

Quenching of flame propagation with heat loss

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Received 1 April 2002

The steady propagation of a planar laminar premixed flame, with a one-step exothermic reaction and linear heat loss, is studied. The corresponding travelling wave equations are solved numerically. The dependence of the flame velocity on the heat loss parameter is determined and compared with known results obtained by asymptotic expansion and other approximations. Due to the introduction of an ignition temperature the problem can be reduced to a bounded interval (of length L) and the graph of flame speed versus heat loss parameter can be parametrised by L . The numerical method is tested in the case of a step function nonlinearity when the exact solution of the differential equations can also be calculated.

KEY WORDS: laminar flame, heat loss, travelling wave

1. Introduction

The theory of the propagation of laminar flames is an important part of combustion theory and has been extensively studied for a range of different complex chemical reactions, see [1–3], for example. The question of flame quenching and propagation inhibition arises naturally in the course of investigating flame propagation. The qualitative features of flame quenching can be studied in the simple case of a first-order reaction, when the reactant A is burnt into a product during an exothermic reaction in the presence of heat loss [2–6]. In this paper the steady propagation of a planar laminar premixed flame is studied in this model case with linear heat loss.

The equations governing our model, written in a moving frame, are [2,3,5–7]

$$mA'(z) = \rho DA''(z) - \mu k(T)\rho A(z), \quad (1)$$

$$C_p m T'(z) = \lambda T''(z) + qk(T)\rho A(z) - h(T(z) - T_a), \quad (2)$$

where

$$k(T) = \begin{cases} \frac{k_0}{\mu} \exp\left(\frac{-E}{R(T - T_1)}\right) & \text{if } T \geq T_1, \\ 0 & \text{otherwise.} \end{cases} \quad (3)$$

See appendix for the list of symbols. (Primes denote differentiation with respect to the travelling wave coordinate z .) Equations (1)–(2) are subject to the following boundary conditions:

$$A \rightarrow A_0, T \rightarrow T_a \quad \text{as } z \rightarrow -\infty, \quad A' \rightarrow 0, T' \rightarrow 0 \quad \text{as } z \rightarrow +\infty. \quad (4)$$

Here A_0 denotes the initial fuel concentration and T_a is the ambient temperature. The boundary conditions at $+\infty$ determine the limit of the functions A and T as follows:

- if $h = 0$ (adiabatic case), then $A \rightarrow 0$ and $T \rightarrow T_b$ as $z \rightarrow +\infty$;
- if $h > 0$ (heat loss case), then $A \rightarrow A_s$ and $T \rightarrow T_a$ as $z \rightarrow +\infty$,

where $0 \leq A_s < A_0$ is to be determined. In the adiabatic case the value of T_b is determined by the other parameters of the system, namely

$$T_b = T_a + \frac{qA_0}{\mu C_p}.$$

In the heat loss case the value of A_s is determined by the differential equations. The ignition temperature T_I is introduced to avoid the so-called cold boundary difficulty. Namely, a necessary condition for the existence of a solution is $T_a \leq T_I$. We shall assume $T_I > 0$. This condition has advantages from the numerical point of view and also excludes the existence of a continuum of solutions [8]. The solution of our problem tends to the one without an ignition temperature as $T_I \rightarrow 0$ [8]. The function k is obtained by a shift from the usual Arrhenius function, hence the reaction term is modified in the whole temperature range. This modification, however, does not cause any qualitative change in the solutions and it has the advantage that the source term is continuous, hence the solutions are in C^2 , which is useful from the numerical point of view.

Our system had been widely studied by various methods. The main results can be broadly classified as

- Existence results, giving conditions on the parameters for the existence and non-existence (extinction) of travelling wave solutions [1,9–14].
- Approximating formulas for the mass flux and the profiles obtained by asymptotic expansion [4,5,9,11,15].
- Lower and upper estimates for the mass flux obtained by analytic methods [3,9,12,14].
- Numerical results for the mass flux and the profiles [16–22,31].

In the adiabatic case there are results in all the above four categories. In the heat loss case the numerical solution is not so well documented as it might seem, as is pointed out in [19]. The majority of the numerical simulations use the time dependent system, e.g., [22–24]. The steady problem can be solved by pseudo arclength continuation methods that use first an Euler predictor step and then a Newton–Raphson iteration along the bifurcation curve [25]. This method was implemented for the numerical simulation of the planar one-dimensional flame propagation [26], and was applied for the investigation of chemically complex systems, see, e.g., [27]. Complex systems have also been

investigated with radiative heat loss [28,29]. However, according to our knowledge, the only paper where the simple system (1)–(4) was solved numerically and the numerical results are compared to those obtained by asymptotic expansion is [19]. In that paper graphs of the flame speed versus the heat loss parameter are computed and compared to those obtained by high activation energy asymptotics. The ignition temperature is not included in their model description. They used the transformation $y = \tanh(z)$ of the independent variable to reduce the problem to a bounded interval, which caused problems in the computation of the tail of the profiles. In [19] a different boundary condition is used at the rear of the wave compared to ours and the method of finite differences is used to discretise the problem.

The aim of our work is the systematic numerical study of the system in the case of $h > 0$, i.e., to determine the dependence of the mass flux m on the heat loss parameter h together with the concentration and temperature profiles. The results of this paper are theoretical. First, our numerical results confirm the qualitative picture of the graphs of the flame speed versus the heat loss parameter obtained by high activation energy asymptotics. Second, our results show the range of validity of the asymptotic expansion. The novelties in this work are as follows.

- The problem is reduced analytically to a bounded interval (of length L) using the ignition temperature. Therefore the tail of the profiles can be calculated analytically hence there is no need to enlarge the interval of integration to get the required accuracy. So we can easily avoid the problem of having artificial turning points because of insufficient computational range of integration [27]. We also get rid of the translation invariance of the problem that may cause difficulties in the convergence of the iteration.
- In the continuation algorithm the length L can be used as a parameter in the graph of flame speed versus heat loss parameter. Changing the value of L it is easy to find the turning point. It was found that there exists a critical value $L = L_{\min}$, such that for $L < L_{\min}$ there is no solution of the problem and for $L > L_{\min}$ there are two solutions.
- Results obtained by three different methods: numerical integration, asymptotic expansion, lower and upper estimates are compared systematically.
- The system is solved analytically with a step function nonlinearity, and the numerical method is tested in that case.

In the next section we shall present the non-dimensional model and recall the main known theoretical results in order to compare our numerical simulations with them. In section 3 our numerical results are presented for both cases. The MATLAB package was used for the computations. In the final section the numerical method is tested in the case of a step function nonlinearity when the exact solution can also be calculated.

