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Quenching of flame propagation through endothermic reaction

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The propagation of a premixed laminar flame supported by an exothermic chemical reaction under adiabatic conditions but subject to inhibition through a parallel endothermic chemical process is considered. The temperature dependence of the reaction rates is assumed to have a generalised Arrhenius type form with an ignition temperature, below which there is no reaction. The heat loss through the endothermic reaction, represented by the dimensionless parameter α, has a strong quenching effect on wave initiation and propagation. The temperature profile can have a front or a pulse structure depending on the relative value of the ignition temperatures and on the value of the parameters α and β, the latter represents the rate at which inhibitor is consumed relative to the consumption of fuel. The wave speed-cooling parameter (α) curves are determined for various values of the other parameters. These curves can have three different shapes: monotone decreasing, $\supset$-shaped or S-shaped, with the possibility of having one, two or three different flame velocities for the same value of the cooling parameter α.

KEY WORDS: laminar flame, step function, travelling wave

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1. Introduction

In this paper we consider the propagation of a flame supported by an exothermic chemical reaction under adiabatic conditions but subject to inhibition through a parallel endothermic chemical process. In particular, we will be concerned with determining the marginal conditions for the establishment of constant-velocity constant-form flame structures and the dependence of the flame speed in such cases on the reaction parameters. Such information is of interest as we seek to develop alternatives to halon-based fire extinguishants since the adoption of the Montreal protocol.

Our model involves two chemical steps:

$$A \to P + \text{ heat}, \quad \text{rate} = k_1(T)a,$$
$$W \to Q - \text{ heat}, \quad \text{rate} = k_2(T)w.$$

The first step has a positive exothermicity (negative reaction enthalpy) $Q_1 > 0$, the second step has a negative exothermicity, $Q_2 < 0$. The temperature dependence of the steps is assumed to have the form

$$k_i(T) = k_{i0}\kappa_i(T), \quad i = 1, 2,$$

where

$$\kappa_i(T) = 0 \quad \text{if } T \leqslant T_i; \qquad \kappa_i(T) > 0 \quad \text{if } T > T_i. \tag{1}$$

T_i $(i = 1, 2)$ are the ignition temperatures, below which there is no reaction. We note that for $T \leqslant T_i$ condition (1) is not satisfied by the Arrhenius temperature dependence but for small ignition temperatures it is a very good approximation. Moreover, it has the advantage that the cold boundary difficulty does not occur in this case. The solution of our problem tends to the one without an ignition temperature as $T_i \to 0$ [1]. For $T > T_i$ we take two main examples for $\kappa_i(T)$. It can be the usual Arrhenius function

$$\kappa_i(T) = \mathrm{e}^{-E_i/RT} \quad (T > T_i),$$

where E_i $(i = 1, 2)$ are the activation energies, or it can take the simpler form

$$\kappa_i(T) \equiv 1 \quad (T > T_i).$$

In the second case κ_i are step functions. The motivation for studying this special case is twofold. First, the differential equations governing our model can be solved analytically and the joining conditions give rise to nonlinear algebraic equations, which are relatively easy to solve numerically. Hence we obtain the "exact" solution of the problem in this case. Therefore, this case can serve as a test problem for the numerical investigation. Second, the step function can be considered as a simplified version of Arrhenius' law, namely, below the ignition temperature there is no reaction, whereas above that temperature the reaction rate does not depend on temperature. Therefore some qualitative features of the model can be revealed via this special case.

Previous work on flame quenching [2–7] has concerned heat removal through physical processes such as conduction or radiation. In the present case, the "heat loss" process is controlled by the concentration of the endothermic species W, which is consumed during the process at a rate which depends on the temperature.

The effect of the addition of sprays or particles (both reactive or inert) on premixed flame propagation had been investigated experimentally and theoretically [8–10]. These studies have shown that the propagation speed of a premixed flame is decreased by the addition of dust (or spray) through negative thermal (and sometimes chemical) feedback. The main parameters on which the flame speed depended were found to be the virtual heat capacity of the particles and the particle size. The speed was found to decrease either monotonically or to have an S-shaped form (depending on the value of the particle-size parameter).

The modification of our system (with a second-order reaction) was investigated numerically and with high activation energy asymptotics [11,12]. From this previous work, we expect the important parameters to be represented by the dimensionless groups:

$$\alpha = \frac{(-Q_2)k_{20}W_0}{Q_1 k_{10} A_0}, \qquad \beta = \frac{k_{20}\mu_W}{k_{10}\mu_A},$$

where A_0, W_0 are the initial concentrations of A and W, and μ_A, μ_W are the molar masses.

The aim of this work is to determine the dependence of the dimensionless flame velocity c on those parameters, find critical values of α (dependent on other parameters) at which flame extinction occurs and to determine the temperature and concentration profiles.

In the general case (section 2), when the functions κ_i are assumed to satisfy only the assumptions in (1), we can determine some qualitative properties of the solutions. It turns out that we can have two different types of front waves or pulse waves in temperature. We give conditions in terms of α, β and T_i for the existence of these solutions. In the case when κ_1 and κ_2 are step functions (sections 3 and 4) we explicitly determine the dependence of c on α for any value of β and T_i, and thus determine the extinction value of α belonging to the turning point of the (α, c) diagram. We found a new feature of this diagram, namely in the case $T_1 > T_2$ it can have two turning points, that is we can have three solutions (with three different flame velocities) for the same values of the parameters. We note that all calculations are made for arbitrary values of the Lewis numbers, but for simplicity the results are presented in the case when $L_A = L_W = 1$.

2. Model and general results

2.1. Model

The nondimensional equations governing our model, written in a reference frame moving with the flame front, are [7,13–15]:

$$b''(y) - cb'(y) + a(y)f_1\big(b(y)\big) - \alpha w(y)f_2\big(b(y)\big) = 0, \tag{2}$$

$$\frac{1}{L_A}a''(y) - ca'(y) - a(y)f_1\big(b(y)\big) = 0, \tag{3}$$

$$\frac{1}{L_W}w''(y) - cw'(y) - \beta w(y)f_2\big(b(y)\big) = 0, \tag{4}$$

on $-\infty < y < \infty$ with boundary conditions

$$b(y) \to 0, \quad a(y) \to 1, \quad w(y) \to 1 \qquad \text{as } y \to -\infty, \tag{5}$$

$$b'(y) \to 0, \quad a'(y) \to 0, \quad w'(y) \to 0 \qquad \text{as } y \to +\infty \tag{6}$$

and with the assumption that

$$b(y) > 0, \quad a(y) \geqslant 0, \quad w(y) \geqslant 0, \quad c > 0, \qquad -\infty < y < \infty. \tag{7}$$

This assumption excludes the trivial solution $b \equiv 0$, $a \equiv 1$, $w \equiv 1$. Here the nondimensional variables a, b, w represent the fuel concentration, temperature and the concentration of the inhibitor. The Lewis numbers L_A and L_W and the parameters α, β are nonnegative. The scaled ignition temperatures are $b_{\mathrm{I}}, b_{\mathrm{II}} \in [0, 1)$. Therefore the functions f_1 and f_2 are assumed to satisfy the following conditions:

$$f_1(b) = 0, \quad \text{if } 0 \leqslant b \leqslant b_{\mathrm{I}}; \qquad f_1(b) > 0, \quad \text{if } b > b_{\mathrm{I}}; \tag{8}$$

$$f_2(b) = 0, \quad \text{if } 0 \leqslant b \leqslant b_{\mathrm{II}}; \qquad f_2(b) > 0, \quad \text{if } b > b_{\mathrm{II}}. \tag{9}$$

It is also assumed that f_1, f_2 are bounded functions that are differentiable except at most at the point b_{I}, respectively b_{II}, where they have right limit

$$\varphi_1 = \lim_{b \to b_{\mathrm{I}}^+} f_1(b), \qquad \varphi_2 = \lim_{b \to b_{\mathrm{II}}^+} f_2(b). \tag{10}$$

As it was mentioned above, we have two examples in mind, Arrhenius dependence for temperatures above the ignition temperature and a step function that jumps from zero to 1 at the ignition temperature.

In the next section we assume that a, b, w, c satisfy (2)–(7) and we derive some qualitative properties of the solution. In the following three subsections we determine the structure of the temperature profile. Throughout this section it is assumed only that f_1 and f_2 satisfy (8)–(9), their concrete forms are not specified.

2.2. *Qualitative properties of the solutions*

Proposition 1. The functions a and w are nonincreasing.

Proof. Multiplying equation (3) with $L_A e^{-L_A c y}$ and integrating over (y, ∞) we get

$$a'(y) e^{-L_A c y} = -\int_y^\infty e^{-L_A c s} a(s) f_1\big(b(s)\big)\, ds$$

yielding $a'(y) \leqslant 0$ for all y. Similarly from equation (4) we obtain $w'(y) \leqslant 0$. □

Proposition 2. The limits

$$a_+ = \lim_{+\infty} a, \qquad b_+ = \lim_{+\infty} b, \qquad w_+ = \lim_{+\infty} w$$

exist and

$$a_+ + b_+ - \frac{\alpha}{\beta} w_+ = 1 - \frac{\alpha}{\beta}. \tag{11}$$

Moreover, if $\varphi_1 > 0$ and there exists y^*, such that $b(y) > b_{\mathrm{I}}$ for all $y > y^*$, then $a_+ = 0$. If $\varphi_2 > 0$ and there exists y^*, such that $b(y) > b_{\mathrm{II}}$ for all $y > y^*$, then $w_+ = 0$.

Proof. The existence of a_+ and w_+ follows from the monotonicity of the functions a and w and condition (6). To prove the existence of b_+ and derive (11) we can combine equations (2)–(4) to eliminate the reaction terms, integrate once and apply boundary conditions (5)–(6), for the details see [12].

If $b(y) > b_{\mathrm{I}}$ for all $y > y^*$, then

$$\lim_{y\to\infty} f_1\big(b(y)\big) > 0$$

since the value of the limit is $f_1(b_+) > 0$ if $b_+ > b_{\mathrm{I}}$, and it is $\varphi_1 > 0$ if $b_+ = b_{\mathrm{I}}$. Hence from equation (3) $a_+ = 0$. Similarly, from equation (4) we get $w_+ = 0$. □

Proposition 3. There exist y_1 and y_2, such that $b(y_1) > b_{\mathrm{I}}$ and $b(y_2) > b_{\mathrm{II}}$.

