MATHEMATICAL INVESTIGATION OF THE COLD BOUNDARY DIFFICULTY IN FLAME PROPAGATION THEORY

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1. Introduction. Our aim in this paper is to describe a rigorous mathematical answer to the well-known paradox called the "cold boundary difficulty" in flame propagation theory. We essentially report here on some work done by J. M. Roquejoffre (see [23], [24], [25] where it appears in detail) in collaboration with the first two authors.

This cold boundary difficulty lies in the fact that the governing equations modelling a steady planar premixed flame propagating in an infinite tube (that is, the simplest problem of flame propagation theory) admit no solution, whereas such solutions are expected to exist on an experimental basis: steady planar premixed flames are actually observed (although not in infinite tubes !).

The origin of the difficulty is the following: when modelled using the (widely accepted) Arrhenius law, the chemical reaction rate does not vanish in the fresh mixture. Therefore, the temperature of the fresh gases keeps increasing because of the small but non-zero reaction rate, and no steady state exists. This explains why the cold boundary difficulty has been "solved" by modifying the expression of the reaction term, for instance using an ignition temperature assumption.

In this paper, we mathematically solve the cold boundary difficulty in the following sense; we show that the unmodified model (with the actual Arrhenius term) leads to a well-posed initial value problem, and that the unique time-dependent solution of the Arrhenius model remains close to a steady planar flame during a long time (in fact, during a time which is larger and larger as the activation energy of the chemical reaction increases), before it diverges from the steady flame for even larger values of the time t. Our rigorous analysis therefore reaches the same conclusions as the multiple-time-scale asymptotic analysis of Zeldovich [29].

The paper is organised as follows. In section 2, we describe the governing equations used in our analysis and present the cold boundary difficulty. Mathematical results showing the existence and uniqueness of a time-dependent solution of the Arrhenius model and of a steady solution of a modified (ignition temperature) model are presented in Section 3. The long-time behaviour of the time-dependent solution is examined in Section 4, which leads us to the "mathematical solution" of the cold boundary difficulty in Section 5. Lastly, we illustrate our analysis by showing a numerical example in Section 6.

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2. Governing equations. We start with the classical isobaric approximation of flame propagation theory (see e.g. [5], [7], [17], [27]): we consider a planar unsteady premixed flame propagating in an infinite channel with the assumption of one-step chemistry. The governing equations describing this phenomenon involve the conservation equations for mass, momentum, energy and mass of reactant, and an isobaric equation of state. In Eulerian coordinates, these equations take the form

$$
(2.1) \qquad \begin{cases} \rho_\tau + (\rho u)_\xi = 0 \ , \\ \rho u_\tau + \rho u u_\xi = -p_\xi \ , \\ \rho C_p T_\tau + \rho u C_p T_\xi = (\lambda T_\xi)_\xi + mQ\omega(\rho Y, T) + P_\tau \ , \\ \rho Y_\tau + \rho u Y_\xi = -m\omega(\rho Y, T) + (\rho D Y_\xi)_\xi \ , \\ \rho R^0 T = mP(\tau) \ . \end{cases}
$$

We use standard notations: in (2.1), ξ and τ are the space and time coordinates respectively, ρ is the mixture density, u is the mixture velocity, T is the mixture temperature and Y is the mass fraction of the reactant; in the framework of the isobaric approximation, $P(\tau)$ is the average pressure, which is assumed to depend only on time, and $p(\xi, \tau)$ is the small pressure variation around this average value. Moreover, C_p is the specific heat at constant pressure of the mixture, which is assumed to be constant, λ is the mixture thermal conductivity, $Q > 0$ is the heat released by the reaction per unit mass of reactant, m is the molecular weight of the reactant, D is its diffusion coefficient, and R^0 is the universal gas constant. Lastly, $\omega(\rho Y, T)$ is the chemical reaction rate, and has the form

$$
(2.2) \qquad \omega(\rho Y, T) = \frac{\rho Y}{m} \ F(T) = \mathcal{B} \ \frac{\rho Y}{m} \ T^\alpha \ \exp\left(-\frac{E}{R^0 T}\right) \ ,
$$

where $\mathcal{B}$, α and E are three positive constants: $\mathcal{B}$ is called the Arrhenius prefactor, and E is the activation energy of the chemical reaction.