2. Non-dimensional equations

In order to make equations (1)–(2) non-dimensional, we introduce the following variables:

$$y = \alpha z, \quad a(y) = \frac{A(z)}{A_0}, \quad b(y) = \frac{T(z) - T_a}{T_b - T_a}, \quad (5)$$

where

$$\varepsilon = \frac{R(T_b - T_1)}{E}, \quad \alpha = \sqrt{k_0 e^{-1/\varepsilon} \frac{\rho C_p}{\lambda}}.$$

Substituting (5) into equations (1)–(2) and introducing the parameters

$$L_e = \frac{\lambda}{D\rho C_p}, \quad c = m \sqrt{\frac{C_p}{\rho \lambda k_0}} e^{1/\varepsilon}, \quad \gamma = \frac{h}{\rho C_p k_0} e^{1/\varepsilon}, \quad b_1 = \frac{T_1 - T_a}{T_b - T_a} \quad (6)$$

we obtain

$$\frac{1}{L_e} a''(y) - ca'(y) - a(y)f(b(y)) = 0, \quad (7)$$

$$b''(y) - cb'(y) + a(y)f(b(y)) - \gamma b(y) = 0, \quad (8)$$

where

$$f(b) = \begin{cases} \exp\left(\frac{b-1}{\varepsilon(b-b_1)}\right) & \text{if } b \geq b_1, \\ 0 & \text{otherwise.} \end{cases} \quad (9)$$

The boundary conditions are

$$a \rightarrow 1, \quad b \rightarrow 0 \quad \text{as } y \rightarrow -\infty, \quad a' \rightarrow 0, \quad b' \rightarrow 0 \quad \text{as } y \rightarrow +\infty. \quad (10)$$

The boundary conditions at $+\infty$ determine the limits of a and b as follows:

- if $\gamma = 0$ (adiabatic case), then $a \rightarrow 0$ and $b \rightarrow 1$ as $y \rightarrow +\infty$;
- if $\gamma > 0$ (heat loss case), then $a \rightarrow a_s$ and $b \rightarrow 0$ as $y \rightarrow +\infty$,

where $0 \leq a_s < 1$ is to be determined. Besides these boundary conditions we assume that

$$a \text{ and } b \text{ are bounded, non-negative functions on } \mathbf{R}. \quad (11)$$

Summarising, we will deal with the following two problems.

- **Problem (AD).** Let $\gamma = 0$ and f be given in (9). Solve (7), (8), (10), (11) for a , b and c .
- **Problem (HL).** Let $\gamma > 0$ and f be given in (9). Solve (7), (8), (10), (11) for a , b and c .

That is, for a given value of the scaled heat loss parameter γ , the value of the scaled mass flux c (velocity) and the profiles a (concentration) and b (temperature) are to be determined.

The adiabatic case has been widely investigated. In the case of unit Lewis number ($L_e = 1$) the system can be reduced to a single equation and shooting methods can be applied to find the value c_{ad} of the dimensionless mass flux, for which problem (AD) has a solution [10,12,13]. In the general case (L_e is an arbitrary positive number) Leray–Schauder degree theory can be applied to prove the existence of a value c_{ad} , for which problem (AD) has a solution [9]. The nonlinear system (7)–(8) cannot be solved analytically hence approximations are applied to get the velocity and the profiles. These approximations are based on the fact that, for small values of ε (i.e., high values of the activation energy), the reaction term has a considerable effect only in a narrow layer called the flame-sheet. In the case of $L_e = 1$ the second-order formula for the velocity is

$$c_{ad} = \varepsilon(1 - b_1)\sqrt{2}[1 + \varepsilon(I(b_1) - 3)], \tag{12}$$

where

$$I(b_1) = \int_0^\infty 1 - \sqrt{1 - e^{-\omega s}(1 + \omega s)} \, ds, \quad \omega = \frac{1}{1 - b_1}.$$

Formula (12) can be found in [3,15,19] for $b_1 = 0$ (when the ignition temperature is not involved). A similar formula is available in the general case $L_e > 0$ (see [15]).

These formulas are based on formal asymptotic expansion. However, upper and lower bounds may be established rigorously for c_{ad} [6,14]. An iterative technique for obtaining successively narrower upper and lower bounds (converging to a common limit) for the velocity has been developed by Johnson and Nachbar [3,12]. In the case $L_e = 1$ the first upper and lower bound are

$$2I_1 < c_{ad}^2 < 2I_2, \tag{13}$$

where

$$I_1 = \int_0^1 \frac{(1 - s)f(s)}{s} \, ds, \quad I_2 = \int_0^1 \frac{(1 - s)f(s)}{s^2} \, ds.$$

In [14] a different method is applied to establish an upper and a lower bound for the velocity. The upper bound is given in (14) (the lower bound is the same as that in (13)). The left inequality of (14) was obtained by Zeldovich and Frank-Kamanetski (see [6]). Thus we have

$$2I_0 < c_{ad}^2 < \frac{2I_1}{1 - \sqrt{2I_1}}, \tag{14}$$

where

$$I_0 = \int_0^1 (1 - s)f(s) \, ds.$$

The comparison of the different bounds can be seen in figure 1.