Proof. First we show the existence of y_1. Let us assume the contrary $b(y) \leqslant b_{\mathrm{I}}$ for all y. Then $f_1(b(y)) \equiv 0$, hence multiplying equation (2) with e^{-cy} and integrating over (y, ∞) we get

$$b'(y)\mathrm{e}^{-cy} = -\alpha \int_y^\infty \mathrm{e}^{-cs} w(s) f_2\big(b(s)\big)\,\mathrm{d}s$$

yielding $b'(y) \leqslant 0$ for all y. Boundary conditions (5) then imply that b is the trivial solution $b \equiv 0$ contradicting (7).

To prove the existence of y_2, assume the contrary $b(y) \leqslant b_{\mathrm{II}}$ for all y. Then $f_2(b(y)) \equiv 0$, and following the argument given above, we obtain $b'(y) \geqslant 0$ for all y and $b'(y) > 0$ if $b(y) > b_{\mathrm{I}}$. Hence b can attain the value b_{I} at most once and the limit

$$f_{1+} = \lim_{y\to\infty} f_1\big(b(y)\big)$$

exists. From equation (2) we get

$$a_+ f_{1+} = 0. \tag{12}$$

Adding the equations (2) and (3) and integrating over $(-\infty, \infty)$ we obtain

$$a_+ + b_+ = 1. \tag{13}$$

Equation (12) gives two possibilities. First, $a_+ = 0$, then from (13) $b_+ = 1$ contradicting to $b(y) \leqslant b_{\mathrm{II}} < 1$. Second, $f_{1+} = 0$ implying $b(y) \leqslant b_{\mathrm{I}}$ that yields $b \equiv 0$ again, which contradicts (7). □

Proposition 4. If $b(y^*) = b_{\mathrm{II}}$, then $b(y) \geqslant b_{\mathrm{II}}$ for all $y > y^*$.

Proof. Let us assume the contrary, i.e., that there exists $y_1 > y^*$, such that $b(y_1) < b_{\mathrm{II}}$. Then there exists $y_2 \in (y^*, y_1)$, such that

$$b(y_2) < b_{\mathrm{II}}, \qquad b'(y_2) < 0. \tag{14}$$

We show that

$$b(y) < b_{\mathrm{II}} \quad \text{for all } y > y_2. \tag{15}$$

Namely, let us assume that there exists $y_3 > y_2$, such that

$$b(y_3) = b_{\mathrm{II}} \quad \text{and} \quad b(y) < b_{\mathrm{II}} \quad \text{for all } y \in (y_2, y_3). \tag{16}$$

Then multiplying equation (2) with e^{-cy} and integrating on (y_2, y) we get

$$b'(y)\mathrm{e}^{-cy} = b'(y_2)\mathrm{e}^{-cy_2} - \int_{y_2}^{y} \mathrm{e}^{-cs} a(s) f_1\bigl(b(s)\bigr)\,\mathrm{d}s < 0 \quad \text{for all } y \in (y_2, y_3). \tag{17}$$

Thus b is decreasing on (y_2, y_3) implying that $b(y_3) < b_{\mathrm{II}}$, which contradicts (16). Hence we have (15) and, consequently, (17) for all $y \in (y_2, \infty)$. Going to the limit $y \to \infty$ in (17) we obtain $b'(y_2) \geqslant 0$ contradicting (14) and completing the proof. □

Corollary 1. If $b(y^*) = b_{\mathrm{II}}$, then $b'(y^*) \geqslant 0$.

Proposition 5. If $b(y^*) = b_{\mathrm{II}}$ and $b'(y^*) > 0$, then $b(y) < b_{\mathrm{II}}$ and $b'(y) > 0$ for all $y < y^*$.

Proof. The inequality $b(y) < b_{\mathrm{II}}$ follows directly from proposition 4. Hence $f_2(b(y)) = 0$ for all $y < y^*$. Then multiplying equation (2) with e^{-cy} again and integrating on (y, y^*) we get

$$b'(y)\mathrm{e}^{-cy} = b'\bigl(y^*\bigr)\mathrm{e}^{-cy^*} + \int_{y}^{y^*} \mathrm{e}^{-cs} a(s) f_1\bigl(b(s)\bigr)\,\mathrm{d}s > 0 \quad \text{for all } y < y^*.$$

Thus we have $b'(y) > 0$ for all $y < y^*$. □

Proposition 6. If $b_{\mathrm{I}} < b_{\mathrm{II}}$, then b attains the value b_{I} once, and there is no open interval where $b(y) \equiv b_{\mathrm{II}}$.

Proof. According to proposition 3 the function b attains the values b_{I} and b_{II} at least once. We can assume that b attains b_{II} first at zero, because the differential equations are translationally invariant. Then by proposition 5 the function b is increasing for $y < 0$, hence it attains the value b_{I} exactly once in $(-\infty, 0)$. According to proposition 4 $b(y) \geqslant b_{\mathrm{II}} > b_{\mathrm{I}}$ for $y > 0$, therefore b cannot attain b_{I} in $(0, \infty)$. It remains to prove that $b(y)$ cannot be the constant b_{II} in any open (nonempty) interval in $(0, \infty)$. This result follows from

$$a(y) > 0 \quad \text{for all } -\infty < y < \infty \tag{18}$$

(see equation (2)). We now prove the inequality. Since a is nonincreasing and $a \geqslant 0$, therefore only the case $a(y) \equiv 0$ in (y_1, ∞) has to be excluded. As it was shown above b attains the value b_{I} exactly once in $(-\infty, 0)$. Let us denote that point by l. It can be easily seen that $a(y) = 1 - K\mathrm{e}^{cL_A y}$ in $(-\infty, l]$ with some constant K. Hence $a(y) > 0$ in that interval. In the interval (l, ∞) $b(y) > b_{\mathrm{I}}$, therefore the function $y \mapsto f_1(b(y))$ is smooth. Hence the solution of the initial value problem corresponding to the differential equation (3) is unique. Therefore a cannot be everywhere zero in any open subinterval, because otherwise it would be zero in (l, ∞), which contradicts $a(l) > 0$. Thus (18) is proved and the proof is complete. □

The results formulated in the above propositions enable us to determine the qualitative structure of the temperature profiles. These depend strongly on the value of b_{I} relative to b_{II}, therefore we shall consider the cases $b_{\mathrm{I}} < b_{\mathrm{II}}$, $b_{\mathrm{I}} = b_{\mathrm{II}}$ and $b_{\mathrm{I}} > b_{\mathrm{II}}$ separately. We can assume, since the differential equations (2)–(4) are translationally invariant and according to proposition 5 the function b is increasing before it reaches the value b_{II}, that in all cases

$$b(0) = \min\{b_{\mathrm{I}}, b_{\mathrm{II}}\} \quad \text{and} \quad b(y) < \min\{b_{\mathrm{I}}, b_{\mathrm{II}}\} \quad \text{for } y < 0. \tag{19}$$

The structure of the temperature profiles depend strongly also on the continuity of f_i. If f_i are continuous, i.e., $\varphi_i = 0$ (see (10)), then uniqueness of the solution of the initial value problem corresponding to the differential equation (2) implies that the function b cannot be the constant b_{II} in any open interval in the case $b_{\mathrm{I}} \geqslant b_{\mathrm{II}}$ as well (it is true in the case $b_{\mathrm{I}} < b_{\mathrm{II}}$ generally according to proposition 6). The structure of the temperature profiles can be more complex in the case $\varphi_i > 0$, i.e., when f_1 and f_2 have a jump at b_{I} and at b_{II}, respectively. (In that case uniqueness of the initial value problem is not guaranteed.) Since the main object of the paper is the step function case, when the characterisation of the temperature profiles is different in the two cases, we shall assume

(H1) $\varphi_i > 0$ for $i = 1, 2$.

We cannot exclude the possibility of oscillatory solutions, although we have been unable to find such solutions. To exclude this possibility we make the following assumptions where appropriate.

(H2) The function b attains the value b_{I} at most twice.
(H3) If $b(y^*) = b_{\mathrm{II}}$ and $b'(y^*) = 0$, then $b(y) \equiv b_{\mathrm{II}}$ for all $y > y^*$.

2.3. The structure of the temperature profile in the case $b_{\mathrm{I}} < b_{\mathrm{II}}$

In this case (19) reads as

$$b(0) = b_{\mathrm{I}} \quad \text{and} \quad b(y) < b_{\mathrm{I}} \quad \text{for } y < 0.$$

The structure of the temperature profile in $(0, \infty)$ is described in the next proposition.

Proposition 7. Assume that (H3) and $b_{\mathrm{I}} < b_{\mathrm{II}}$ hold. Then there exists $l > 0$, such that $b(l) = b_{\mathrm{II}}$ and

$$b_{\mathrm{I}} < b(y) < b_{\mathrm{II}}, \quad \text{for } 0 < y < l; \qquad b_{\mathrm{II}} < b(y) \quad \text{for } l < y < \infty.$$

Proof. Let l be the first point where b attains the value b_{II}. The existence of such an l follows from proposition 3. We have to prove the second inequality. Assume that there exists $y^* > l$, such that $b(y^*) = b_{\mathrm{II}}$. Then corollary 1 implies that $b'(y^*) = 0$, hence from (H3) $b(y) \equiv b_{\mathrm{II}}$ for all $y > y^*$, which contradicts to proposition 6.

Typical temperature profiles for this case are shown in figure 2. □

2.4. *The structure of the temperature profile in the case $b_{\mathrm{I}} = b_{\mathrm{II}}$*

In this case proposition 4 implies that

$$b_+ \geqslant b_{\mathrm{I}}. \tag{20}$$

According to the value of b_+ we can have two different temperature profiles:

- front profiles, if $b_+ > b_{\mathrm{I}}$;
- pulse profiles, if $b_+ = b_{\mathrm{I}}$.

In this case (19) reads as

$$b(0) = b_{\mathrm{I}} \quad \text{and} \quad b(y) < b_{\mathrm{I}} \quad \text{for } y < 0. \tag{21}$$

The structure of the temperature profile in $(0, \infty)$ is described in the next proposition.

Proposition 8. Assume that (H3) and $b_{\mathrm{I}} = b_{\mathrm{II}}$ hold. Then exactly one of the following two possibilities holds.