2.1. Steady flames: the cold boundary difficulty. Let us first consider the case of steady planar flames. For a steady solution of (2.1), the mass conservation equation (2.1.a) writes

$$
(2.3) \qquad (\rho u)_\xi = 0 \ ,
$$

whence $\rho u = c$, an unknown constant. Setting $G(T) = \dfrac{mP}{R^0 T} F(T)$ (P is constant for a steady solution), we can then rewrite (2.1) under the following form:

$$
(2.4) \qquad \begin{cases} cC_p T_\xi = QYG(T) + (\lambda T_\xi)_\xi \ , \\ cY_\xi = -YG(T) + (\rho D Y_\xi)_\xi \ , \end{cases}
$$

$$
(2.5) \qquad \begin{cases} \rho = \dfrac{mP}{R^0 T} \ , \\ u = \dfrac{c}{\rho} \ , \\ p_\xi = -cu_\xi \ . \end{cases}
$$

It therefore appears that equations (2.4) are decoupled from (2.5). In fact, one only studies system (2.4) in order to determine T, Y and the real constant c (see e.g. Theorem 2 below), since solving system (2.5) for the variables ρ, u and p is then straightforward.

The boundary conditions associated with equations (2.4) are of the following type:

$$\left\{\begin{array}{l} T(-\infty) = T_u \ , \ Y(-\infty) = Y_u \ , \\ T(+\infty) = T_b \ , \ Y(+\infty) = 0 \ , \end{array}\right. \tag{2.6}$$

where T_u and T_b are the temperatures of the fresh mixture and of the burnt gases respectively, and where Y_u is the mass fraction of reactant in the fresh mixture ahead of the flame; the last equality in (2.6) states that complete consumption of the reactant occurs in the flame. These values satisfy $0 < T_u < T_b$ (the burnt gases are hotter than the unburnt mixture), and $0 < Y_u \leq 1$ (the fresh mixture actually contains some reactant). Furthermore, the burnt gas temperature is simply given by writing the overall energy balance equation (obtained by integrating from $-\infty$ to $+\infty$ the sum of the first equation (2.4.a) and of the second equation (2.4.b) multiplied by Q):

$$T_b = T_u + \frac{QY_u}{C_p} \ . \tag{2.7}$$

The problem (2.4)-(2.6) (or the simpler problem which arises in the so-called "equidiffusional" case, that is when the Lewis number $\mathcal{L} = \dfrac{\lambda}{\rho C_p D}$ is constant and equal to unity; see (3.21) below), has been investigated by many authors (see Aronson-Weinberger [1], Johnson [10], Johnson-Nachbar [11], Kanel' [12], [13], Kolmogorov *et al.* [14], Zeldovich [28], Zeldovich *et al.* [30], [31], and more recently Berestycki *et al.* [6], Marion [19], [20], Berestycki-Larrouturou [4], [5]), under various hypotheses under the nonlinear reaction term G.

This investigation raises the well-known "cold boundary difficulty", on which a lot of ingenuity has been spent for several years (see for instance Buckmaster-Ludford [7], Clavin [8], Williams [27], just to mention some prominent work on the question). The difficulty is the following: the value of the reaction rate $\omega(\rho Y, T)$ does not vanish in the fresh mixture, because $G(T_u) \neq 0$. It is then easy to see that (2.4)-(2.6) has no solution (the fact that $\lim\limits_{x \to -\infty} [cC_pT_\xi - (\lambda T_\xi)_\xi] \neq 0$ contradicts the fact that T is bounded in the neighbourhood of $-\infty$). ¿From the physical point of view, the origin of the difficulty is clear: the state (Y_u, T_u) prescribed at $-\infty$ is not an equilibrium state, and the problem is therefore ill-posed.

On the other hand, there is a well-established experimental evidence that steady planar premixed flames do exist, and solutions of (2.4)-(2.6) are therefore expected to exist.