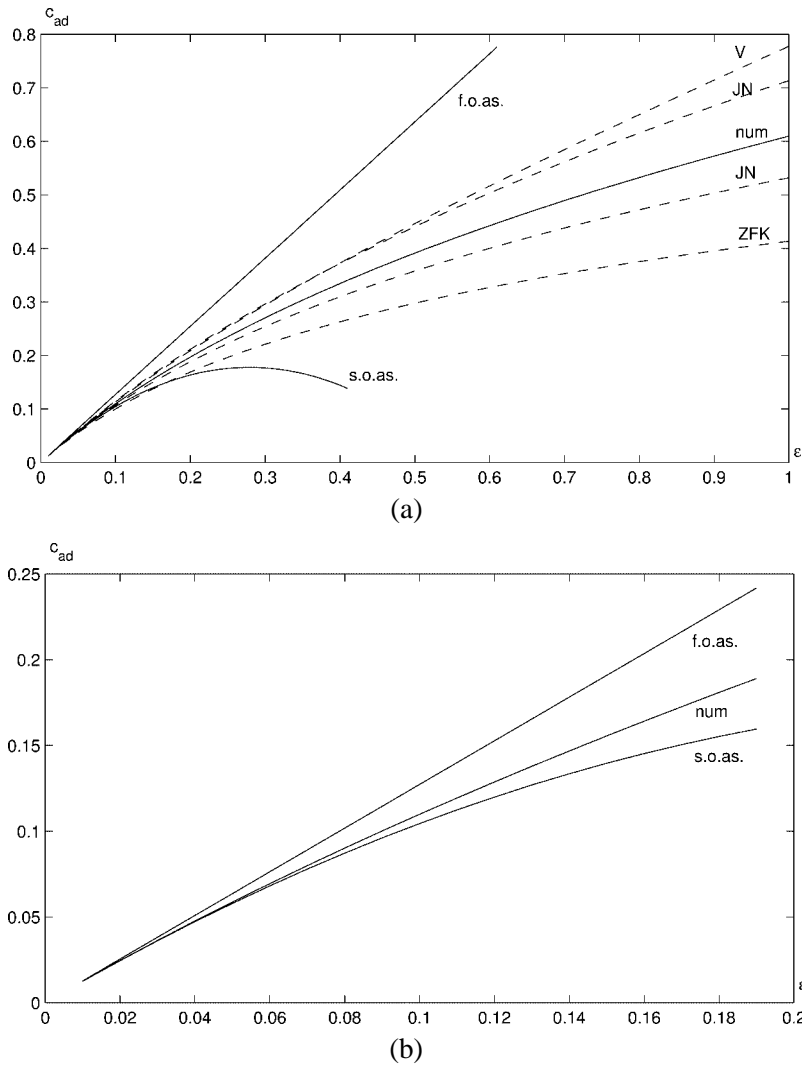


Figure 1. The dependence of c_{ad} on ϵ for $b_I = 0.1$. (a) The numerical value of c_{ad} , the upper and lower bounds for c_{ad} given by (13), (14) and the first and second order terms of the asymptotic expansion of c_{ad} given by (12) are shown. The curves given by (13) are labelled with JN, the curves given by (14) are denoted by ZFK (lower estimate) and by V (upper estimate). (b) The numerical value of c_{ad} and the first and second order terms of its asymptotic expansion for small ϵ .

The heat loss case is less well understood. Some qualitative properties of the solution can be derived by elementary calculations. It is easy to show that if a , b and c are solutions of problem (HL), then a is strictly decreasing, $c > 0$ and

$$a(+\infty) = 1 - \frac{\gamma}{c} \int_{-\infty}^{+\infty} b(s) ds.$$

In [11] it is proved in the case $L_e = 1$ that $c < c_{ad}$, if problem (HL) has a solution for c . The existence of the solution can again be proved by a Leray–Schauder degree argument. Giovangigli proved [11] that in the case $L_e = 1$ for any $c \in (0, c_{ad})$ there exists $\gamma > 0$, such that problem (HL) has a solution. Moreover, $\gamma \rightarrow 0$ as $c \rightarrow 0$ or $c \rightarrow c_{ad}$. As a consequence, there is an extinction value γ_{ext} of γ , such that for $\gamma > \gamma_{ext}$ there is no solution of problem (HL). The shape of the (γ, c) curve has been determined only for small values of ε using formal asymptotic expansions [3–5,11]. In our case (when the ignition temperature is also involved) it can be given as

$$\frac{\gamma}{\varepsilon^3} = -(1 - b_1)^3 \left(\frac{c}{c_{ad}}\right)^2 \log\left(\frac{c}{c_{ad}}\right)^2. \tag{15}$$

Our aim is to determine the (γ, c) curve numerically and to compare it to the curve given by (15) for small values of ε . In order to get all this curve the boundary-value problem (HL) must be solved, since one part of this curve belongs to unstable solutions of the corresponding time dependent problem.

3. Numerical results

3.1. Adiabatic case

Problem (AD) has been investigated numerically by several authors, e.g., [16–18, 20–22]. Here we present our numerical results briefly in order to test our numerical method in the simpler case and to get numerical values for the adiabatic wave velocity for our case as these differ from those in the literature since, in our system, an ignition temperature is involved. We consider the case of unit Lewis number, $L_e = 1$, in which case $a + b = 1$ and the system can be reduced to a single equation. Thus the problem to be solved is

$$b''(y) - c_{ad}b'(y) + (1 - b(y))f(b(y)) = 0, \tag{16}$$

$$b \rightarrow 0 \text{ as } y \rightarrow -\infty, \quad b \rightarrow 1 \text{ as } y \rightarrow +\infty. \tag{17}$$

Since this problem is translationally invariant we can assume $b(0) = b_1$. According to (9) we have $f(b(y)) = 0$ for $y < 0$, hence the problem can be solved analytically on $(-\infty, 0]$ as

$$b(y) = b_1 e^{c_{ad}y} \quad \text{for } y < 0. \tag{18}$$

Therefore our problem is reduced to one on the half-line $[0, +\infty)$

$$b''(y) - c_{ad}b'(y) + (1 - b(y))f(b(y)) = 0, \tag{19}$$

$$b(0) = b_1, \quad b'(0) = c_{ad}b_1, \quad b \rightarrow 1 \text{ as } y \rightarrow +\infty. \tag{20}$$

(The second boundary condition ensures the smoothness of the solution.) In order to apply a numerical method the problem has to be reduced to a bounded interval. Therefore choosing a large number $L > 0$ we solve

$$b''(y) - c_{\text{ad}}b'(y) + (1 - b(y))f(b(y)) = 0, \quad (21)$$

$$b(0) = b_1, \quad b'(0) = cb_1, \quad b(L) = 1. \quad (22)$$

In [9,30] it is proved that the solution of (21)–(22) converges to that of (19)–(20) as L tends to infinity.

We apply the finite-difference method to solve (21)–(22). We introduce the grid points $0 = y_1 < y_2 < \dots < y_N = L$ and $b_i = b(y_i)$ for $i = 1, 2, \dots, N$. The value of b_1 and b_N are given by the boundary conditions (22) as

$$b_1 = b_1, \quad b_N = 1.$$

Hence we have $N - 1$ unknowns b_2, \dots, b_{N-1} and c . We also have $N - 1$ equations, namely the differential equation (21) is satisfied in y_2, \dots, y_{N-1} and a final equation given by the remaining boundary condition $b'(0) = c_{\text{ad}}b_1$. This system can be solved by the Newton–Raphson method (starting from a linear profile as an initial guess). The length of the interval (L) was increased until c_{ad} reached the same value, to within the required accuracy.

The dependence of c_{ad} on ε is shown in figure 1 for $b_1 = 0.1$. The upper and lower bounds for c_{ad} given by (13) and (14) and the first and second order terms of the asymptotic expansion of c_{ad} given by (12) are also shown in figure 1. The temperature and concentration profiles can be seen in figure 2 for $\varepsilon = 0.01$, $\varepsilon = 0.1$ and $\varepsilon = 1$. We observe that the length of the interval L has to be chosen larger as ε is decreased to have good approximation of problem (19)–(20) with problem (21)–(22).