1. $b_{\mathrm{I}} < b(y)$ for all $0 < y < \infty$.
2. There exists $l > 0$, such that $b(l) = b_{\mathrm{I}}$ and

$$b_{\mathrm{I}} < b(y), \quad \text{for } 0 < y < l; \qquad b(y) \equiv b_{\mathrm{I}}, \quad \text{for } l \leqslant y < \infty.$$

We shall refer to these as type 1 and type 2 temperature profiles.

Proof. According to proposition 3 we have $b(y) > b_{\mathrm{I}}$ for small $y > 0$. If there is no point $l > 0$ where $b(l) = b_{\mathrm{I}}$, then case 1 holds. If there exists $l > 0$ where $b(l) = b_{\mathrm{I}}$, then let us assume that this is the first positive value where b attains b_{I}. Then by corollary 1 $b'(l) = 0$ (since $b_{\mathrm{II}} = b_{\mathrm{I}}$) and by (H3) $b(y) \equiv b_{\mathrm{I}}$ for $y > l$. □

It is obvious that the front profiles belong to type 1 and the pulse profiles can belong either to type 1 or to type 2. However, the two classifications of the temperature profiles differ only in the marginal cases between the two classes. The border between type 1 and type 2 profiles ($l = \infty$) belongs to type 1. The border between front and pulse profiles ($b_+ = b_{\mathrm{I}}$ and $b(y) > b_{\mathrm{I}}$ for $y > 0$) belongs to the pulses. We note that in the case $\varphi_i = 0$ we can have only type 1 profiles and the profiles are classified only according to the value of b_+ as fronts and pulses.

For some regions of the parameter plane (α, β) we can determine the type of the temperature profiles in this general case. A more detailed description will be given in the step function case.

Proposition 9. Assume that $b_{\mathrm{I}} = b_{\mathrm{II}}$ holds.

1. If b is a type 1 temperature profile and $\varphi_i > 0$ ($i = 1, 2$), then $\alpha \leqslant \beta(1 - b_{\mathrm{I}})$.
2. If b is a type 2 temperature profile, $f_1 \equiv f_2$ and $\beta > 1$, then $\alpha > \beta(1 - b_{\mathrm{I}})$.

Proof. 1. From proposition 2 we get $a_+ = 0 = w_+$. Hence (11) reads as

$$b_+ = 1 - \frac{\alpha}{\beta} \tag{22}$$

and the desired inequality follows from (20) and (22).

2. Now $b_+ = b_{\mathrm{I}}$ and we will show that

$$a_+ \leqslant \alpha w_+. \tag{23}$$

Once this is shown we have from (11) that

$$(1 - b_{\mathrm{I}})\beta - \alpha \leqslant \alpha w_+(\beta - 1) < 0.$$

Hence, we only have to prove (23). Since b is a type 2 profile, $b(y) \equiv b_{\mathrm{I}}$ in $[l, \infty)$. Multiplying equation (2) by e^{-cy} and integrating on (y, l) for some $y \in (0, l)$ we get

$$b'(y)\mathrm{e}^{-cy} = \int_y^l \mathrm{e}^{-cs}\big(a(s) - \alpha w(s)\big) f_1\big(b(s)\big)\,\mathrm{d}s. \tag{24}$$

It can be shown that $a - \alpha w$ cannot have infinitely many zeros in $[0, l]$, hence $a(s) - \alpha w(s)$ does not change sign in an interval $[l_1, l]$ for some $l_1 \in (0, l)$. Therefore b' does not change sign in that interval. Since $b(y) > b_{\mathrm{I}}$ in $(0, l)$, $b'(y) < 0$ in (l_1, l), and from (24) we have $a(s) - \alpha w(s) < 0$ for $s \in (l_1, l)$. Then going to the limit $s \to l$ we obtain (23). □

Remark 1. In the case of step functions $b_{\mathrm{I}} = b_{\mathrm{II}}$ implies $f_1 \equiv f_2$ and we will show that for $\beta \geqslant 1$ there are no type 2 temperature profiles. Hence, in this case, the line $\alpha = \beta(1 - b_{\mathrm{I}})$ separates the regions of front and pulse solutions.

Typical temperature profiles for this case are shown in figure 4.

2.5. *The structure of the temperature profile in the case $b_{\mathrm{I}} > b_{\mathrm{II}}$*

In this case proposition 4 implies

$$b_+ \geqslant b_{\mathrm{II}}. \tag{25}$$

According to the value of b_+ we can have three different temperature profiles:

- front 1 profiles, if $b_+ > b_{\mathrm{I}}$;
- front 2 profiles, if $b_{\mathrm{II}} < b_+ \leqslant b_{\mathrm{I}}$;
- pulse profiles, if $b_+ = b_{\mathrm{II}}$.

In this case (19) reads as

$$b(0) = b_{\mathrm{II}} \quad \text{and} \quad b(y) < b_{\mathrm{II}} \quad \text{for } y < 0. \tag{26}$$

The structure of the temperature profile in $(0, \infty)$ is described in the next proposition.

Proposition 10. Assume that (H1)–(H3) and $b_{\mathrm{I}} > b_{\mathrm{II}}$ hold. Then exactly one of the following three possibilities holds.

1. There exists $l > 0$, such that $b(l) = b_{\mathrm{I}}$ and

$$b_{\mathrm{II}} < b(y) < b_{\mathrm{I}}, \quad \text{for } 0 < y < l; \qquad b_{\mathrm{I}} < b(y), \quad \text{for } l < y < \infty.$$

2. There exist $L > l > 0$, such that $b(l) = b_{\mathrm{I}} = b(L)$ and

$$b_{\mathrm{II}} < b(y) < b_{\mathrm{I}}, \quad \text{for } 0 < y < l; \qquad b_{\mathrm{I}} < b(y), \quad \text{for } l < y < L;$$
$$b_{\mathrm{II}} < b(y) < b_{\mathrm{I}}, \quad \text{for } L < y < \infty.$$

3. There exist $\Lambda > L > l > 0$, such that $b(l) = b_{\mathrm{I}} = b(L)$, $b(\Lambda) = b_{\mathrm{II}}$ and

$$b_{\mathrm{II}} < b(y) < b_{\mathrm{I}}, \quad \text{for } 0 < y < l; \qquad b_{\mathrm{I}} < b(y), \quad \text{for } l < y < L;$$
$$b_{\mathrm{II}} < b(y) < b_{\mathrm{I}}, \quad \text{for } L < y < \Lambda; \qquad b(y) \equiv b_{\mathrm{II}}, \quad \text{for } \Lambda \leqslant y < \infty.$$

We shall refer to these as type 1, type 2 and type 3 temperature profiles.

Proof. Let l be the first point where b attains the value b_{I}. The existence of such an l follows from proposition 3. If there is no point $L > l$ where $b(L) = b_{\mathrm{I}}$, then 1 holds. If such an L exists, then by (H2) we have $b(y) < b_{\mathrm{I}}$ for all $y > L$. If $b(y) > b_{\mathrm{II}}$ for all $y > L$, then 2 holds. If there exists $\Lambda > L$ where $b(\Lambda) = b_{\mathrm{II}}$, then from corollary 1 $b'(\Lambda) = 0$, hence (H3) implies $b(y) \equiv b_{\mathrm{II}}$ in $[\Lambda, \infty)$, i.e., 3 holds. □

Typical temperature profiles for this case are shown in figures 7–9. It is obvious that front 1 profiles belong to type 1, front 2 profiles can belong either to type 1 or to type 2, and the pulse profiles can belong either to type 2 or to type 3. However, the two classifications of the temperature profiles differ again only in the marginal cases between the two classes, as in the case $b_{\mathrm{I}} = b_{\mathrm{II}}$. We note that when $\varphi_i = 0$ we can only have type 1 and type 2 profiles and the profiles are classified only according to the value of b_+ as front 1, front 2 profiles and pulses.

For some regions of the (α, β) parameter plane we can determine the type of the temperature profiles in this general case. A more detailed description will be given in the step function case.

Proposition 11. Assume that $b_{\mathrm{I}} > b_{\mathrm{II}}$.

1. If b is a type 1 temperature profile and $\varphi_i > 0$ $(i = 1, 2)$, then $\alpha \leqslant \beta(1 - b_{\mathrm{I}})$.
2. If b is a type 2 temperature profile and $\varphi_2 > 0$, then $\alpha \leqslant \beta(1 - b_{\mathrm{II}})$.

Proof. 1. From proposition 2 we get $a_+ = 0 = w_+$. Hence (11) reads as

$$b_+ = 1 - \frac{\alpha}{\beta}. \tag{27}$$

For a type 1 profile $b_+ \geqslant b_{\mathrm{I}}$, therefore the desired inequality follows from (27).

2. From proposition 2 we get $w_+ = 0$. Hence (11) reads as

$$a_+ + b_+ = 1 - \frac{\alpha}{\beta} \tag{28}$$

and the inequality follows from $a_+ \geqslant 0$, (25) and (28). □

3. Method for solving the differential equations in the step function case

In this section we present a method to solve problem (2)–(7) when f_1 and f_2 are the step functions

$$f_1(b) = \begin{cases} 1 & \text{if } b > b_{\mathrm{I}}, \\ 0 & \text{otherwise}, \end{cases} \qquad f_2(b) = \begin{cases} 1 & \text{if } b > b_{\mathrm{II}}, \\ 0 & \text{otherwise}. \end{cases} \tag{29}$$

In this case the system of differential equations is piecewise linear, i.e., the real line **R** can be divided into segments, in which the differential equations are linear with constant coefficients, hence the solutions can be given explicitly. The joining conditions at the endpoints of the segments give a system of nonlinear algebraic equations that has to be solved to obtain the solution. Here we consider the solutions that satisfy hypotheses (H1)–(H3), but the algorithm presented below works also in the more general case, when instead of (H2) it is assumed only that the number of points where b attains the value b_{I} is finite.

We denote the points where b attains the value b_{I} or b_{II} with $l_1 < l_2 < \cdots < l_{n+1}$. If $b \equiv b_{\mathrm{II}}$ in $[y^*, \infty)$, then let $l_{n+1} = y^*$ and the points $y > y^*$ do not appear in the set $\{l_1, \ldots, l_{n+1}\}$. Let

$$b_k = b(l_k) \quad \text{for } k = 1, 2, \ldots, n+1. \tag{30}$$

Hence the value of b_k is b_{I} or b_{II}. As mentioned above, we can assume $l_1 = 0$, because of the translational invariance of the problem. For convenience we will use the notation $l_0 = -\infty$ and $l_{n+2} = \infty$. The points $l_1, \ldots, l_{n+1}$ divide the real line into $n+2$ segments, in each of which the differential equations are linear. Let

$$\varepsilon_k = f_1\big(b(y)\big), \quad \delta_k = f_2\big(b(y)\big) \quad \text{for } y \in (l_k, l_{k+1}),\ k = 0, 1, \ldots, n+1, \tag{31}$$

that is ε_k and δ_k can be 0 or 1.