In fact, the difficulty is essentially mathematical: the actual value of the reaction rate ω inside the fresh mixture is non zero, but is extremely small compared to the reaction term value inside the flame: this is due to the fact that the activation energy

E is large, i.e., that the ratio $\dfrac{E}{RT}$ is large for temperatures T in the considered range of temperature $[T_u, T_b]$. In practice, the ratio $\dfrac{e^{-E/RT_u}}{e^{-E/RT_b}}$ may well be of the order of e^{-50} .

In other words, the characteristic time τ_u of the chemical reaction in the fresh mixture (at temperature T_u) is extremely large (as large as a big number of billions of years !). One may therefore think, if one believes in the Arrhenius expression of the chemical reaction term (2.2), that the experimentally observed "steady premixed flames" are not really steady; but they are evolving over a characteristic time which is of the same order of magnitude as τ_u. Therefore, although there exists no steady solution in the mathematical sense to system (2.1), where the quantity $F(T_u)$ is small but positive, one may expect that (2.1) has an unsteady solution, *which remains "during a long time" "very close" to a steady flame.* This is exactly what comes out from the work of J. M. Roquejoffre [23], [25], which we now describe.

2.2. Unsteady solutions. We therefore turn to the unsteady solutions of (2.1).

It is now well known that the unsteady solutions of (2.1) are more easily investigated using instead of (2.1) the Lagrangian form of (2.1). Thus, we introduce the change of coordinates $(\xi, \tau) \longleftrightarrow (x, t)$ where $x(\xi, \tau)$ represents the mass-weighted Lagrangian coordinate of the particle which is located at the abcissa ξ at time τ (inversely, $\xi(x,t)$ is the position at time t of the fluid particle whose Lagrangian coordinate is x), and where $t = \tau$. This change of variables is defined by the relation

$$\int_{\xi(0,t)}^{\xi(x,t)} \rho(x',t)dx' = x \tag{2.8}$$

which imply $x_\xi = \rho$, $x_\tau = -\rho u$ (we refer to e.g. [15], [17] for the details about this transformation). The Lagrangian form of the flame propagation equations (2.1) can then be derived: for any quantity w we have

$$w_\tau = w_t - \rho u w_x \ , \ w_\xi = \rho w_x \ , \tag{2.9}$$

and (2.1) becomes

$$\begin{cases} \rho_t + \rho^2 u_x = 0 \ , \\ u_t + p_x = 0 \ , \\ T_t = \dfrac{mQ}{C_p}\dfrac{\omega(\rho Y, T)}{\rho} + \dfrac{1}{C_p}(\lambda\rho T_x)_x + \dfrac{1}{\rho C_p}P'(t) \ , \\ Y_t = -m\dfrac{\omega(\rho Y, T)}{\rho} + (\rho^2 D Y_x)_x \ , \\ \rho R^0 T = mP(t) \ , \ \omega(\rho Y, T) = \dfrac{\rho Y}{m}F_\epsilon(T) \ . \end{cases} \tag{2.10}$$

We now use the notation F_ϵ instead of F for the reaction term in order to stress the dependence of this term on the activation energy: ϵ is a (small) positive parameter, proportional to the inverse of the activation energy.

Introducing the Lewis number $\mathcal{L} = \dfrac{\lambda}{\rho C_p D}$, we can rewrite (2.10) as

$$(2.11) \qquad \begin{cases} T_t = \dfrac{Q}{C_p} Y F_\epsilon(T) + \dfrac{1}{C_p}(\lambda\rho T_x)_x + \dfrac{1}{\rho C_p} P'(t) \ , \\ \\ Y_t = -Y F_\epsilon(T) + \dfrac{1}{C_p \mathcal{L}}(\lambda\rho Y_x)_x \ , \end{cases}$$

$$(2.12) \qquad \begin{cases} \rho R^0 T = m P(t) \ , \\ \\ u_x = \left(\dfrac{1}{\rho}\right)_t \ , \\ \\ p_x = -u_t \ . \end{cases}$$

Thus, the use of the Lagrangian coordinate x uncouples the equations (2.11) for the "combustion variables" T and Y (which take the form of a reaction-diffusion system) from the equations (2.12) for the "hydrodynamical variables" ρ, u and p (which reduces to a system of linear partial differential equations).

