specific heat ($\mathrm{J\,kg^{-1}K^{-1}}$) respectively), h is an overall heat transfer coefficient ($\mathrm{W\,m^{-2}K^{-1}}$), S is surface area ($\mathrm{m^2}$), V is volume ($\mathrm{m^3}$), E is activation energy ($\mathrm{J\,mol^{-1}}$), Q is the heat of reaction ($\mathrm{J\,kg^{-1}}$), A is the pre-exponential reaction constant ($\mathrm{s^{-1}}$) and R is the Universal gas constant ($8.314\,\mathrm{J\,mol^{-1}K^{-1}}$). In these equations y represents the mass fraction of fuel and the temperature T (K) is non-dimensionalised with respect to the activation temperature E/R, rather than the ambient temperature.

A schematic of the propagating combustion wave is given in Figure 1. As indicated in Figure 1, the boundary conditions are

$$\xi = +\infty: \quad u = u_a, \; y = 1, \tag{2.3a}$$

$$\xi = -\infty: \quad u = u_a, \; y = 0. \tag{2.3b}$$

A point of discussion is relevant here concerning the approach to solving (2.1) and (2.2). If one was seeking to solve these equations without first applying some

https://doi.org/10.1017/S1446181100013638 Published online by Cambridge University Press

asymptotic limit, and with full account taken of the ambient temperature as a parameter, then the approach of using an ignition temperature (such as that used by Bayliss and Matkowsky [3]) would be necessary, coupled with a rescaling of temperature with a consequent adjustment to the form of the reaction term. We do not use an ignition temperature here since the asymptotic analysis considered later in Section 3 naturally brings in an inner region where the reaction dominates, but is negligible outside such a zone. The boundary conditions (2.3), giving the same boundary condition on temperature, are a result of the slow decay to the original ambient temperature T_a (non-dimensionally u_a) at $\xi = -\infty$ on the equilibrium side. Later it is assumed that $u_a = 0$ with little lost in the main results—particularly concerning extinction.

3. Exact integral and asymptotic analysis, finite Lewis number

3.1. Exact integral By multiplying (2.2) by $1/\beta$ and adding it to (2.1), we have the derived result

$$\frac{d^2}{d\xi^2}\left(u + \frac{y}{\beta L}\right) + c\frac{d}{d\xi}\left(u + \frac{y}{\beta}\right) - \ell(u - u_a) = 0. \tag{3.1}$$

Integrating this result from $-\infty$ to $+\infty$ implies the following result for wave speed:

$$c = \beta\ell\int_{-\infty}^{+\infty}(u - u_a)\,d\xi. \tag{3.2}$$

Note that as $\ell \to 0$, so the temperature tail shown in Figure 1 extends to infinity with c reaching its adiabatic value. In this work ℓ will always be considered small, that is $o(1)$. The cooling tail is in fact characterised by a length of $O(\ell^{-1})$.

3.2. Outer zone asymptotics Away from the reaction zone, the solution for temperature and fuel in the preheat and equilibrium zones must satisfy

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} - \ell(u - u_a) = 0,$$
$$\frac{1}{L}\frac{d^2y}{d\xi^2} + c\frac{dy}{d\xi} = 0.$$

This is on the basis of $u \ll 1$ in the preheat zone, and $y \to 0$ in the equilibrium zone. For $\xi > 0$ on the cold (pre-heat) side, the solutions fitting the boundary conditions are

$$u = u_a + (u_f - u_a)e^{-m\xi}, \tag{3.3}$$
$$y = 1 - e^{-L\xi},$$

where

$$m \equiv \frac{c}{2} + \frac{1}{2}\sqrt{c^2 + 4\ell} \quad (> 0), \tag{3.4}$$

and u_f represents the flame temperature, that is, $u_f \equiv u|_{\xi=0}$. For $\xi < 0$ on the hot (equilibrium) side, the solutions fitting the boundary conditions are

$$u = u_a + (u_f - u_a)e^{n\xi}, \tag{3.5}$$

$$y = 0, \tag{3.6}$$

where

$$n \equiv -\frac{c}{2} + \frac{1}{2}\sqrt{c^2 + 4\ell} \quad (> 0). \tag{3.7}$$

Substituting these approximate solutions into the wave speed equation (3.2) implies

$$\begin{aligned} c &\approx \beta\ell \int_{-\infty}^{0_-} (u - u_a)\, d\xi + \beta\ell \int_{0_+}^{+\infty} (u - u_a)\, d\xi \\ &\approx \beta\ell(u_f - u_a)\left[\int_{-\infty}^{0} e^{n\xi}\, d\xi + \int_{-\infty}^{0} e^{m\xi}\, d\xi\right] \approx \beta\ell(u_f - u_a)\left(\frac{1}{n} + \frac{1}{m}\right), \end{aligned}$$

that is,

$$c \approx \beta\sqrt{c^2 + 4\ell}\,(u_f - u_a). \tag{3.8}$$

Note as $\ell \to 0$ so $u_f \to u_{\text{ad}} \equiv u_a + 1/\beta$, so that adiabatic conditions satisfy (3.8) as a special case.