In sections 2.3–2.5 we have determined the qualitative structure of the temperature profile in the general case. Now we shall use this characterisation in the case of step functions. We have established that the solutions belong to one of the six types summarised in table 1. (Assuming that b satisfies (H1)–(H3).) The table also shows the

Table 1
The six possible types of the temperature profiles. The number of segments determined by the points $l_1, \ldots, l_{n+1}$ and the values of $b_k, \varepsilon_k, \delta_k$ for $k = 1, 2, \ldots, n+1$ are shown.

Type	Number of segments $(n+2)$	Value of b_k	Value of ε_k	Value of δ_k
$b_{\rm I} < b_{\rm II}$ front	3	$b_1 = b_{\rm I}, b_2 = b_{\rm II}$	$\varepsilon_1 = 1, \varepsilon_2 = 1$	$\delta_1 = 0, \delta_2 = 1$
$b_{\rm I} = b_{\rm II}$ front	2	$b_1 = b_{\rm I} = b_{\rm II}$	$\varepsilon_1 = 1$	$\delta_1 = 1$
$b_{\rm I} = b_{\rm II}$ pulse	3	$b_1 = b_{\rm I} = b_{\rm II} = b_2$	$\varepsilon_1 = 1, \varepsilon_2 = 0$	$\delta_1 = 1, \delta_2 = 0$
$b_{\rm I} > b_{\rm II}$ front 1	3	$b_1 = b_{\rm II}, b_2 = b_{\rm I}$	$\varepsilon_1 = 0, \varepsilon_2 = 1$	$\delta_1 = 1, \delta_2 = 1$
$b_{\rm I} > b_{\rm II}$ front 2	4	$b_1 = b_{\rm II}, b_2 = b_{\rm I}$	$\varepsilon_1 = 0, \varepsilon_2 = 1$	$\delta_1 = 1, \delta_2 = 1$
		$b_3 = b_{\rm I}$	$\varepsilon_3 = 0$	$\delta_3 = 1$
$b_{\rm I} > b_{\rm II}$ pulse	5	$b_1 = b_{\rm II}, b_2 = b_{\rm I}$	$\varepsilon_1 = 0, \varepsilon_2 = 1$	$\delta_1 = 1, \delta_2 = 1$
		$b_3 = b_{\rm I}, b_4 = b_{\rm II}$	$\varepsilon_3 = 0, \varepsilon_4 = 0$	$\delta_3 = 1, \delta_4 = 0$

number of segments determined by the points $l_1, \ldots, l_{n+1}$ and the values of $b_k, \varepsilon_k, \delta_k$ for $k = 1, 2, \ldots, n+1$.

We now follow the algorithm described below to determine the profiles and the flame velocity in each case.

Step 1

We choose the type of the solution we wish to determine. We note that the type of solution depends also on the parameters α and β, hence it can happen that the chosen type of solution does not exist for the given values of α and β.

Once the type is chosen, the value of n is given together with b_k, ε_k and δ_k (for $k = 1, \ldots, n+1$) according to table 1. We consider $c, l_2, \ldots, l_{n+1}$ to be given ($l_1 = 0$ is assumed) and express the solution in terms of them. In the final step we derive a system of $n+1$ algebraic equations that determine the value of the various unknowns.

Step 2

We solve the differential equations in each segment (l_k, l_{k+1}) for $k = 0, 1, \ldots, n+1$. In the interval (l_k, l_{k+1}) system (2)–(4) takes the form

$$b''(y) - cb'(y) + \varepsilon_k a(y) - \delta_k \alpha w(y) = 0, \tag{32}$$

$$\frac{1}{L_A} a''(y) - ca'(y) - \varepsilon_k a(y) = 0, \tag{33}$$

$$\frac{1}{L_W} w''(y) - cw'(y) - \delta_k \beta w(y) = 0. \tag{34}$$

First we solve equations (33) and (34), since these are independent homogeneous linear differential equations, and then we use their solution to solve the inhomogeneous linear differential equation (32). The general solution of equations (33) and (34) can be written in the form

$$a(y) = A_k e^{\lambda_{k1} y} + B_k e^{\lambda_{k2} y} \quad (k = 0, 1, \dots, n+1), \tag{35}$$

$$w(y) = C_k e^{\nu_{k1} y} + D_k e^{\nu_{k2} y} \quad (k = 0, 1, \dots, n+1), \tag{36}$$

where $\lambda_{k1} > \lambda_{k2}$ are the solutions of

$$\lambda^2 - L_A c\lambda - \varepsilon_k L_A = 0 \tag{37}$$

and $\nu_{k1} > \nu_{k2}$ are the solutions of

$$\nu^2 - L_W c\nu - \delta_k L_W \beta = 0. \tag{38}$$

The general solution of equation (32) can be written as

$$b(y) = E_k + F_k e^{cy} + R_{k1} e^{\lambda_{k1} y} + R_{k2} e^{\lambda_{k2} y} + R_{k3} e^{\nu_{k1} y} + R_{k4} e^{\nu_{k2} y} \quad (k = 0, 1, \dots, n+1). \tag{39}$$

Before proceeding to step 3 we outline the remaining part of the algorithm. The coefficients A_k, B_k, C_k, D_k ($4n+8$ unknowns) are determined by the joining conditions that a and w are continuously differentiable at $l_1, \dots, l_{n+1}$ ($4n+4$ equations) and by the boundary conditions (5)–(6) (4 equations). The coefficients $R_{k1}, R_{k2}, R_{k3}, R_{k4}$ are determined by A_k, B_k, C_k, D_k. The coefficients E_k and F_k are determined by the boundary conditions (30). Finally, we will have $n+1$ equations arising from the continuity of the derivative of b at the points $l_1, \dots, l_{n+1}$. These equations determine the $n+1$ unknowns $c, l_2, \dots, l_{n+1}$. The resulting system of nonlinear algebraic equations has to be solved numerically.

Step 3

We determine the coefficients A_k, B_k, C_k, D_k for $k = 0, 1, \dots n+1$. First we make use of boundary conditions (5). Since $\varepsilon_0 = \delta_0 = 0$, therefore from (37) and (38):

$$\lambda_{01} = L_A c, \quad \lambda_{02} = 0, \quad \nu_{01} = L_W c, \quad \nu_{02} = 0. \tag{40}$$

Hence (5) yields

$$B_0 = 1, \quad D_0 = 1. \tag{41}$$

To use boundary conditions (6) we note that

$$\lambda_{n+1,1} > 0, \quad \nu_{n+1,1} > 0. \tag{42}$$

Hence (6) yields

$$A_{n+1} = 0, \quad C_{n+1} = 0. \tag{43}$$

The joining conditions expressing the continuous differentiability of a at l_k (for $k = 1, \dots, n+1$) read as

$$A_{k-1}\mathrm{e}^{\lambda_{k-1,1}l_k} + B_{k-1}\mathrm{e}^{\lambda_{k-1,2}l_k} = A_k\mathrm{e}^{\lambda_{k1}l_k} + B_k\mathrm{e}^{\lambda_{k2}l_k}, \tag{44}$$

$$A_{k-1}\lambda_{k-1,1}\mathrm{e}^{\lambda_{k-1,1}l_k} + B_{k-1}\lambda_{k-1,2}\mathrm{e}^{\lambda_{k-1,2}l_k} = A_k\lambda_{k1}\mathrm{e}^{\lambda_{k1}l_k} + B_k\lambda_{k2}\mathrm{e}^{\lambda_{k2}l_k}. \tag{45}$$

Similarly, for w we have

$$C_{k-1}\mathrm{e}^{\nu_{k-1,1}l_k} + D_{k-1}\mathrm{e}^{\nu_{k-1,2}l_k} = C_k\mathrm{e}^{\nu_{k1}l_k} + D_k\mathrm{e}^{\nu_{k2}l_k}, \tag{46}$$

$$C_{k-1}\nu_{k-1,1}\mathrm{e}^{\nu_{k-1,1}l_k} + D_{k-1}\nu_{k-1,2}\mathrm{e}^{\nu_{k-1,2}l_k} = C_k\nu_{k1}\mathrm{e}^{\nu_{k1}l_k} + D_k\nu_{k2}\mathrm{e}^{\nu_{k2}l_k}. \tag{47}$$

These $4n + 4$ equations together with the 4 equations in (41) and (43) give a system of $4n + 8$ linear equations for the $4n + 8$ unknowns A_k, B_k, C_k, D_k ($k = 0, 1, \dots, n + 1$). If $c, l_1, \dots, l_{n+1}$ are given, then A_k, B_k, C_k, D_k can be obtained explicitly.

Step 4

We now determine the coefficients E_k, F_k, R_{ki} for $k = 0, 1, \dots, n + 1$, $i = 1, 2, 3, 4$. It is easy to see that $\varepsilon_0 = \delta_0 = 0$ implies that

$$b(y) = b_1\mathrm{e}^{cy}$$

for $y < 0$, hence

$$E_0 = R_{01} = R_{02} = R_{03} = R_{04} = 0, \quad F_0 = b_1. \tag{48}$$

The values of R_{ki} can be readily obtained by the method of undetermined coefficients. Namely, we substitute (35), (36) and (39) into (32) and put the coefficients of $\mathrm{e}^{\lambda_{k1}y}$, $\mathrm{e}^{\lambda_{k2}y}$, $\mathrm{e}^{\nu_{k1}y}$ and $\mathrm{e}^{\nu_{k2}y}$ equal to zero, to obtain

$$R_{k1} = \frac{\varepsilon_k A_k}{\lambda_{k1}(c - \lambda_{k1})}, \qquad R_{k2} = \frac{\varepsilon_k B_k}{\lambda_{k2}(c - \lambda_{k2})},$$

$$R_{k3} = \frac{\delta_k \alpha C_k}{\nu_{k1}(\nu_{k1} - c)}, \qquad R_{k4} = \frac{\delta_k \alpha D_k}{\nu_{k2}(\nu_{k2} - c)}. \tag{49}$$

Since the values of A_k, B_k, C_k, D_k have already been determined, expression (49) gives the values of R_{ki}.