Let us now write initial and boundary conditions associated with (2.11)-(2.12). The form of the equations suggests which conditions should be used in order to get a possibly well-posed problem: first, we need an initial condition and two boundary conditions for the unknowns T and Y of the parabolic system (2.11). We will therefore write the following conditions for the temperature and mass fraction:

$$(2.13) \qquad T(x,0) = T^0(x) \ , \ Y(x,0) = Y^0(x) \ ,$$

$$(2.14) \qquad \begin{cases} T(-\infty,t) = T_u(t) \ , \ Y(-\infty,t) = Y_u(t) \ , \\ T(+\infty,t) = T_b(t) \ , \ Y(+\infty,t) = Y_b(t) \ , \end{cases}$$

where the functions $T_u(t)$, $Y_u(t)$, $T_b(t)$, $Y_b(t)$ are defined by

$$(2.15) \qquad \begin{cases} T_u'(t) = \dfrac{Q}{C_p} Y_u(t) F_\epsilon[T_u(t)] + \dfrac{1}{\rho_u(t) C_p} P'(t) \ , \ T_u(0) = T_{u0} \ , \\ \\ T_b'(t) = \dfrac{Q}{C_p} Y_b(t) F_\epsilon[T_b(t)] + \dfrac{1}{\rho_b(t) C_p} P'(t) \ , \ T_b(0) = T_{b0} \ , \\ \\ Y_u'(t) = -Y_u(t) F_\epsilon[T_u(t)] \ , \ Y_u(0) = Y_{u0} \ , \\ \\ Y_b'(t) = -Y_b(t) F_\epsilon[T_b(t)] \ , \ Y_b(0) = Y_{b0} \ ; \end{cases}$$

in (2.15), we have set $T_u^0 = T^0(-\infty)$, $T_b^0 = T^0(+\infty)$, $Y_u^0 = Y^0(-\infty)$, $Y_b^0 = Y^0(+\infty)$, and $\rho_u(t) = \rho(-\infty,t)$, $\rho_b(t) = \rho(+\infty,t)$. Of course, the differential system (2.15) has been deduced from (2.11).

Moreover, since the second and third equations in (2.12) give u_x and p_x, a single boundary condition might be adequate for the velocity and for the pressure; we write

$$u(-\infty,t) = u_u \ , \ p(-\infty,t) = p_u(t) \tag{2.16}$$

(the boundary value u_u is not allowed to vary with time from (2.12.c), since we need p_x to vanish at $-\infty$ from (2.16)).

Lastly, we need an additional condition in order to determine the evolution of the pressure $P(t)$. Since $mP(t) = \rho_u(t)R^0T_u(t)$, it suffices to specify the value of $\rho_u(t)$. But we also need u_x to vanish at $-\infty$ from (2.16), and (2.12) then says that $\rho_u(t)$ is not allowed to vary with time, so that we write

$$\rho(-\infty,t) = \rho_u \ , \tag{2.17}$$

a given constant.

We will see below that problem (2.11)-(2.17), which was proposed by Ludford [18], is a well-posed initial-boundary value problem.

3. Existence and uniqueness results. In this section, we will mainly state two existence and uniqueness results, one for time-dependent solutions of (2.11)-(2.17), and one for steady solutions of a similar problem where the reaction term is appropriately modified in order to remove the cold boundary difficulty.