3.3. Inner zone asymptotics In the inner reaction zone we re-scale the temperature and space. Thus we define

$$u = u_{\text{ad}} + \frac{\phi}{\beta} = u_a + \frac{1}{\beta} + \frac{\phi}{\beta} \tag{3.9a}$$

and

$$\chi = \sqrt{\beta}\,\xi, \tag{3.9b}$$

where u_{ad} is the adiabatic temperature and χ is the rescaled space variable. Consequently in this zone, the exponential in the reaction zone can be written

$$\begin{aligned} e^{-1/u} &\equiv \exp\left[-\left(u_{\text{ad}} + \frac{\phi}{\beta}\right)^{-1}\right] \\ &\approx \exp\left[-\frac{1}{u_{\text{ad}}}\left(1 - \frac{\phi}{\beta u_{\text{ad}}}\right)\right] \approx \exp\left(-\frac{1}{u_{\text{ad}}} + \frac{\phi}{\beta u_{\text{ad}}^2}\right), \end{aligned}$$

and the two differential equations in the inner zone to leading order in β^{-1} become

$$\frac{d^2\phi}{d\chi^2} + ye^{-1/u_{\rm ad}}e^{\phi/\beta u_{\rm ad}} = 0 \quad \text{and} \tag{3.10}$$
$$\frac{1}{L}\frac{d^2y}{d\chi^2} - ye^{-1/u_{\rm ad}}e^{\phi/\beta u_{\rm ad}} = 0$$

so that to leading order, the equation eliminating the reaction rate (3.1) becomes

$$\frac{d^2\phi}{d\chi^2} + \frac{1}{L}\frac{d^2y}{d\chi^2} = 0.$$

Integrating this equation once yields

$$\frac{d\phi}{d\chi} + \frac{1}{L}\frac{dy}{d\chi} = c_1, \tag{3.11}$$

where c_1 is a constant. Matching with the equilibrium solutions at $\xi = -\infty$ (see (3.5)–(3.7)) requires

$$\left.\frac{d\phi}{d\chi}\right|_{-\infty} = \sqrt{\beta}\left.\frac{du}{d\xi}\right|_{0_-} = \sqrt{\beta}(u_f - u_a) = \frac{n}{\sqrt{\beta}}(1 + \phi|_{-\infty}). \tag{3.12}$$

Consequently under the $\beta \to \infty$ limit (3.12) gives $\left.\frac{d\phi}{d\chi}\right|_{-\infty} = 0$, and so c_1 is zero.

Note that for ℓ small, then from (3.7),

$$n = -\frac{c}{2} + \frac{c}{2}\sqrt{1 + 4\frac{\ell}{c^2}} \approx \frac{\ell}{c} \quad (\ell \text{ small}). \tag{3.13}$$

Consequently integrating (3.11) a second time yields

$$\phi + y/L = c_2, \tag{3.14}$$

where c_2 is a constant. Matching on the hot side again gives

$$\frac{\phi|_{-\infty}}{\beta} = u|_{\xi=0_-} - u_{\rm ad}, \quad \text{with } y|_{-\infty} = 0. \tag{3.15}$$

If we define

$$\phi_f \equiv \beta(u_f - u_{\rm ad}), \tag{3.16}$$

then the condition (3.15a) becomes $\phi|_{-\infty} = \phi_f$, so that c_2 is simply ϕ_f. Noting then from (3.14) that $y = -L(\phi - \phi_f)$, we then obtain the single equation in the inner zone from (3.10):

$$\frac{d^2\phi}{d\chi^2} = Le^{-1/u_{\rm ad}}(\phi - \phi_f)e^{\phi/\beta u_{\rm ad}^2},$$

with boundary conditions on the equilibrium side ($\xi = -\infty$):

$$\phi|_{-\infty} = \phi_f, \quad \left.\frac{d\phi}{d\chi}\right|_{-\infty} = 0.$$

This single differential equation can be integrated once to give

$$\frac{1}{2}\left(\frac{d\phi}{d\chi}\right)^2 = Le^{-1/u_{ad}} \int_{\phi'=\phi_f}^{\phi} (\phi' - \phi_f)e^{\phi'/\beta u_{ad}^2}\, d\phi'.$$