The values of E_k and F_k for $k = 1, \dots, n$ can be obtained from the boundary conditions (30)

$$b(l_k) = b_k, \quad b(l_{k+1}) = b_{k+1}. \tag{50}$$

Introducing

$$G_k = R_{k1}\mathrm{e}^{\lambda_{k1}l_k} + R_{k2}\mathrm{e}^{\lambda_{k2}l_k} + R_{k3}\mathrm{e}^{\nu_{k1}l_k} + R_{k4}\mathrm{e}^{\nu_{k2}l_k},$$
$$H_k = R_{k1}\mathrm{e}^{\lambda_{k1}l_{k+1}} + R_{k2}\mathrm{e}^{\lambda_{k2}l_{k+1}} + R_{k3}\mathrm{e}^{\nu_{k1}l_{k+1}} + R_{k4}\mathrm{e}^{\nu_{k2}l_{k+1}},$$

(50) reads as

$$b_k = E_k + F_k\mathrm{e}^{cl_k} + G_k, \quad b_{k+1} = E_k + F_k\mathrm{e}^{cl_{k+1}} + H_k$$

yielding

$$E_k = \frac{(b_k - G_k)e^{cl_{k+1}} + (H_k - b_{k+1})e^{cl_k}}{e^{cl_{k+1}} - e^{cl_k}}, \tag{51}$$

$$F_k = \frac{b_k - G_k + H_k - b_{k+1}}{e^{cl_k} - e^{cl_{k+1}}}. \tag{52}$$

The value of E_{n+1} and F_{n+1} are given by the equation

$$b(l_{n+1}) = b_{n+1} \tag{53}$$

and the boundary condition (6). The boundary condition, (42) and (53) imply

$$F_{n+1} = 0, \qquad E_{n+1} = b_{n+1} - G_{n+1}.$$

Step 5

We determine the unknowns $c, l_2, \ldots, l_{n+1}$ from the joining conditions for b (recall that $l_1 = 0$). The function b has to be continuously differentiable at $l_1, \ldots, l_{n+1}$, that is the left-hand side limit and the right-hand side limit of b' has to be the same at those points. Hence we have $n + 1$ equations for the $n + 1$ unknowns $c, l_2, \ldots, l_{n+1}$. This matching condition in l_k reads as

$$\begin{aligned} &F_{k-1}ce^{cl_k} + R_{k-1,1}\lambda_{k-1,1}e^{\lambda_{k-1,1}l_k} + R_{k-1,2}\lambda_{k-1,2}e^{\lambda_{k-1,2}l_k} \\ &\quad + R_{k-1,3}\nu_{k-1,1}e^{\nu_{k-1,1}l_k} + R_{k-1,4}\nu_{k-1,2}e^{\nu_{k-1,2}l_k} \\ &\quad = F_kce^{cl_k} + R_{k1}\lambda_{k1}e^{\lambda_{k1}l_k} + R_{k2}\lambda_{k2}e^{\lambda_{k2}l_k} + R_{k3}\nu_{k1}e^{\nu_{k1}l_k} + R_{k4}\nu_{k2}e^{\nu_{k2}l_k}. \end{aligned} \tag{54}$$

This system can be solved by the Newton–Raphson method for $c, l_2, \ldots, l_{n+1}$. It turned out that for certain values of α and β this system has 2 or 3 solutions that are difficult to find with this method. Therefore we solved the system for $\alpha, l_2, \ldots, l_{n+1}$ with a given value of c, then we got a unique solution. Hence the (α, c) diagram is parametrised by c. Once the values of $\alpha, l_2, \ldots, l_{n+1}$ are obtained, it has to be checked that the value of $b(y)$ lies between b_k and b_{k+1} for all $y \in (l_k, l_{k+1})$.

4. Results

The algorithm detailed in the previous section was implemented as a computer program. The parameters of the program are

$$n, b_{\mathrm{I}}, b_{\mathrm{II}}, c, \beta, b_1, \ldots, b_{n+1}, \varepsilon_1, \ldots, \varepsilon_{n+1}, \delta_1, \ldots, \delta_{n+1}.$$

The input of the program is the $(n + 1)$-dimensional vector

$$(\alpha, l_2, \ldots, l_{n+1}).$$

The output of the program is the $(n+1)$-dimensional vector the coordinates of which are obtained as the difference of the left-hand side and the right-hand side of the equations in (54). Thus the program defines a function $\mathcal{F}:\mathbf{R}^{n+1} \to \mathbf{R}^{n+1}$. The solution of the equation

$$\mathcal{F}(x) = 0$$

was obtained by the Newton–Raphson method. We will present the explicit form of system (54) only in the cases $n = 0$ and $n = 1$. As mentioned above, all the results determined numerically are for unit Lewis numbers, i.e., $L_A = L_W = 1$. However, all calculations are made for arbitrary Lewis numbers.

4.1. Case $b_{\mathrm{I}} < b_{\mathrm{II}}$

According to proposition 7 we have $n = 1$ and the values of $b_k, \varepsilon_k, \delta_k$ are given in the first row of table 1. Now system (54) reads as

$$\left(b_{\mathrm{I}} - \frac{\eta_2}{\eta_2 - c}\right)\mathrm{e}^{cl_2} + \frac{c}{\eta_2 - c}\mathrm{e}^{\eta_2 l_2} - b_{\mathrm{II}} + 1 = 0, \tag{55}$$

$$\beta\frac{c - \xi_2}{\xi_2}\left(b_{\mathrm{I}} - \frac{\eta_2}{\eta_2 - c}\right)\mathrm{e}^{cl_2} = \alpha, \tag{56}$$

where

$$\eta_{1,2} = \frac{1}{2}\left(L_A c \pm \sqrt{L_A^2 c^2 + 4L_A}\right), \qquad \xi_{1,2} = \frac{1}{2}\left(L_W c \pm \sqrt{L_W^2 c^2 + 4L_W\beta}\right). \tag{57}$$

The first equation can be solved for l_2 if c is given. It can be easily seen that there is a critical value c_{crit} of c, such that for $c < c_{\mathrm{crit}}$ there is no solution for l_2 and there are two solutions if $c > c_{\mathrm{crit}}$. It can be shown that the condition

$$b_{\mathrm{I}} < b(y) < b_{\mathrm{II}} \quad \text{for all } y \in (0, l_2)$$

is satisfied only if l_2 is the smaller solution of (55). When l_2 is determined equation (56) gives the value of α belonging to the given c. It is easy to see that the condition

$$b_{\mathrm{II}} < b(y) \quad \text{for all } y > l_2$$

is equivalent to

$$b_+ > b_{\mathrm{II}}$$

which yields from (11)

$$1 - \frac{\alpha}{\beta} > b_{\mathrm{II}}. \tag{58}$$

Hence a part of the (α, c) diagram determined by (55)–(56) must be cut off by the condition (58). The (α, c) diagram is shown in figure 1 for different values of β. The temperature profiles for different values of c and fixed value $\beta = 2$ can be seen in figure 2. The value $c = 2.57232$ is the critical value of the velocity, below which equation (55) has no solution for l_2 when $\beta = 2$.

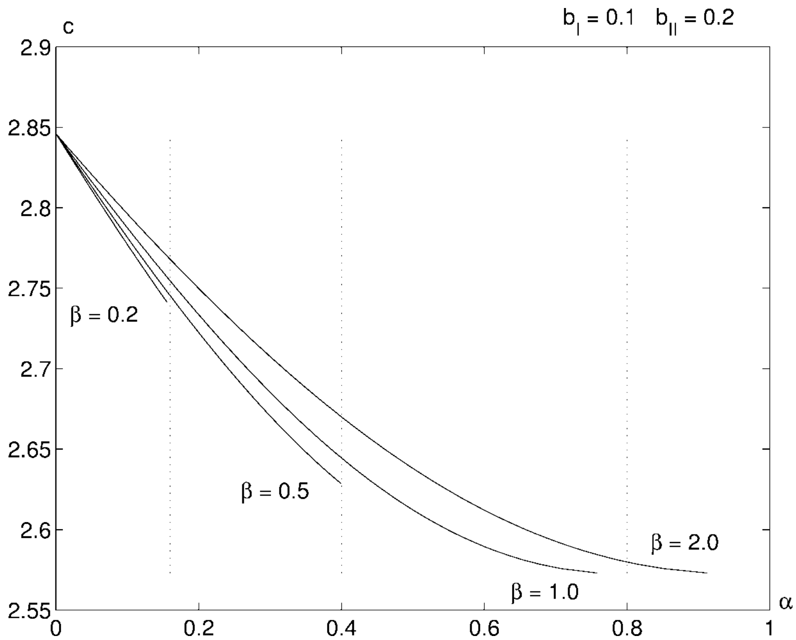

Figure 1. The (α, c) diagram for various values of β in the case $b_{\mathrm{I}} = 0.1$, $b_{\mathrm{II}} = 0.2$. The dotted lines are drawn at $\alpha = \beta(1 - b_{\mathrm{II}})$.

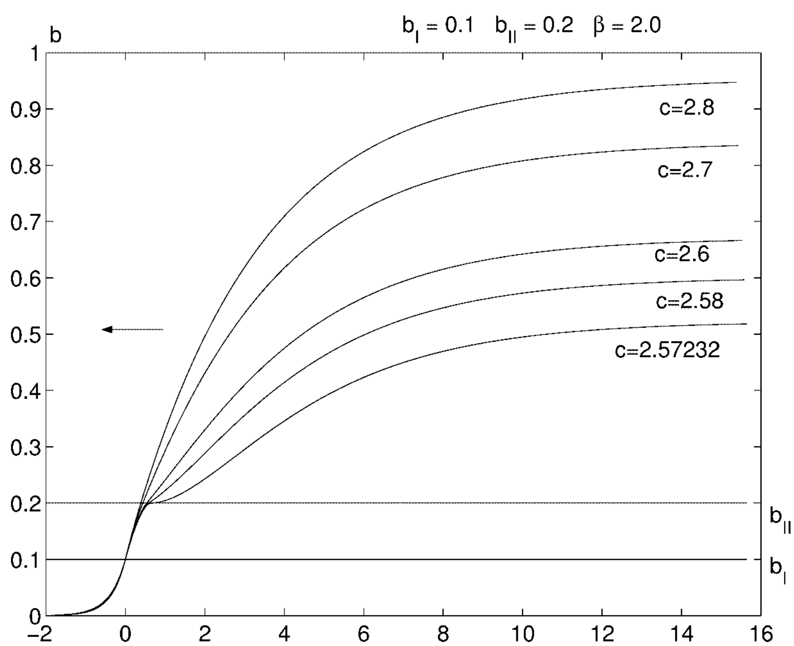

Figure 2. Temperature profiles for different values of c and fixed value $\beta = 2$ in the case $b_{\mathrm{I}} = 0.1$, $b_{\mathrm{II}} = 0.2$. The value $c = 2.57232$ is the critical value of the velocity, below which there is no solution.