3.1 Normalized equations. Let us first rewrite (2.11)-(2.17) in a simpler normalized form. For the sake of simplicity, we will assume in the sequel that the product $\lambda\rho$ is constant, which will simplify the expression of the diffusive terms in (2.11) (we refer to [24] for the analogous existence and uniqueness result with genuinely non linear diffusive terms). We can then choose the reference values for x, t, T, Y, P, ρ, u and p such that, in normalized variables, (2.11)-(2.17) becomes

$$\left\{ \begin{aligned} & T_t = Yf_\epsilon(T) + T_{xx} + \frac{\gamma-1}{\gamma}\frac{T_u'(t)}{T_u(t)}T \ , \\ & Y_t = -Yf_\epsilon(T) + \frac{1}{\mathcal{L}}Y_{xx} \ , \end{aligned} \right. \tag{3.1}$$

$$T(x,0) = T^0(x) \ , \ Y(x,0) = Y^0(x) \ , \tag{3.2}$$

$$\left\{ \begin{aligned} & T(-\infty,t) = T_u(t) \ , \ Y(-\infty,t) = Y_u(t) \ , \\ & T(+\infty,t) = T_b(t) \ , \ Y(+\infty,t) = Y_b(t) \ , \end{aligned} \right. \tag{3.3}$$

$$\left\{ \begin{aligned} & T_u'(t) = \gamma Y_u(t) f_\epsilon[T_u(t)] \ , \ T_u(0) = T_u^0 = T^0(-\infty) \ , \\ & T_b'(t) = Y_b(t) f_\epsilon[T_b(t)] + \frac{\gamma-1}{\gamma}\frac{T_u'(t)}{T_u(t)}T_b(t) \ , \ T_b(0) = T_b^0 = T^0(+\infty) \ , \\ & Y_u'(t) = -Y_u(t) f_\epsilon[T_u(t)] \ , \ Y_u(0) = Y_u^0 = Y^0(-\infty) \ , \\ & Y_b'(t) = -Y_b(t) f_\epsilon[T_b(t)] \ , \ Y_b(0) = Y_b^0 = Y^0(+\infty) \ , \end{aligned} \right. \tag{3.4}$$

$$\begin{cases} \rho T = T_u(t) \ , \\ \rho_t + \rho^2 u_x = 0 \ , \\ p_x = -u_t \ , \end{cases} \tag{3.5}$$

$$\begin{cases} \rho(-\infty, t) = 1 \ , \\ u(-\infty, t) = u_u \ , \\ p(-\infty, t) = p_u(t) \ . \end{cases} \tag{3.6}$$

Referring to [23] for the details about this normalization, we simply mention here that the nonlinearity f_ϵ is proportional to F_ϵ, and that the ratio $\frac{\gamma - 1}{\gamma}$ in (3.1) and (3.4) comes from Mayer's relation $\frac{\gamma - 1}{\gamma} = \frac{R^0}{mC_p}$, where γ is the specific heat ratio of the mixture.

3.2. Existence and uniqueness of unsteady solutions. Problem (3.1)-(3.6) has been studied in [23], where the differential system (3.4), the reaction-diffusion problem (3.1)-(3.3) and lastly problem (3.5)-(3.6) are investigated in this order in three consecutive steps. Before stating the main result of [23] about the solutions of (3.1)-(3.6), we need to describe the mathematical hypotheses. Introducing a function Γ satisfying

$$\begin{cases} \Gamma \in \mathcal{C}^\infty(I\!R, I\!R) \ , \\ \Gamma \equiv 0 \ \text{ on } (-\infty, -1) \ , \\ \Gamma \equiv 1 \text{ on } (1, +\infty) \ , \end{cases} \tag{3.7}$$

and setting

$$\begin{cases} T^0(x) = T_u^0 + (T_b^0 - T_u^0)\Gamma(x) + \phi^0(x) \ , \\ Y^0(x) = Y_u^0 + (Y_b^0 - Y_u^0)\Gamma(x) + \psi^0(x) \ , \end{cases} \tag{3.8}$$

we will assume that

$$\phi^0 \in H^4(I\!R) \cap L^1(I\!R) \ , \ \psi^0 \in H^4(I\!R) \cap L^1(I\!R) \ , \tag{3.9}$$

$$T_{min} = \inf_{x \in I\!R} T^0(x) > 0 \ , \ \inf_{x \in I\!R} Y^0(x) \geq 0 \ . \tag{3.10}$$

Moreover, we assume that

$$\begin{cases} f_\epsilon \in \mathcal{C}^3(I\!R_+, I\!R_+) \ , \\ f_\epsilon \text{ is bounded and Lipschitz-continuous on } I\!R_+ \ . \end{cases} \tag{3.11}$$