3.2. Heat loss case

Our numerical method works for any value of the Lewis number L_e , however to be specific and to have simpler formulas we present our numerical results in the case of $L_e = 1$. In the heat loss case the problem can be reduced to a bounded interval. The reduction is based on the fact that $f(b) = 0$, when $b < b_1$ and b tends to zero at $+\infty$ and at $-\infty$. Therefore out of a bounded interval $b(y) < b_1$, hence $f(b(y)) = 0$. Again using the translational invariance of the differential equations we can assume that the left endpoint of the interval is at $y = 0$, i.e., $b(0) = b_1$ and $b(y) < b_1$ for all $y < 0$. Let us denote by L the right endpoint of the interval, i.e., $b(L) = b_1$ and $b(y) < b_1$ for all $y > L$. Hence out of the interval $[0, L]$ the differential equations decouple and are both linear. Therefore the exact solution can be given in terms of the (possibly unknown) boundary conditions. In the bounded interval $[0, L]$ we transform the differential equations to integral equations that also contain the boundary conditions determined by the known exact solutions in $(-\infty, 0)$ and in $(L, +\infty)$. The integral equations are the ones solved numerically, since they are easier to solve compared to the differential equations. The derivation of the integral equations is standard and regards

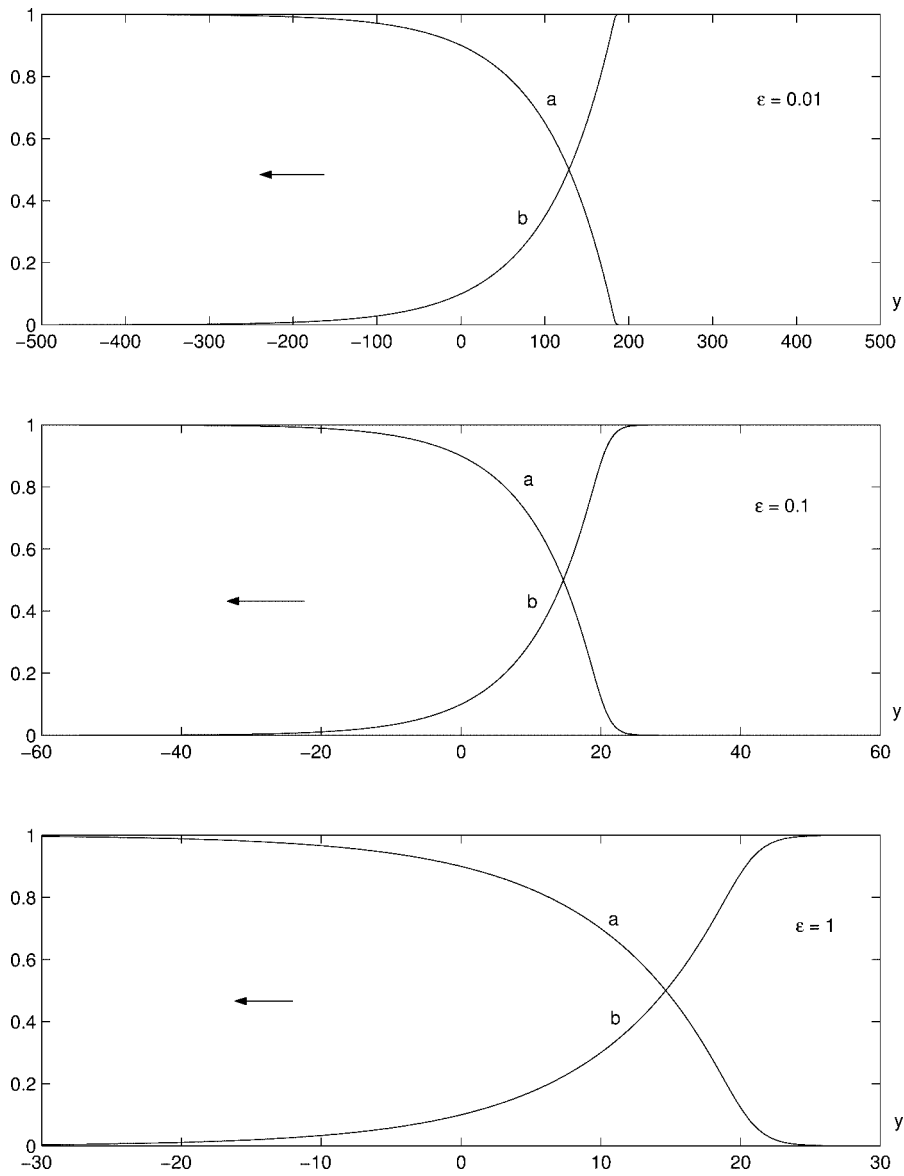


Figure 2. Temperature and concentration profiles in the adiabatic case for three different values of ϵ , when $b_1 = 0.1$. (The direction of propagation of the wave is indicated on the figure.)

the nonlinearity as an inhomogeneous term. Then the integral equations can be obtained using the constant variation formula, or a Green's function. Thus after a little algebra we obtain

Proposition 1. Let us assume that $b_1 > 0$ and that a , b and c are solutions of problem (HL). Let $\mu_1 > 0 > \mu_2$ be solutions of $\mu^2 - c\mu - \gamma = 0$.

1. If $y < 0$, then

$$a(y) = 1 - (1 - a(0))e^{cy}, \quad b(y) = b_1 e^{\mu_1 y}.$$

2. If $y > L$, then

$$a(y) = a(L), \quad b(y) = b_1 e^{\mu_2(y-L)}.$$

3. If $y \in [0, L]$, then

$$a(y) = 1 - b(y) - \frac{\gamma}{c} \left[\frac{b_1}{\mu_1} + \int_0^y b(s) ds + \frac{b_1}{\mu_1} e^{c(y-L)} + e^{cy} \int_y^L e^{-cs} b(s) ds \right], \quad (23)$$

$$b(y) = \frac{1}{\mu_1 - \mu_2} \left[e^{\mu_1 y} \int_y^L e^{-\mu_1 s} a(s) f(b(s)) ds + e^{\mu_2 y} \int_0^y e^{-\mu_2 s} a(s) f(b(s)) ds \right]. \quad (24)$$

Thus the problem to be solved is given on $[0, L]$ with the boundary conditions

$$b(0) = b_1 = b(L). \quad (25)$$

Once this problem is solved the values of $a(0)$ and $a(L)$ are given, hence the solutions are known also for $y < 0$ and for $y > L$.