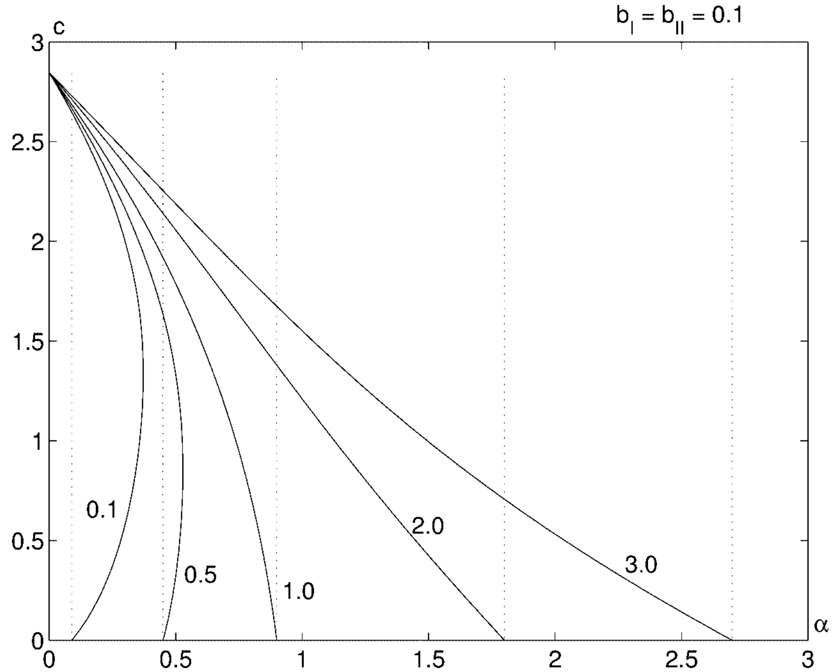

Figure 3. The (α, c) diagram for various values of β in the case $b_{\rm I} = b_{\rm II} = 0.1$. The dotted lines are drawn at $\alpha = \beta(1 - b_{\rm I})$. The points of the diagrams lying on the left-hand side of the corresponding dotted line belong to front solutions, those lying on the right-hand side belong to pulse solutions.

4.2. *Case* $b_{\rm I} = b_{\rm II}$

According to proposition 8 we can have front or pulse type solutions with $n = 0$ and $n = 1$, respectively. The values of $b_k, \varepsilon_k, \delta_k$ are given in the second and third rows of table 1.

In the case of fronts (54) contains only one equation $(n + 1 = 1)$

$$\alpha = \beta^2 \frac{\eta_2^2 - b_{\rm I}}{\xi_2^2}. \tag{59}$$

(The parameters η_2 and ξ_2 are defined in (57).) This equation gives the (α, c) diagram directly, but according to proposition 9 the condition

$$\alpha < \beta(1 - b_{\rm I}) \tag{60}$$

has to be satisfied. Hence only that part of the (α, c) diagram determined by (59), for which condition (60) holds, is appropriate. If $\beta \geqslant 1$, then (60) is fulfilled at all points of the diagram. For $\beta < 1$ the condition (60) cuts off one part of the diagram, the part of the diagram belonging to the pulse type solutions. In the case of pulse type solutions $n = 1$ and the values of $b_k, \varepsilon_k, \delta_k$ are given in the third row of table 1. Then system (54) has a solution only if $\beta < 1$, i.e., for $\beta \geqslant 1$ there are no pulse solutions. For $\beta < 1$ the part of the (α, c) diagram belonging to the pulse solutions joins smoothly to the other part,

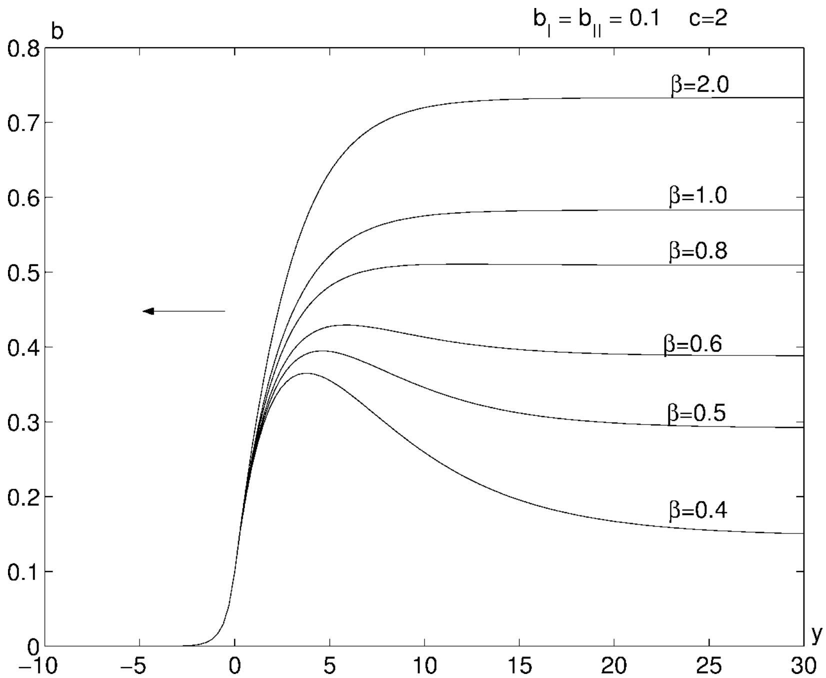

Figure 4. Temperature profiles for different values of β and fixed value $c = 2$ in the case $b_{\mathrm{I}} = b_{\mathrm{II}} = 0.1$.

belonging to the front type solutions, at $\alpha = \beta(1-b_{\mathrm{I}})$. The diagrams for different values of β are shown in figure 3. For every value of β a dotted line is drawn at $\alpha = \beta(1 - b_{\mathrm{I}})$. That is the value of α where the diagram intersects the α axis and at the same time it separates the front and pulse regions. The points of the diagram on the left-hand side of the corresponding dotted line belong to front type temperature profiles, and those on the right-hand side belong to pulse profiles. We can see that for $\beta \geqslant 1$ the entire diagram lies on the left-hand side of the corresponding dotted line. The temperature profiles for $c = 2$ and different values of β can be seen in figure 4. For larger values of β the temperature is monotone increasing. However, as β is reduced there is an overshoot in the temperature profile before the final conditions are attained. This effect becomes more pronounced as β is decreased.

4.3. *Case* $b_{\mathrm{I}} > b_{\mathrm{II}}$

According to proposition 10 we can have front 1, front 2 or pulse type solutions with $n = 1$, $n = 2$ and $n = 3$, respectively. The values of b_k, ε_k, δ_k are given in the last three rows of table 1.

In the case of front 1 solutions system (54) consists of two equations. It has a solution for any value of β, however, only those solutions are appropriate, for which the condition $\alpha < \beta(1-b_{\mathrm{I}})$ holds. There exists a critical value β_2 of β, such that, for $\beta > \beta_2$, all solutions satisfy the condition. Unlike the case $b_{\mathrm{I}} = b_{\mathrm{II}}$ now the (α, c) diagram is not monotone for all values of β. There exists another critical value β_3 of β, such that for

$\beta \geqslant \beta_3$ the diagram is monotone and for $\beta < \beta_3$ it is S-shaped, i.e., there is a range of α for which there are 3 different velocities. Hence, in this case, our system can have 3 solutions for the same parameter values. It will be the object of future work to find out which of them are stable.

In the case of front 2 solutions system (54) consists of three equations. It has a solution only if $\beta < \beta_2$. However, only those solutions are appropriate, for which the condition

$$\beta(1 - b_{\mathrm{I}}) \leqslant \alpha < \beta(1 - b_{\mathrm{II}}) \tag{61}$$

holds. This part of the diagram joins smoothly to the part belonging to front 1 solutions at $\alpha = \beta(1 - b_{\mathrm{I}})$. We found a third critical value β_1 of β, such that for $\beta > \beta_1$ the right-hand side inequality of (61) holds.

In the case of pulse solutions system (54) consists of four equations. It has a solution only if $\beta < \beta_1$. This part of the diagram joins smoothly to the part belonging to front 2 solutions at $\alpha = \beta(1 - b_{\mathrm{II}})$.

Summarising have the following cases according to the structure of the (α, c) diagram.

- If $0 < \beta \leqslant \beta_1$, then the diagram is S-shaped and it consists of three parts belonging to front 1, front 2 and pulse solutions, respectively.
- If $\beta_1 < \beta \leqslant \beta_2$, then the diagram is S-shaped and it consists of two parts belonging to front 1 and front 2 solutions, respectively.
- If $\beta_2 < \beta < \beta_3$, then the diagram is S-shaped and all points belong to front 1 solutions.
- If $\beta_3 \leqslant \beta$, then the diagram is monotone and all points belong to front 1 solutions.

The transition of the (α, c) diagram as β is varied is shown in figure 5, where $b_{\mathrm{I}} = 0.2$ and $b_{\mathrm{II}} = 0.1$. For every value of β a dotted line is drawn at $\alpha = \beta(1-b_{\mathrm{I}})$ where the diagram intersects the α axis and at the same time it separates the front 1 and front 2 regions. The front 2 and pulse regions are separated by the vertical line at $\alpha = \beta(1-b_{\mathrm{II}})$, which is not shown in the figure. The critical values of β can be determined as follows. If $\beta = \beta_1$, then the diagram is tangential to the vertical line drawn at $\alpha = \beta(1-b_{\mathrm{II}})$. For these values of b_{I} and b_{II} this is, approximately, $\beta_1 \approx 0.15$. If $\beta = \beta_2$, then the diagram is tangential to the vertical line drawn at $\alpha = \beta(1 - b_{\mathrm{I}})$. For these values of b_{I} and b_{II} this is, approximately, $\beta_2 \approx 0.26$. If $\beta = \beta_3$, then the two turning points of the diagram coincide. For these values of b_{I} and b_{II} this is, approximately, $\beta_3 \approx 0.3$.