If we let $p' \equiv -(\phi' - \phi_f)/\beta u_{ad}^2$, $p \equiv -(\phi - \phi_f)/\beta u_{ad}^2$, then

$$\frac{1}{2}\left(\frac{d\phi}{d\chi}\right)^2 = L\beta^2 u_{ad}^4 e^{\phi_f/\beta u_{ad}^2} e^{-1/u_{ad}} \int_{p'=0}^{p} p' e^{-p'}\, dp'. \tag{3.17}$$

Upon integration, (3.17) gives

$$\left(\frac{d\phi}{d\chi}\right)^2 = L\beta^2 u_{ad}^4 e^{\phi_f/\beta u_{ad}^2} e^{-1/u_{ad}} \left[\left(\frac{\phi - \phi_f}{\beta u_{ad}^2} - 1\right) e^{(\phi-\phi_f)/\beta u_{ad}^2} + 1\right]. \tag{3.18}$$

This solution for the inner gradient in temperature must now be matched to the outer temperature solution (3.3) on the preheat side where $\xi = +\infty$. Thus

$$\left.\frac{d\phi}{d\chi}\right|_{+\infty} = \sqrt{\beta}\left.\frac{du}{d\xi}\right|_{0_+} = -\sqrt{\beta}\, m(u_f - u_a),$$

which using (3.16) gives

$$\left.\frac{d\phi}{d\chi}\right|_{+\infty} \to -\frac{1}{\sqrt{\beta}} m(1 + \phi_f). \tag{3.19}$$

From (3.9b), $\phi \equiv \beta(u - u_{ad}) = \beta(u - u_a) - 1$, so that as $\chi \to \infty$, $\phi \to -1$. Consequently the matching of gradients ((3.18) and (3.19)) as $\chi \to \infty$ gives the result

$$-\frac{1}{\sqrt{\beta}} m(1 + \phi_f) = -\sqrt{2L\beta^2 u_{ad}^4 e^{\phi_f/\beta u_{ad}^2} e^{-1/u_{ad}} \left[\left(\frac{-1 - \phi_f}{\beta u_{ad}^2} - 1\right) e^{(-1-\phi_f)/\beta u_{ad}^2} + 1\right]}. \tag{3.20}$$

This result matches a leading order outer zone temperature gradient with an inner zone temperature gradient which includes higher order terms. Hence it is recognised that there will therefore be extra terms which strictly could be balanced by taking the outer expansion to the next order—clearly not possible in a tractable way analytically here. That these terms do not affect the leading order calculation of wave speed is confirmed by the earlier paper ([12]) where exactly the same approach was used, and it was shown that there is excellent agreement between numerical results and predictions from the large β asymptotic analysis. This analysis is not the same as that based on large activation energy, and the large β wave speed formula for wave speed does not in any way actually *include* the classical large activation energy result, since (as explained in the introduction) there is no one to one mapping between the two approaches—that is, by definition the parameter β in the current method is composed of the *ratio* of two parameters (non-dimensional activation energy E/RT_{ad} and non-dimensional heat release $Q/c_p T_{\mathrm{ad}}$) in the classical approach. Nevertheless, as the following pages show, there are additional terms initially carried in this non-adiabatic analysis, and recognising that we actually only want the leading estimates of heat loss affected wave speed, we later in this work simplify (3.20) to (3.26) and then (3.33), so that carried in this result are only the main terms necessary to maintain the balance of gradients implied in the limit $\phi \to -1$.

3.4. Wave speed formula for non-adiabatic conditions The result (3.20) is now coupled with the result for c ((3.8)) from the exact integral, which using (3.9b) can be written $c = \sqrt{c^2 + 4\ell}(1 + \phi_f)$.

As stated after (3.13), ℓ is regarded as $o(1)$, so that to leading order (3.21) yields the following connection between ϕ_f, ℓ and c:

$$c \approx c(1 + 4\ell/c^2)^{1/2}(1 + \phi_f),$$

that is,

$$1 \approx (1 + 2\ell/c^2 + \cdots)(1 + \phi_f). \tag{3.21}$$

Thus

$$1 \approx 1 + \frac{2\ell}{c^2} + \phi_f \quad \Rightarrow \quad \phi_f \approx -\frac{2\ell}{c^2}. \tag{3.22}$$