The integrals in (23) and (24) can be transformed to the interval $[0, 1]$ introducing the new variable

$$\bar{y} = \frac{y}{L}$$

and new parameters

$$\bar{c} = cL, \quad \bar{\gamma} = \gamma L^2, \quad \bar{\mu}_i = \mu_i L.$$

Hence system (23)–(25) takes the following form, after dropping the bars for convenience,

$$a(y) = 1 - b(y) - \frac{\gamma}{c} \left[\frac{b_1}{\mu_1} + \int_0^y b(s) ds + \frac{b_1}{\mu_1} e^{c(y-1)} + e^{cy} \int_y^1 e^{-cs} b(s) ds \right], \quad (26)$$

$$b(y) = \frac{L^2}{\mu_1 - \mu_2} \left[e^{\mu_1 y} \int_y^1 e^{-\mu_1 s} a(s) f(b(s)) ds + e^{\mu_2 y} \int_0^y e^{-\mu_2 s} a(s) f(b(s)) ds \right], \quad (27)$$

$$b(0) = b_1 = b(1). \quad (28)$$

Thus the reduced problem is the following.

Problem (RHL). Let $\gamma > 0$ and $b_1 > 0$. Solve (26)–(28) for a, b, c, L .

It turned out that it is simpler to consider γ as an unknown instead of L and solve the above system for a, b, c, γ in terms of L . Then we obtain a curve in the (γ, c) plane parametrised by L .

System (26)–(28) can be discretised by introducing the grid points $0 = y_1 < y_2 < \dots < y_N = 1$ and $a_i = a(y_i), b_i = b(y_i)$ for $i = 1, 2, \dots, N$. Let $\bar{a} = (a_1, \dots, a_N) \in \mathbf{R}^N$ and $\bar{b} = (b_1, \dots, b_N) \in \mathbf{R}^N$. Approximating the integrals in the r.h.s. of (26)–(27) using the values a_i, b_i we get the discretised problem in the form

$$\bar{a} = g_1(\gamma, c, \bar{b}), \tag{29}$$

$$\bar{b} = g_2(\gamma, c, \bar{a}, \bar{b}), \tag{30}$$

$$\bar{b}_1 = b_1 = \bar{b}_N. \tag{31}$$

This system of $2N + 2$ equations can be solved for the $2N + 2$ unknowns $\gamma, c, \bar{a}, \bar{b}$ using the Newton–Raphson method, if a very good initial guess is known. To find the initial guess we exploit the fact that, for large ε , the function f is close to a step function, and in the case of step function, the solution can be expressed analytically (see the next section). Hence choosing first a large value of ε (e.g., $\varepsilon = 100$) and using the exact solution of the problem for the step function as an initial guess the Newton–Raphson method converges to the solution of system (29)–(31). Then a continuation method was used, i.e., the value of ε was decreased succesively and, for the new value of ε , the initial guess can be chosen as the solution obtained for the previous value of ε . For small values of ε ($\varepsilon < 0.1$) the solution obtained by high activation energy asymptotics can also be used as an initial guess. We note that once a point of the (γ, c) curve is found (i.e., for a given value of L the value of γ and c and the vectors \bar{a}, \bar{b} are known), then those can be used as initial guess for another (close) value of L (in this case ε is unchanged).

Using this method the (γ, c) curve was determined for different values of ε in the case $b_1 = 0.1$. Results for $\varepsilon = 0.1$ are shown in figure 3. We found that there is a critical value $L = L_{\min}$ depending on ε , such that for $L < L_{\min}$ there is no solution of system (29)–(31) and for $L > L_{\min}$ there are two solutions. Therefore the (γ, c) curve consists of two parts: an upper branch (u.b.) and a lower branch (l.b.) joining at the point given by L_{\min} . The value of L increases from L_{\min} to $+\infty$ along both branches.

The scaled temperature profiles for certain points on the curve are shown in figure 4. We observe that, as c approaches the adiabatic value c_{ad} (i.e., as L is increasing in the upper branch), then the scaled maximum temperature approaches 1 (the maximum value in the adiabatic case) and that there is an initial steep increase in the profile followed by a long decay zone, because the heat loss parameter γ is small. The entire profiles are given by proposition 1. They are shown in figure 5 for one point of the lower branch and for two points of the upper branch.

Figure 6 shows the comparison of the numerical (γ, c) curves (for $\varepsilon = 0.5, \varepsilon = 0.1$ and for $\varepsilon = 0.05$) with that one obtained by formal asymptotic expansion for small ε given by expression (15). In order to plot the curves in the same scale and to be in

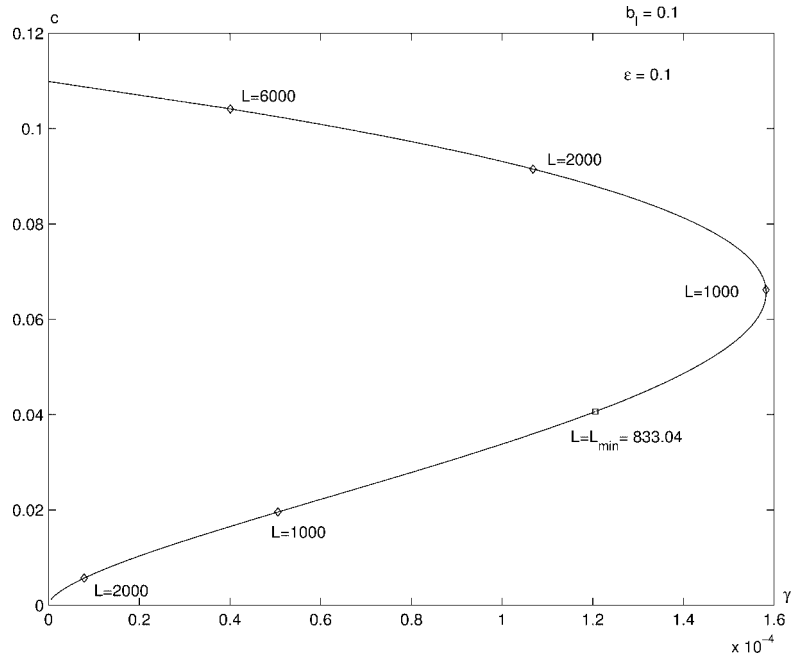


Figure 3. The dependence of the velocity c on the heat loss parameter γ for $\epsilon = 0.1$ and $b_I = 0.1$. The curve is parametrised by L .