In figure 6 the (α, c) diagram is shown for $\beta = 0.1$, $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. This value of β is below the critical value β_1, hence all of the three type solutions exist. The dotted lines are drawn at $\alpha = \beta(1 - b_{\mathrm{I}})$ and at $\alpha = \beta(1 - b_{\mathrm{II}})$. These lines separate the front 1, front 2 and pulse regions.

The profiles are shown in figures 7–9. In figure 7 $\alpha = 0.0788$ to which three different velocity values and three front 1 type solutions belong. In figure 8 $\alpha = 0.087$

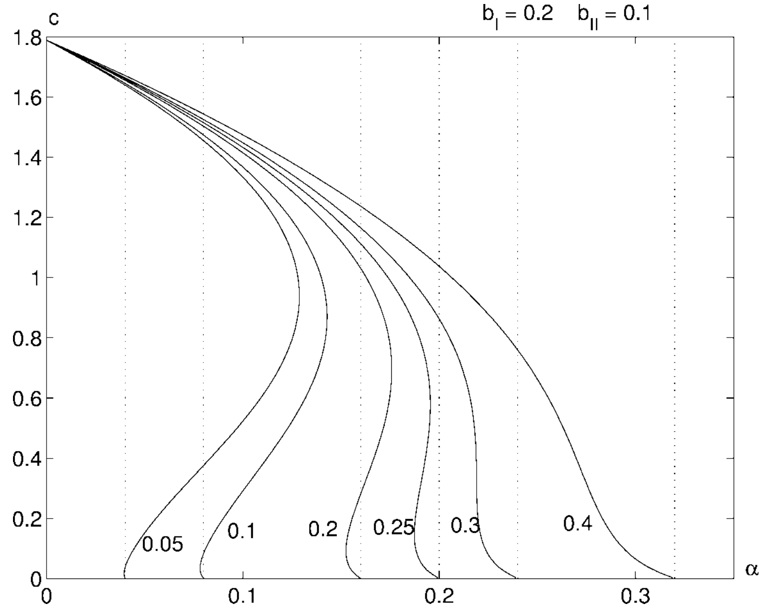

Figure 5. The (α, c) diagram for various values of β (shown in the figure) in the case $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. The dotted lines are drawn at $\alpha = \beta(1 - b_{\mathrm{I}})$. The points of the diagrams lying on the left-hand side of the corresponding dotted line belong to front 1 solutions, those lying on the right-hand side belong to front 2 or pulse solutions.

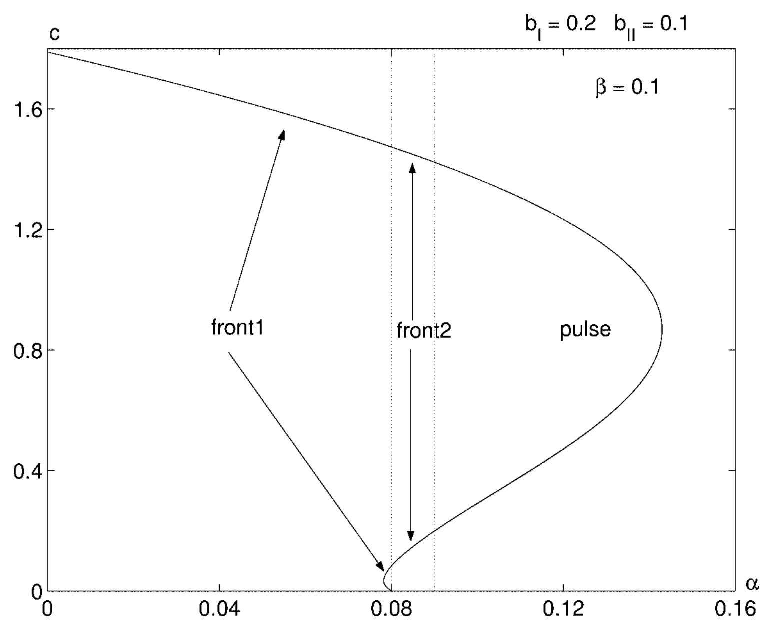

Figure 6. The (α, c) diagram for $\beta = 0.1$, $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. The dotted lines are drawn at $\alpha = \beta(1 - b_{\mathrm{I}})$ and at $\alpha = \beta(1 - b_{\mathrm{II}})$ separating the regions belonging to front 1, front 2 and pulse solutions.

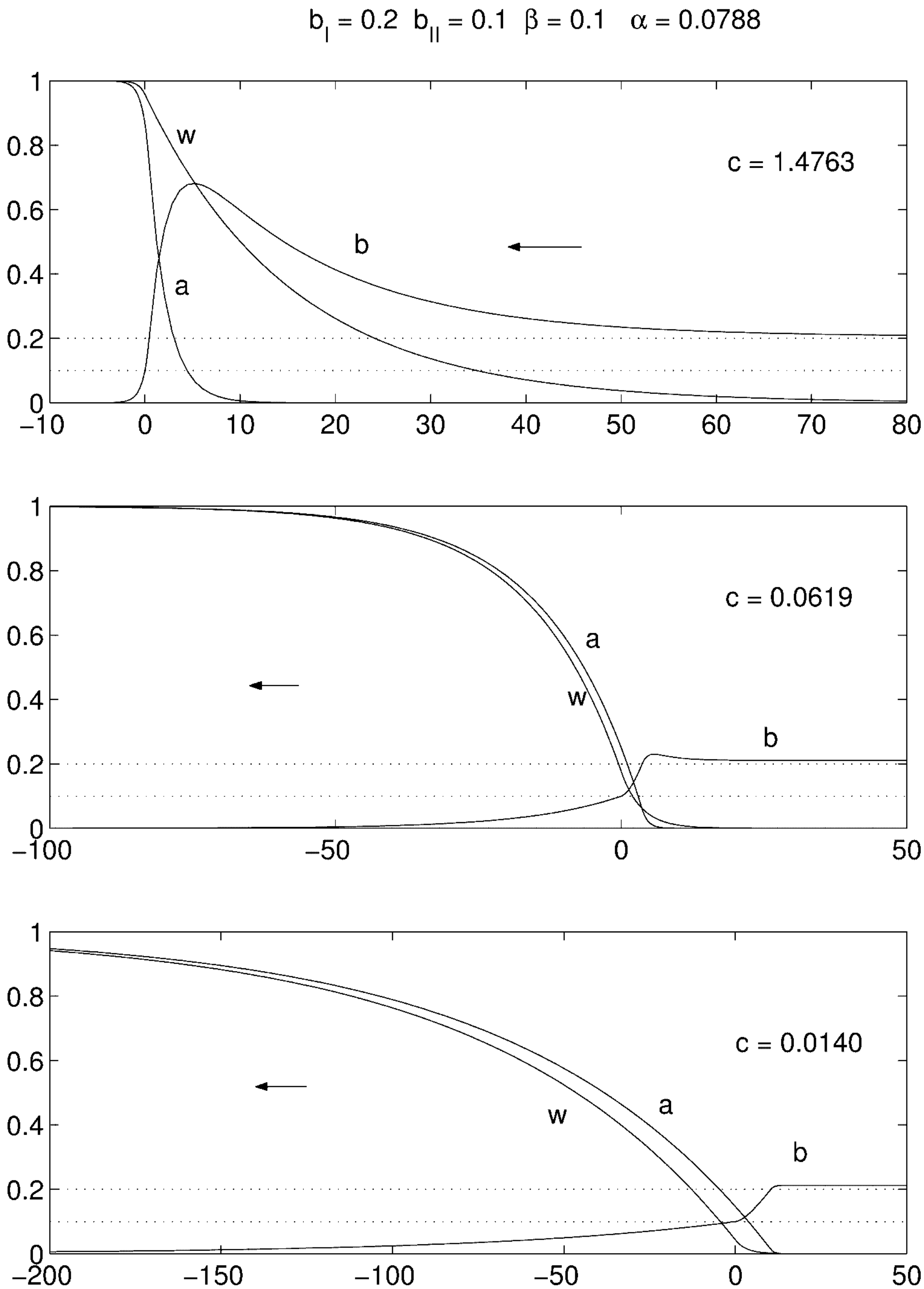

Figure 7. Temperature (b), fuel concentration (a) and inhibitor concentration (w) profiles for three different values of c (shown in the figure) belonging to the parameter value $\alpha = 0.078$ in the case $\beta = 0.1$, $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. For this value of α there are three front 1 type temperature profiles.