Performing a similar expansion for m in (3.4) we find

$$m \approx \frac{c}{2} + \frac{c}{2}\left(1 + \frac{2\ell}{c^2} + \cdots\right), \quad \text{that is,} \quad m \approx c + \frac{\ell}{c} \tag{3.23}$$

and thus

$$m(1 + \phi_f) \approx c - \frac{\ell}{c}. \tag{3.24}$$

Substituting results (3.22)–(3.24) into (3.20) then yields the following transcendental

https://doi.org/10.1017/S1446181100013638 Published online by Cambridge University Press

equation for the wave speed c:

$$c - \frac{\ell}{c} = \sqrt{2L\beta^3 u_{\mathrm{ad}}^4 e^{\phi_f/\beta u_{\mathrm{ad}}^2} e^{-1/u_{\mathrm{ad}}} \left[\left(\frac{-1-\phi_f}{\beta u_{\mathrm{ad}}^2} - 1 \right) e^{(-1-\phi_f)/\beta u_{\mathrm{ad}}^2} + 1 \right]}$$
$$= \sqrt{2L\beta^3 u_{\mathrm{ad}}^4 e^{-1/u_{\mathrm{ad}} - 1/\beta u_{\mathrm{ad}}^2} \left[e^{\phi_f/\beta u_{\mathrm{ad}}^2} e^{1/\beta u_{\mathrm{ad}}^2} - 1 - \frac{1+\phi_f}{\beta u_{\mathrm{ad}}^2} \right]}$$
$$= \sqrt{2L\beta^3 u_{\mathrm{ad}}^4 e^{-1/u_{\mathrm{ad}} - 1/\beta u_{\mathrm{ad}}^2} \left[\frac{-1 + 2\ell/c^2}{\beta u_{\mathrm{ad}}^2} - 1 + e^{-2\ell/\beta c^2 u_{\mathrm{ad}}^2 + 1/\beta u_{\mathrm{ad}}^2} \right]}, \tag{3.25}$$

where $u_{\mathrm{ad}} = u_a + 1/\beta$.

Thus for a given ℓ and β, one formally can find the wave speed c. The expression (3.25) becomes a little easier to manipulate with little loss of generality if we make the approximation $u_a \to 0$ (see [12]) so that $u_{\mathrm{ad}} \approx 1/\beta$ and consequently the result (3.25) becomes the simpler expression

$$c - \frac{\ell}{c} = \sqrt{\frac{2L}{\beta} e^{-2\beta} \left[e^{\beta(1-2\ell/c^2)} - 1 - \beta \left(1 - \frac{2\ell}{c^2} \right) \right]}. \tag{3.26}$$

For adiabatic conditions $\ell \to 0$ with $c \to c_{\mathrm{ad}}$, (3.26) collapses down to

$$c_{\mathrm{ad}} = \sqrt{\frac{2L}{\beta} e^{-2\beta} [e^{\beta} - 1 - \beta]}, \tag{3.27}$$

which for $L = 1$ is the same result as in Weber *et al.* [12]. Equation (3.26) and the adiabatic solution (3.27) are plotted for $L = 1$ in Figure 2 for low heat loss, and clearly confirm the well-known result that for a given β with small heat loss ℓ there are two main solutions with an extinction point where the two solutions merge. Theoretically there are also other low c solutions, from the full formula, but it is unlikely that these are practically relevant. Numerical solutions of the full system (2.1), (2.2) and (2.3) are also marked on this plot as the dashed lines.

For large β, yet further simplification of (3.26) and (3.27) can be made where the terms other than the exponential in the square bracket are small in comparison to the exponential term. Hence we obtain

$$c \approx \sqrt{(2L/\beta) e^{-\beta - 2\beta\ell/c^2}} \tag{3.28a}$$

and

$$c_{\mathrm{ad}} \approx \sqrt{(2L/\beta) e^{-\beta}}. \tag{3.28b}$$

Although (3.28a) is not plotted, it is close to the curves 'b' and 'c' illustrated in Figure 2 for $\ell = 0.00001$ and $\ell = 0.00002$.

https://doi.org/10.1017/S1446181100013638 Published online by Cambridge University Press

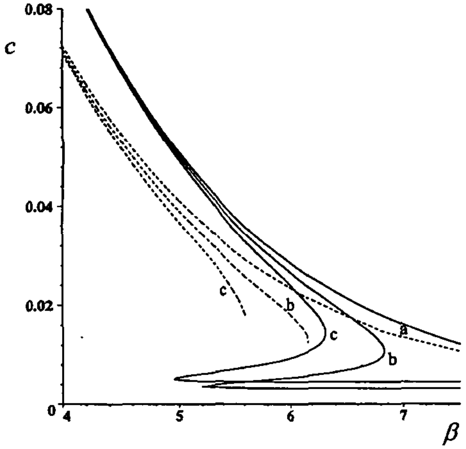

FIGURE 2. Non-adiabatic wave-speed formula given in (3.26) (solid lines) and numerical solutions to the full system (dashed lines) for Lewis number $L = 1$ and various heat losses (a) $\ell = 0$, (b) $\ell = 0.00001$, (c) $\ell = 0.00002$. Note the multiple wave speeds for the non-adiabatic cases and the subsequent extinction point.