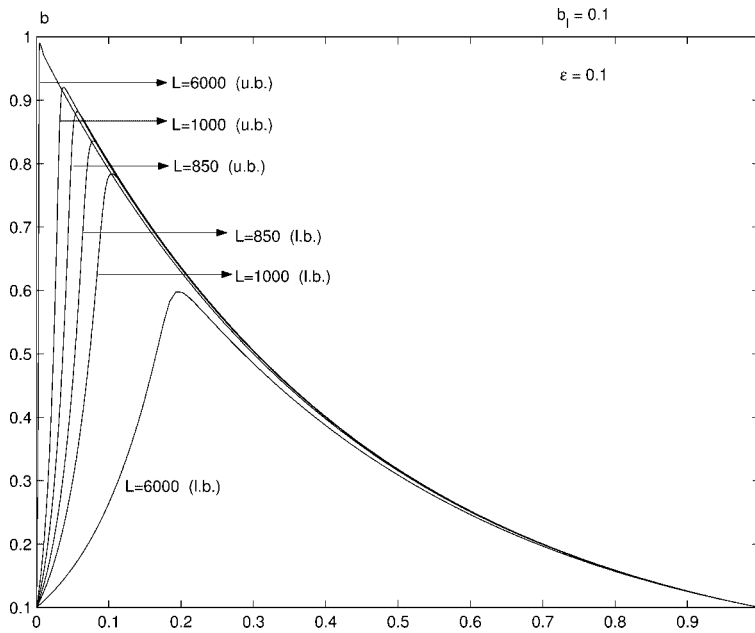


Figure 4. The temperature profiles transformed to the interval $[0, 1]$, i.e., the solution b of (27) for six different values of c , when $\epsilon = 0.1$ and $b_I = 0.1$. (The value of c is determined by L according to figure 3.)

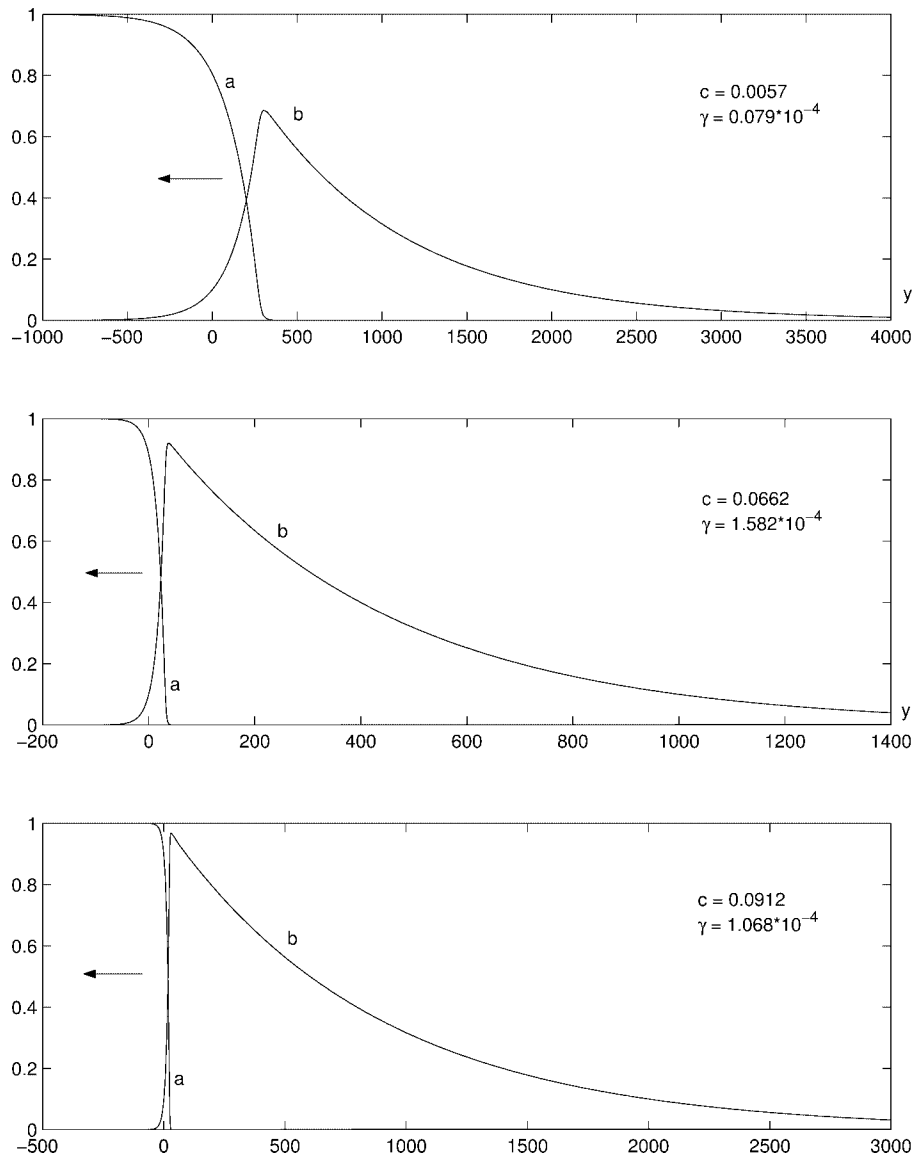


Figure 5. Temperature and concentration profiles in the heat loss case for three different values of c , when $\varepsilon = 0.1$ and $b_I = 0.1$. The corresponding L values (see figure 3) are $L = 2000$ in the lower branch and $L = 1000$ and $L = 2000$ in the upper branch. (The direction of propagation of the wave is indicated on the figure.)

accordance with traditional notation the unit in the γ axis is ε^3 and that in the c axis is c_{ad} . Hence the extinction point in the limit case is at