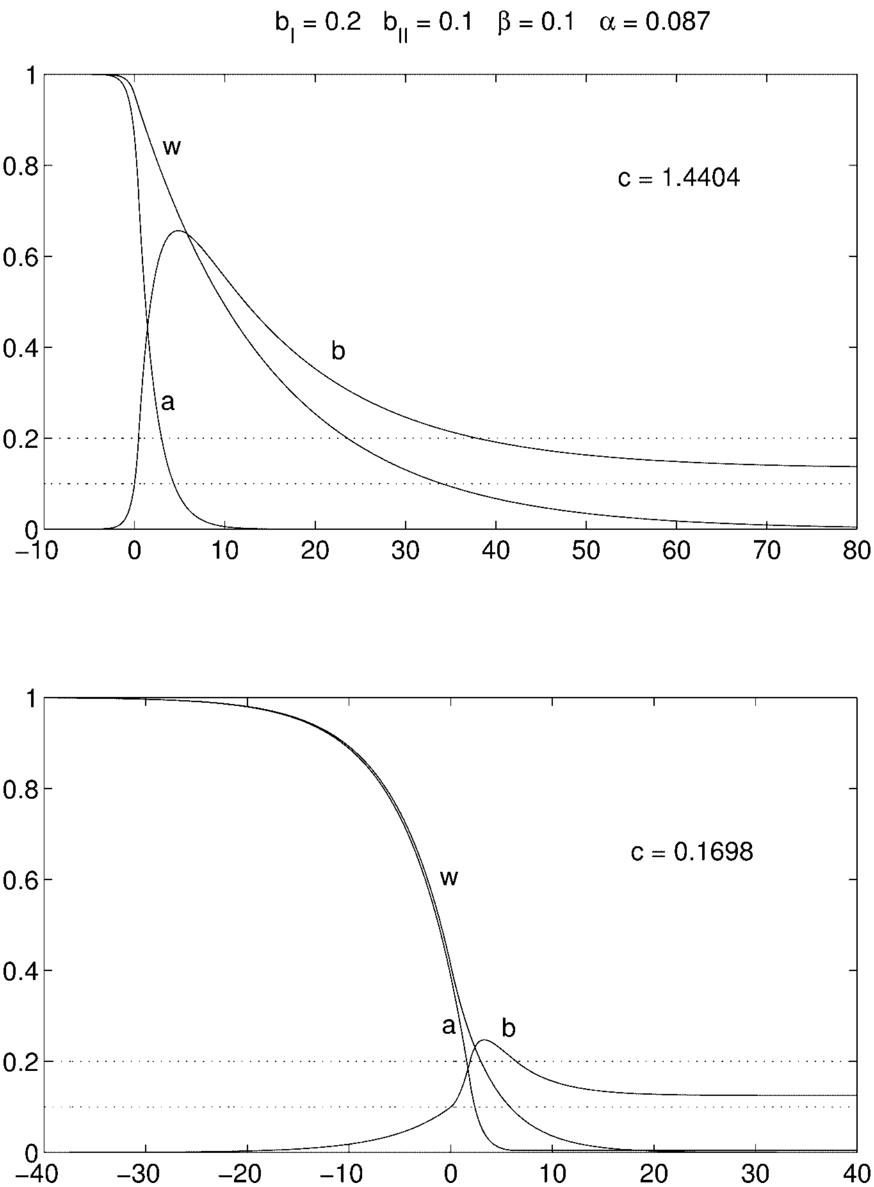

Figure 8. Temperature (b), fuel concentration (a) and inhibitor concentration (w) profiles for two different values of c (shown in the figure) belonging to the parameter value $\alpha = 0.087$ in the case $\beta = 0.1$, $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. For this value of α there are two front 2 type temperature profiles.

to which two different velocity values and two front 2 type solutions belong. In figure 9 $\alpha = 0.12$ to which two different velocity values and two pulse type solutions belong. Comparing the fuel (a) and the inhibitor (w) profiles, we can say that generally the fuel is consumed earlier, but for very small values of the velocity (see figure 7) the inhibitor can be consumed faster.

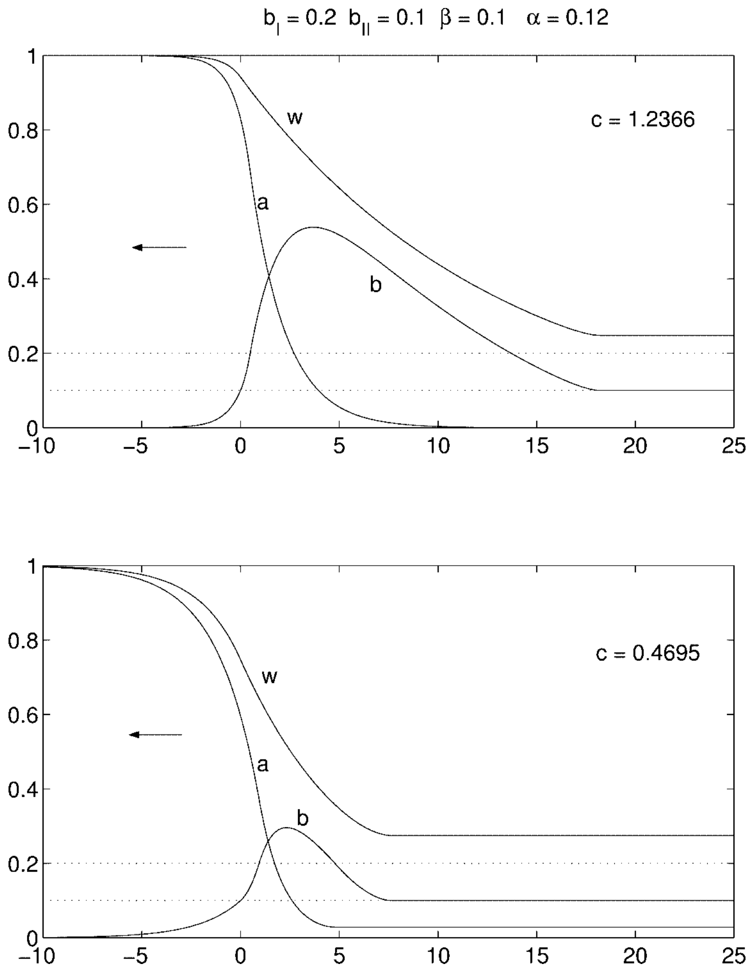

Figure 9. Temperature (b), fuel concentration (a) and inhibitor concentration (w) profiles for two different values of c (shown in the figure) belonging to the parameter value $\alpha = 0.12$ in the case $\beta = 0.1$, $b_{\mathrm{I}} = 0.2$, $b_{\mathrm{II}} = 0.1$. For this value of α there are two pulse type temperature profiles.

5. Conclusions

We have studied the propagation of a flame supported by an exothermic chemical reaction under adiabatic conditions and subject to inhibition through a parallel endothermic chemical process. The temperature dependence of the reaction rates was assumed to have a generalised Arrhenius type form with an ignition temperature, below which there is no reaction. The behaviour of the solutions of our model (2)–(7) depends on the (scaled) ignition temperatures b_{I} and b_{II} and on the dimensionless parameters α and β. We can think of α as a heat loss parameter – it represents the heat lost in the endothermic decay of the inhibitor relative to that produced by the exothermic combustion of the fuel. The parameter β represents the rate at which inhibitor is consumed relative to the consumption of fuel. The heat loss through the endothermic reaction has a strong quenching effect on wave initiation, combustion waves forming only when $\alpha < \alpha_{\rm crit}$. This effect is, in some respects, analogous to the extinction of wave propagation when heat is lost through Newtonian cooling.

In section 2 we have identified the different types of behaviour that can be supported by our general model, i.e., when the concrete form of the temperature dependence of the reaction rates was not specified. (It was assumed only that f_1 and f_2 satisfy (8)–(9).) We found that the structure of the temperature profile depends mainly on the value of $b_{\rm I}$ relative to $b_{\rm II}$. If $b_{\rm I} < b_{\rm II}$, then it has a front structure. If $b_{\rm I} \geqslant b_{\rm II}$, then it can be either a front or a pulse. Which type occurs depends most strongly on the parameters α and β, the other parameters (the Lewis numbers and the concrete form of the functions f_1 and f_2) are not especially significant in determining its qualitative structure.

Then we investigated our model in detail in the case when f_1 and f_2 are step functions. In this case the system of differential equations is piecewise linear, i.e., the real line **R** can be divided into segments, in which the differential equations are linear with constant coefficients, hence the solutions can be given explicitly. The joining conditions at the endpoints of the segments give a system of nonlinear algebraic equations that has to be solved numerically to obtain the solution. In section 3 an algorithm was presented to execute this procedure.

The results obtained in the step function case were presented in section 4. We determined the wave speed (c), cooling parameter (α), curves for various values of the parameters β, $b_{\rm I}$ and $b_{\rm II}$. It can have three different shapes, hence we get other forms of quenching, than in the case of Newtonian cooling. In the case $b_{\rm I} < b_{\rm II}$ and for larger values of β in the case $b_{\rm I} \geqslant b_{\rm II}$ the flame velocity depends monotonically on α (see figures 1, 3 and 5). For moderate values of β, in the case $b_{\rm I} \geqslant b_{\rm II}$, the (α, c) diagram has a turning point as in the case of Newtonian cooling [2–7]. Hence we can expect a saddle-node bifurcation in our case at $\alpha_{\rm crit}$ (see figures 3 and 5). For small values of β, in the case $b_{\rm I} > b_{\rm II}$, the (α, c) diagram is S-shaped (see figures 5 and 6) as was observed in [9]. Hence we can have three different flame velocities for the same value of the cooling parameter α.

Acknowledgement

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References

[1] M. Marion, Qualitative properties of a nonlinear system for laminar flames without ignition temperature, Nonlinear Anal. 9 (1985) 1269–1292.
[2] J.D. Buckmaster, The quenching of deflagration waves, Combustion and Flame 26 (1976) 151–162.
[3] V. Giovangigli, Nonadiabatic plane laminar flames and their singular limits, SIAM J. Math. Anal. 21 (1990) 1305–1325.

[4] D.G. Lasseigne, T.L. Jackson and L. Jameson, Stability of freely propagating flames revisited, Combust. Theory Modelling 3 (1999) 591–611.

[5] P.L. Simon, S. Kalliadasis, J.H. Merkin and S.K. Scott, Quenching of flame propagation with heat loss (submitted for publication).

[6] 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.

[7] F.A. Williams, *Combustion Theory* (Addison-Wesley, 1985).

[8] J.B. Greenberg, A.C. McIntosh and J. Brindley, Linear stability analysis of laminar premixed spray flames, Proc. Roy. Soc. London Ser. A 457 (2001) 1–31.

[9] T. Mitani, A flame inhibition theory by inert dust and spray, Combust. Flame 43 (1981) 243–253.

[10] T. Mitani and T. Niioka, Extinction phenomena of premixed flames with alkali metal compounds, Combust. Flame 55 (1984) 13–21.

[11] B.F. Gray, S. Kalliadasis, A. Lazarovici, C. Macaskill, J.H. Merkin and S.K. Scott, The suppression of an exothermic branched-chain flame through endothermic reaction and radical scavenging (submitted for publication).

[12] A. Lazarovici, S. Kalliadasis, J.H. Merkin and S.K. Scott, Flame quenching through endothermmic reaction (submitted for publication).

[13] J.D. Buckmaster and G.S.S. Ludford, *Theory of Laminar Flames* (Cambridge University Press, 1982).

[14] J. Warnatz, U. Maas and R.W. Dibble, *Combustion. Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation* (Springer, 2001).

[15] Ya.B. Zeldovich, G.I. Barenblatt, V.B. Librovich and G.M. Makhviladze, *The Mathematical Theory of Combustion and Explosions* (Consultants Bureau, 1985).