3.5. Extinction heat loss and wave speeds From (3.28), for large β we can deduce an approximate extinction condition since

$$\beta\ell = c^2 \ln(c_{ad}/c), \tag{3.29}$$

so that $d(\beta\ell)/dc = 0$ when $c = 2c\ln(c_{ad}/c)$, which implies that at this turning point,

$$c_{ext}/c_{ad} = 1/\sqrt{e} = 0.607\ldots, \tag{3.30}$$

where the subscript ext stands for extinction and so

$$\beta\ell_{ext}/c_{ad}^2 = 1/(2e) = 0.184\ldots \quad \Rightarrow \quad \ell_{ext} = L/(\beta^2 e^{1+\beta}), \tag{3.31a,b}$$

where the second expression uses the approximate formula for c_{ad}^2 from (3.28b).

Figure 3 plots out the simpler expression, derived from (3.29):

$$\beta\ell_{ext}/c_{ad}^2 = (c/c_{ad})^2 \ln(c_{ad}/c), \tag{3.32}$$

which essentially encapsulates the major effect of heat loss which is either to predict a critical extinction heat loss, or for a given heat loss, a critical extinction value for the ratio β of activation energy to heat release.

However this approximation is not really accurate enough in determining the extinction heat loss ℓ_{ext}. For the case plotted in Figure 2 for $\ell = 0.00002$, it can be seen that the critical β value from the full formula is about 6.3, with the corresponding

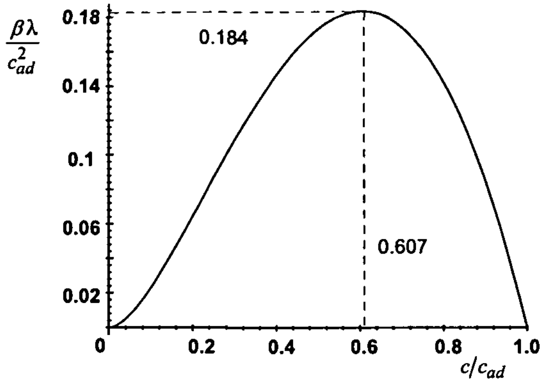

FIGURE 3. Approximate extinction heat loss and wave speed for combustion waves (finite Lewis number).

critical wave speed to be near 0.01 (refer to the solid line (c) in Figure 2). From the above approximate formula, for $\ell = 0.00002$, the critical β is about 6, with $c_{ad} \approx 0.03$, so that $c \approx 0.607 \times 0.03 \approx 0.018$, so that the error is in the region of 6%.

A better approximation is to regard only $\ell/c \ll 1$ in (3.26). Near extinction conditions this is always true. One then obtains

$$c \approx \sqrt{\frac{2L}{\beta} e^{-2\beta} \left[e^{\beta(1-2\ell/c^2)} - 1 - \beta\left(1 - \frac{2\ell}{c^2}\right)\right]}. \tag{3.33}$$

Differentiating and insisting that $d\ell/dc$ is zero for the turning points leads to the following relation at extinction:

$$c \approx 2\frac{\beta\ell}{c}\sqrt{\frac{2L}{\beta}e^{-2\beta}} \frac{e^{\beta(1-2\ell/c^2)} - 1}{\sqrt{e^{\beta(1-2\ell/c^2)} - 1 - \beta(1 - 2\ell/c^2)}}. \tag{3.34}$$

By defining

$$r \equiv \beta(1 - 2\ell/c^2), \tag{3.35}$$

and dividing (3.34) by (3.33), it can then be deduced that at extinction

$$\beta = r + \frac{e^r - 1 - r}{e^r - 1}, \tag{3.36}$$

and reversing definition (3.35), and using (3.33) for c^2, we have also at extinction that

$$\ell_{ext} = \frac{L}{\beta^2} e^{-2\beta} \frac{(e^r - 1 - r)^2}{e^r - 1}. \tag{3.37}$$