$$\gamma_{ext} = (1 - b_I)^3 e^{-1}, \quad c_{ext} = e^{-0.5}.$$

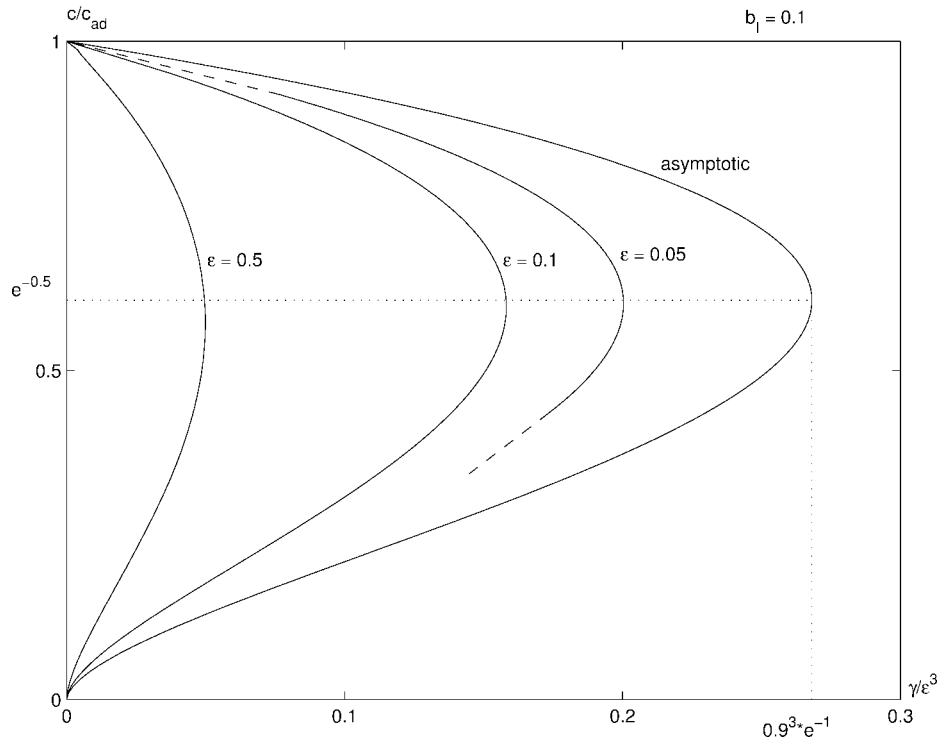


Figure 6. Comparison of the numerical (γ, c) curves (for $\varepsilon = 0.5$, $\varepsilon = 0.1$ and $\varepsilon = 0.05$) with that one obtained by formal asymptotic expansion for small ε given by expression (15). The unit in the γ axis is ε^3 and that in the c axis is c_{ad} ($b_I = 0.1$).

This figure shows the extent to which the asymptotic values can be used in a given range of ε values.

The extinction point was calculated for further values of ε , see figure 7. It is seen that the asymptotic value of the extinction velocity, $c_{\text{ext}} = e^{-0.5}$ is a good approximation for a relatively wide range of ε , but the asymptotic value of the extinction heat loss parameter $\gamma_{\text{ext}} = (1 - b_I)^3 e^{-1}$ is reasonable only for very small values of ε .

4. The case of step function nonlinearity

In this section we solve problem (AD) and problem (HL), when f is the step function

$$f(b) = \begin{cases} 1 & \text{if } b \geq b_I, \\ 0 & \text{otherwise.} \end{cases} \quad (32)$$

Throughout this section $L_e = 1$ and $b_I \in (0, 1)$ are assumed.

The motivation of studying this special case is twofold. First, the differential equations can be solved analytically and only the boundary conditions are to be solved numerically.

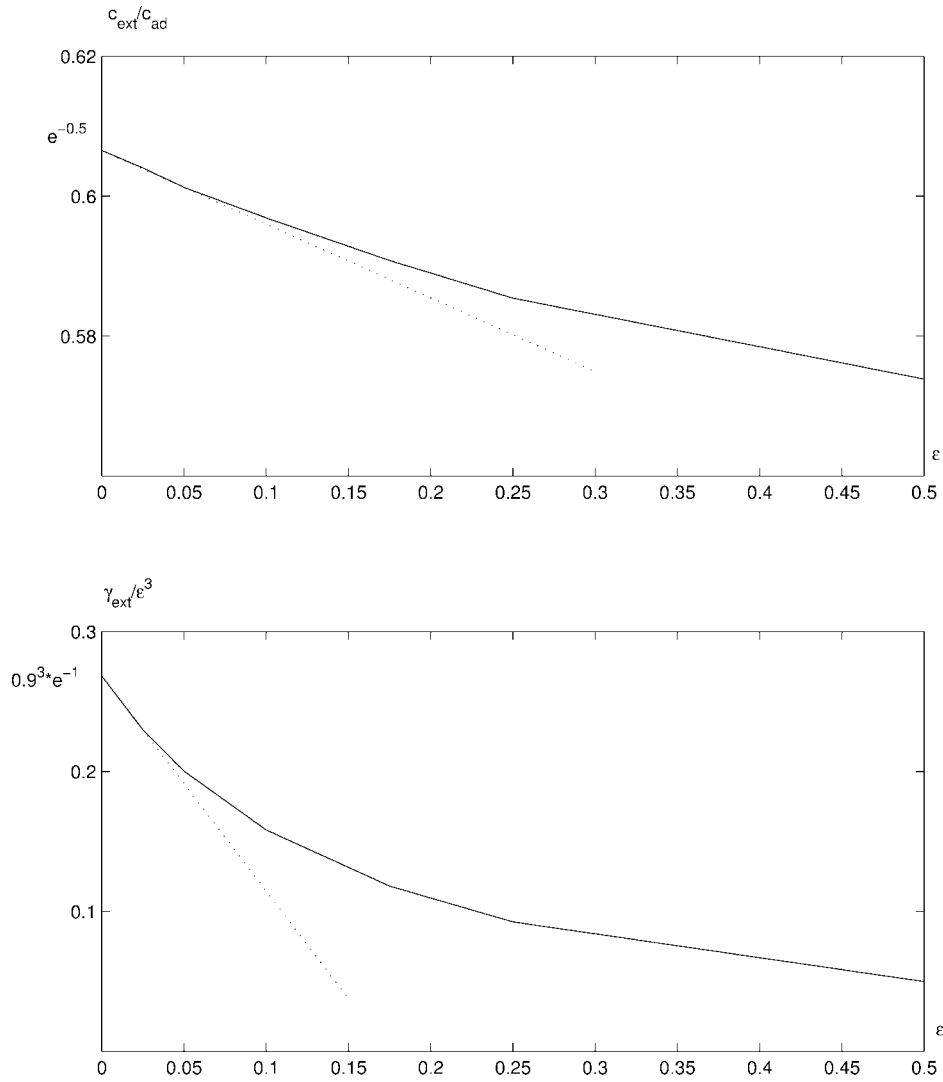


Figure 7. The dependence of the extinction velocity c_{ext} and extinction value of the heat loss parameter γ_{ext} on ϵ . The unit in the γ axis is ϵ^3 and that in the c axis is c_{ad} ($b_1 = 0.1$).

ically, hence we obtain the “exact” solution of the problem in this special case. Therefore, this case can serve as a test problem for the numerical method we used for the function f given in (9). Second, the step function can be considered as a simplified version of Arrhenius’ law, namely, below the ignition temperature (b_1) there is no reaction, but 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. Moreover, as mentioned above, the exact solution of this problem can serve as initial guess to the above general problem.

4.1. Adiabatic case

Now problem (AD) can be solved analytically. Since $\gamma = 0$ and $L_e = 1$, therefore using $a = 1 - b$ the problem can be reduced to the single equation

$$b'' - c_{\text{ad}}b' + (1 - b)f(b) = 0.$$

Similarly to the general case we can assume $b(0) = b_1$. Hence the equation can be solved in $(-\infty, 0)$ and in $(0, +\infty)$ separately. In $(-\infty, 0)$ the solution is

$$b(y) = b_1 e^{c_{\text{ad}}y} \quad \text{for } y < 0, \quad (33)$$

according to (18). In $(0, +\infty)$ the equation takes the form

$$b'' - c_{\text{ad}}b' + 1 - b = 0$$

with boundary conditions

$$b(0) = b_1, \quad b'(0) = cb_1, \quad b(+\infty) = 1.$$

The solution is

$$b(y) = 1 - (1 - b_1)e^{\lambda_2 y} \quad \text{for } y > 0, \quad (34)$$

where $\lambda_2 = (c - \sqrt{c^2 + 4})/2$. The second boundary condition implies

$$cb_1 = \lambda_2(b_1 - 1)$$

determining the dimensionless mass flux as

$$c_{\text{ad}} = \frac{1 - b_1}{\sqrt{b_1}}. \quad (35)$$

The temperature profile is given by (33) and (34), the concentration is given by $a = 1 - b$.