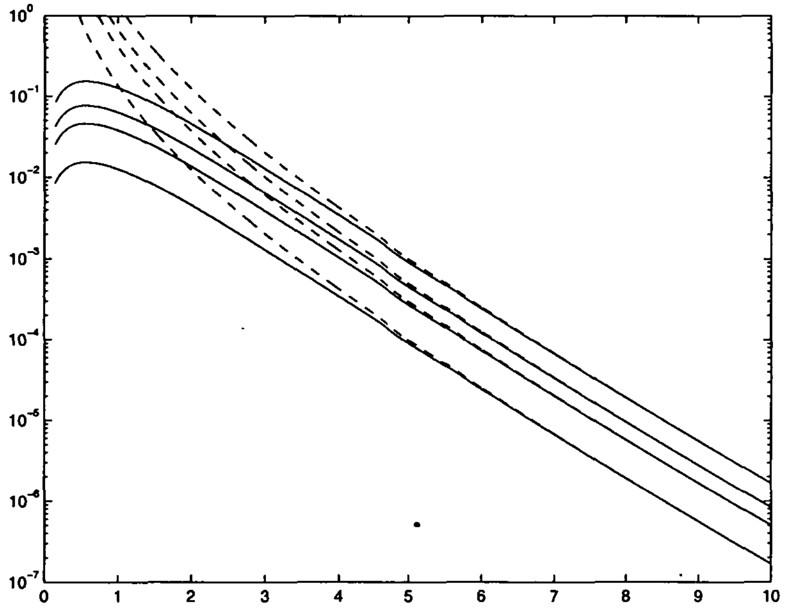

FIGURE 4. Extinction heat loss ℓ_{ext} plotted against ratio β of activation energy to heat release for various Lewis numbers L. The solid lines use (3.36) and (3.37), whilst the dotted lines are the results from the crude approximation resulting in (3.31b).

Equations (3.36) and (3.37) can then be used to calculate to much greater accuracy the extinction heat loss. The results from using these are shown in Figure 4.

It is evident from maxima in the plots in Figure 4 that for very small β the other unrealistic turning points are picked up (shown in Figure 2 bottom left). The realistic section of the curves in Figure 4 is the right-hand part where in the log plot the curves are almost a straight line with constant gradient. The gradient is consistent with (3.31b), but the shift in the values is important for accuracy, and (3.36) and (3.37) represent a significant correction to the standard use of (3.31b) for extinction calculations.

Equations (3.33), (3.36) and (3.37) represent the main findings from the analysis of this paper, namely that by using the large β analysis (as against large activation energy asymptotics) one can obtain a more accurate formula for non-adiabatic wave speeds coupled with extinction conditions.

4. Analysis for solid fuels (infinite Lewis number)

4.1. Exact integral and outer zone asymptotics For infinite Lewis number (solid fuels) a similar analysis is possible with the added benefit that an explicit formula for the ratio of the fuel (y) is possible. For infinite Lewis number L, (2.2) enables the immediate substitution of $ye^{-1/u} = (c/\beta)(dy/d\xi)$ to be made into (2.1) which now becomes

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} + \frac{c}{\beta}\frac{dy}{d\xi} - \ell(u - u_a) = 0. \tag{4.1}$$

The exact integral analysis is similar to the last section with c governed by the integral (see (3.2)): $c = \beta\ell\int_{-\infty}^{+\infty}(u - u_a)\,d\xi$. However unlike in the previous section, the first integration of (4.1) enables an explicit formula for y to be found:

$$y = \frac{\beta\ell}{c}\int_{-\infty}^{\xi}(u - u_a)\,d\xi - \beta(u - u_a) - \frac{\beta}{c}\frac{du}{d\xi},$$

so that a single differential equation in u alone can be formed,

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} + \left[\frac{\beta\ell}{c}\int_{-\infty}^{\xi}(u - u_a)\,d\xi - \beta(u - u_a) - \frac{\beta}{c}\frac{du}{d\xi}\right]e^{-1/u} - \ell(u - u_a) = 0.$$

The outer zone asymptotic analysis for large β yields the same leading order solutions for temperature either side of the combustion wave (see (3.3) and (3.5))

$$u = u_a + (u_f - u_a)e^{-m\xi} \quad \text{and} \quad u = u_a + (u_f - u_a)e^{n\xi},$$

so that one still obtains the same form for the wave speed relationship (3.8)

$$c \approx \beta\sqrt{c^2 + 4\ell}(u_f - u_a). \tag{4.2}$$

4.2. Inner zone asymptotics In the inner zone, the re-scaling of temperature is identical, but matching requirements lead to a different natural scaling for the new inner stretched coordinate η:

$$u = u_{\mathrm{ad}} + \phi/\beta = u_{\mathrm{ad}} + 1/\beta + \phi/\beta, \quad \eta \equiv \beta\xi.$$

Consequently the differential equation (3.35) in the inner zone becomes

$$\beta\frac{d^2\phi}{d\eta^2} + c\frac{d\phi}{d\eta} + \left[\frac{\ell}{\beta c}\int_{\phi_f}^{\phi}\frac{\phi' + 1}{d\phi'/d\eta}\,d\phi' - (\phi + 1) - \frac{\beta}{c}\frac{d\phi}{d\eta}\right]e^{-1/u_{\mathrm{ad}} + \phi/(\beta u_{\mathrm{ad}}^2)}$$
$$- \frac{\ell}{\beta}(1 + \phi) = 0$$

and to leading order

$$\frac{d^2\phi}{d\eta^2} = \frac{1}{c}\frac{d\phi}{d\eta}e^{-1/u_{\mathrm{ad}} + \phi/(\beta u_{\mathrm{ad}}^2)}. \tag{4.3}$$