4.2. Heat loss case

Problem (HL) will be reduced to a system of two algebraic equations that have to be solved numerically. According to proposition 1 problem (HL) can be reduced to a problem given on the bounded interval $[0, L]$. However, in this case it is easier to solve

the differential equation for a in $[0, L]$ directly. Now (7) takes the form

$$a''(y) - ca'(y) - a(y) = 0, \quad y \in (0, L).$$

Hence for $y \in (0, L)$

$$a(y) = d_1 e^{\lambda_1 y} + d_2 e^{\lambda_2 y}, \tag{36}$$

where $\lambda_{1,2} = (c \pm \sqrt{c^2 + 4})/2$. The values of d_1 and d_2 are determined by the following matching conditions at 0 and at L

$$a(0) = d_1 + d_2, \quad c(a(0) - 1) = d_1 \lambda_1 + d_2 \lambda_2, \tag{37}$$

$$a(L) = d_1 e^{\lambda_1 L} + d_2 e^{\lambda_2 L}, \quad 0 = d_1 \lambda_1 e^{\lambda_1 L} + d_2 \lambda_2 e^{\lambda_2 L}. \tag{38}$$

Solving this system for d_1 and d_2 we obtain from (36)

$$a(y) = \frac{c \lambda_1 e^{\lambda_1 L + \lambda_2 y} - c \lambda_2 e^{\lambda_2 L + \lambda_1 y}}{\lambda_1^2 e^{\lambda_1 L} - \lambda_2^2 e^{\lambda_2 L}}. \tag{39}$$

Now, from (24) one can obtain $b(y)$ for $y \in [0, L]$, since $f(b(y)) = 1$. Finally, expressing $b(0)$ and $b(L)$ from (24) and substituting these expressions into (25) we get the following algebraic equations

$$b_1 = K [(\lambda_1 - \lambda_2) \mu_2 e^{\mu_2 L} + (1 + \lambda_2 \mu_2) e^{\lambda_2 L} - (1 + \lambda_1 \mu_2) e^{\lambda_1 L}], \tag{40}$$

$$b_1 = K e^{\mu_2 L} [(\lambda_1 - \lambda_2) \mu_1 e^{\mu_1 L} + (1 + \lambda_2 \mu_1) e^{\lambda_2 L} - (1 + \lambda_1 \mu_1) e^{\lambda_1 L}], \tag{41}$$

where

$$K = \frac{c}{(\mu_1 - \mu_2)(\gamma - 1)(\lambda_1^2 e^{\lambda_1 L} - \lambda_2^2 e^{\lambda_2 L})}.$$

For a given value of L this system can be solved with the Newton–Raphson method for γ and c . Hence varying the value of L between 0 and $+\infty$ we get a curve in the (γ, c) parameter plane. For $L = 0$ we get $\gamma = 0 = c$, for $L = +\infty$ we get $\gamma = 0$, $c = c_{ad} = (1 - b_1)/\sqrt{b_1}$ (see (35)). We note that L_{min} does not occur in this case, i.e., for all $L > 0$ we get a unique solution of (40)–(41). The (γ, c) curve is shown in figure 8. It is qualitatively similar to those obtained by asymptotic expansion for high activation energy ($\varepsilon \rightarrow 0$) and previously by numerical integration for different values of ε . The integral equations were solved also numerically using the same method as in the case of an Arrhenius type nonlinearity, i.e., we applied our method described in section 3.2 to problem (RHL) with replacing f by the step function (32). Hence the numerical method was tested in a case when the exact solution is also known. The numerical values of γ and c together with their exact values (obtained by solving the algebraic system (40)–(41)) are shown in figure 8.

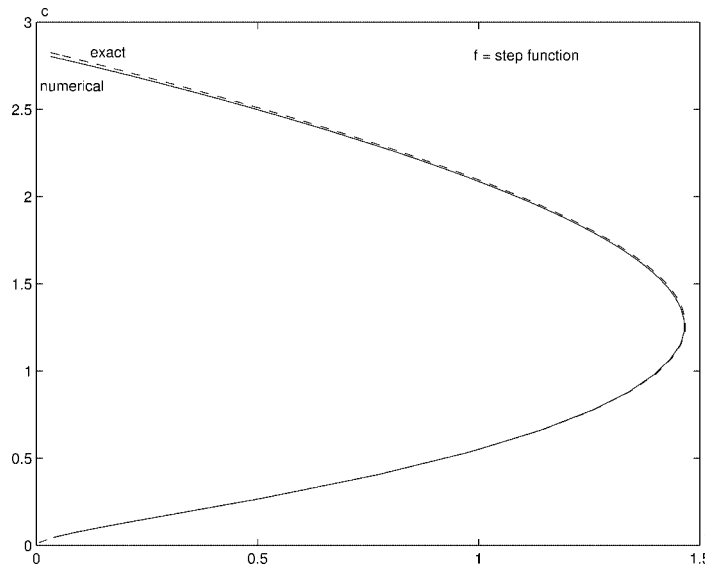


Figure 8. The dependence of the velocity c on the heat loss parameter γ when f is the step function given by (32). The numerical solution (solid curve) is obtained by solving numerically the integral equations (23)–(24) with boundary conditions (25). The exact solution (dashed curve) is obtained by solving analytically the integral equations and then solving numerically the boundary conditions given by (40)–(41).

Acknowledgements

We are grateful to the EPSRC for financial support (Grant GR/N66537/01) and to Professors B.F. Gray and R.O. Weber for helpful discussion.

Appendix. List of symbols

m	mass flux	$\text{kg}/\text{m}^2\text{s}$
A	mass fraction of the reactant A	–
ρ	total density	kg/m^3
T	temperature	K
T_a	ambient temperature	K
T_I	ignition temperature	K
μ	molar mass of A	kg/mol
E	activation energy	J
R	universal gas constant	J/K
k_0	pre-exponential factor	1/s
q	exothermicity of the reaction	J/mol
D	diffusion coefficient of A	m^2/s
C_p	specific heat for constant pressure	J/kgK
λ	thermal conductivity	J/msK
h	heat loss parameter	$\text{J}/\text{m}^3\text{sK}$

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