In a similar way as with the general Lewis number case, the relationship for wave speed (4.2) can be written as $c \approx \sqrt{c^2 + 4\ell}(1 + \phi_f)$, where matching of temperature either side of the reaction zone leads as before to $\phi|_{-\infty} = \phi_f$ and $\phi|_{\infty} = -1$. With ℓ regarded as $o(1)$, the same result for the small drop in temperature at the flame and its connection to heat loss is found from (4.2):

$$\phi_f \approx -2\ell/c^2. \tag{4.4}$$

Integration of the inner zone differential equation (4.3) yields

$$\frac{d\phi}{d\eta} = -\frac{\beta u_{\mathrm{ad}}^2}{c} e^{-1/u_{\mathrm{ad}}} \left(e^{\phi_f/\beta u_{\mathrm{ad}}^2} - e^{\phi/\beta u_{\mathrm{ad}}^2} \right).$$

Matching of this solution for the inner gradient in temperature to the outer temperature solution (3.3) on the preheat side where $\xi = +\infty$ gives

$$\left.\frac{d\phi}{d\eta}\right|_{+\infty} = \left.\frac{du}{d\xi}\right|_{0_+} = -m(u_f - u_a) = -\frac{m}{\beta}(1 + \phi_f).$$

Noting that as $\eta \to \infty$, $\phi \to -1$ and using similar reasoning to the previous section (as (3.24)) that $m(1 + \phi_f) \approx c - \ell/c$, we obtain the analogue of (3.25) for the wave speed for solid fuels ($L = \infty$) with heat losses:

$$c - \frac{\ell}{c} = \frac{\beta^2 u_{\mathrm{ad}}^2}{c} e^{-1/u_{\mathrm{ad}}} \left(e^{-2\ell/\beta c^2 u_{\mathrm{ad}}^2} - e^{-1/\beta u_{\mathrm{ad}}^2} \right). \tag{4.5}$$

4.3. Heat loss and multiple wave speeds for moderate β ratio As with the equivalent result (3.25) for non-infinite Lewis numbers, there is little loss of generality if we take $u_a \to 0$, in which case the result (4.5) becomes

$$c - \frac{\ell}{c} = \frac{1}{c} e^{-\beta} \left(e^{-2\ell\beta/c^2} - e^{-\beta} \right), \tag{4.6}$$

which checks with the result in Weber *et al.* [12] $c = \sqrt{e^{-\beta}(1 - e^{-\beta})}$ for adiabatic conditions, that is, when $\ell \to 0$.

Figure 5 shows the multiple wave speeds that pertain to the formula (4.6) particularly at moderate β values. Marked on this figure are the numerical results as well, and locations where known oscillatory instabilities occur [9] (the maximum and minimum wave speeds in the oscillatory region are shown). The important difference in the case of solid fuels is that this instability is much more readily obtained and on the figure below corresponds to the slow branch of the wave speed plot.

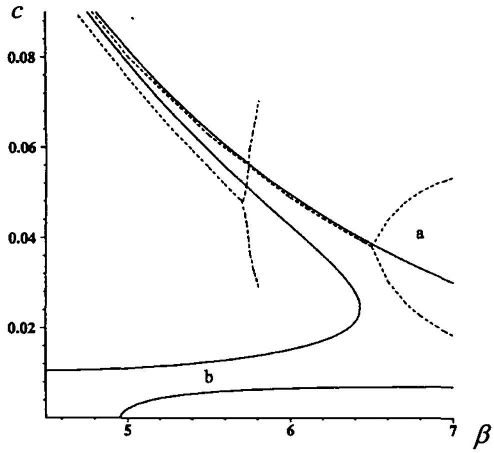

FIGURE 5. Solid fuel ($L = \infty$) wave speeds from (4.6) shown as the solid lines (a) $\ell = 0$, (b) $\ell = 0.00005$. Note the multiple wave speeds for the non-adiabatic case. Also shown are the numerical results (dashed lines); the maximum and minimum wave speeds have been plotted in the oscillatory regions.

4.4. Extinction Further simplification of result (4.4) can be obtained by again regarding $\ell/c \ll 1$, so that we have a very good approximation without losing the main characteristics of the transcendental wave speed formula:

$$c^2 = e^{-\beta}\left(e^{-2\ell\beta/c^2} - e^{-\beta}\right) \quad \text{and} \quad c_{\text{ad}}^2 = e^{-\beta}\left(1 - e^{-\beta}\right), \tag{4.7}$$

leading to

$$\frac{\beta\ell}{c_{\text{ad}}^2} = \frac{1}{2}\hat{c}^2 \ln\left[\hat{c}^2\left(1 - e^{-\beta}\right) + e^{-\beta}\right]. \tag{4.8}$$

This curve is essentially the top part of the shape shown in Figure 5, so that it captures the main dual wave speed phenomenon obtained with heat loss. If one ignored the second and third terms in the square bracket, then one obtains the same approximate expression (3.32) as we had for non-infinite Lewis number combustion waves. The more accurate result however is summarised by (4.7) and (4.8). For the infinite Lewis number case considered in this section, it is found in this case that for β values over about 5, the critical extinction heat loss ℓ_{ext} and wave speed c_{ext} are well approximated by (3.30) and (3.31a). Thus for solid combustion one can still use $c_{\text{ext}}/c_{\text{ad}} \approx 0.61$ and $\beta\ell_{\text{ext}}/c_{\text{ad}}^2 \approx 0.185$.

5. Conclusions

Heat losses and general Lewis number have been added to the combustion wave speed analysis of Weber *et al.* [12] using an asymptotic analysis based on the ratio of activation energy to heat release being large (as against the more traditional analysis of activation energy alone). Multiple wave speed solutions have been obtained—these are more pronounced in the solid fuel case for moderate values of the ratio β. A turning point in the speed curves indicates the extinction condition. This was further analysed to obtain an approximate extinction condition based solely on the ratio of the activation energy to the heat release, the heat loss and the adiabatic wave speed.

These formulae apply over a wider range of activation energies than the classical approximations based on large activation energy asymptotics.

For both gaseous and solid fuels, extinction criteria have been established and good comparison with full numerical solutions has been obtained.

Of particular note is that as reported by Mercer *et al.* [9] for solid fuels, the numerical results clearly show that the oscillatory instability is much more readily observed as the heat loss is increased. Illustrative calculations of maximum and minimum wave speeds have been shown for a typical case with and without heat loss.

References

[1] N. J. Balmforth, R. V. Craster and S. J. A. Malham, "Unsteady fronts in an autocatalytic system", *Proc. Roy. Soc. London Ser. A* **455** (1999) 1401–1433.

[2] A. Bayliss and B. J. Matkowsky, "Two routes to chaos in condensed phase combustion", *SIAM J. Appl. Math.* **50** (1990) 437–459.

[3] A. Bayliss and B. J. Matkowsky, "Nonlinear dynamics of cellular flames", *SIAM J. Appl. Math.* **52** (1992) 396–415.

[4] A. Bayliss and B. J. Matkowsky, "From travelling waves to chaos in combustion", *SIAM J. Appl. Math.* **54** (1994) 147–174.

[5] A. Bayliss, B. J. Matkowsky and M. Minkoff, "Period doubling gained, period doubling lost", *SIAM J. Appl. Math.* **49** (1989) 1047–1063.

[6] T. Boddington, A. Cottrell and P. G. Laye, "A numerical model of combustion in gasless pyrotechnic systems", *Combust. Flame* **76** (1989) 63–69.

[7] J. F. Griffiths and J. A. Barnard, *Flame and combustion*, 3rd ed. (Stanley Thomas, London, 1995).

[8] G. N. Mercer, R. O. Weber, B. F. Gray and S. D. Watt, "Combustion pseudo-waves in a system with reactant consumption and heat loss", *Math. Comput. Modelling* **24** (1996) 29–38.

[9] G. N. Mercer, R. O. Weber and H. S. Sidhu, "An oscillatory route to extinction for solid fuel combustion waves due to heat losses", *Proc. Roy. Soc. London Ser. A* **454** (1998) 2015–2022.

[10] M. J. Metcalf, J. H. Merkin and S. K. Scott, "Oscillating wave fronts in isothermal chemical systems with arbitrary powers of autocatalysis", *Proc. Roy. Soc. London Ser. A* **447** (1994) 155–174.

[11] K. S. Shkadinskii, B. I. Khaikin and A. G. Merzhanov, "Propagation of a pulsating exothermic reaction front in the condensed phase", *Combust. Expl. Shock* **7** (1971) 15–22.

[12] R. O. Weber, G. N. Mercer, H. S. Sidhu and B. F. Gray, "Combustion waves for gases ($Le = 1$) and solids ($Le \to \infty$)", *Proc. Roy. Soc. London Ser. A* **453** (1997) 1105–1118.