Then, the investigation of problem (3.1)-(3.6) begins by considering the system (3.4) of ordinary differential equations (ODEs). The proof of the following result involves classical arguments of the ODE theory (see [23]):

PROPOSITION 1. *Assume that the hypotheses (3.9)-(3.11) hold. Then, there exists a unique solution $[T_u(t), T_b(t), Y_u(t), Y_b(t)]$ to system (3.4). This solution is bounded and exists for all time, and satisfies*

$$\begin{cases} T_u(t) > 0 \ , \ T'_u(t) \geq 0 \ , \\ T_b(t) > 0 \ , \ T'_b(t) \geq 0 \ , \\ Y_u(t) \geq 0 \ , \ Y'_u(t) \leq 0 \ , \ \lim_{t \to +\infty} Y_u(t) = 0 \ , \\ Y_b(t) \geq 0 \ , \ Y'_b(t) \leq 0 \ , \ \lim_{t \to +\infty} Y_b(t) = 0 \ . \end{cases} \tag{3.12}$$

In the sequel, we will use the notations

$$T_u^\infty = \lim_{t \to +\infty} T_u(t) > 0 \ , \ T_b^\infty = \lim_{t \to +\infty} T_b(t) > 0 \ . \tag{3.13}$$

Then, one proves the following result for (3.1)-(3.3):

THEOREM 1. *Assume that the hypotheses (3.9)-(3.11) hold. Then, there exists a unique solution $[T(x,t), Y(x,t)]$ on $\mathbb{R} \times \mathbb{R}_+$ to system (3.1)-(3.4). This solution satisfies*

$$\begin{cases} T, \ Y \in L^\infty_{loc}(\mathbb{R}_+, L^\infty(\mathbb{R})) \ , \\ 0 \leq Y(x,t) \leq \sup_{x \in \mathbb{R}} \ Y^0(x) \ , \\ T(x,t) \geq T_{min} \ . \ \bullet \end{cases} \tag{3.14}$$

To prove Theorem 1, one introduces the unknowns ϕ, ψ defined by

$$\begin{cases} \phi(x,t) = T(x,t) - T_u(t) - (T_b(t) - T_u(t))\Gamma(x) \ , \\ \psi(x,t) = Y(x,t) - Y_u(t) - (Y_b(t) - Y_u(t))\Gamma(x) \ , \end{cases} \tag{3.15}$$

which satisfy homogeneous boundary conditions, and one writes problem (3.1)-(3.3) under the form

$$\frac{d\Phi}{dt} + A\Phi = \mathcal{F}(\Phi, t) \ , \ \Phi(0) = \Phi^0 \ , \tag{3.16}$$

where $\Phi(t) = [\phi(.,t), \psi(.,t)]$ and where the operator A is defined in the appropriate functional space by $A(\phi, \psi) = (-\phi_{xx}, -\frac{\psi_{xx}}{\mathcal{L}})$. The proof then relies on classical arguments of partial differential equations theory, based on the application of the linear semigroup theory (see [15], [23] for the details).

Once problem (3.1)-(3.4) is solved, studying problem (3.5)-(3.6) is an easy task. We refer to [15], [23] for the precise result, since we will restrict now our attention to the combustion variables T and Y.

3.3. Existence and uniqueness of traveling-wave solutions. It is clear that a steady solution in Eulerian coordinates corresponds to a traveling wave solution in Lagrangian variables, since the identities $T_\tau = 0$, $Y_\tau = 0$ then imply $T_t - cT_x = 0$, $Y_t - cY_x = 0$ from (2.3) and (2.9).

We therefore wish to consider traveling-wave solutions. In order to remove the cold boundary difficulty, we modify the reaction term. We consider a non linear function $f_{0\epsilon}$ satisfying

$$(3.17) \qquad \begin{cases} f_{0\epsilon} \in C^3(\mathbb{R}_+, \mathbb{R}_+) , \\ f_{0\epsilon} \text{ is bounded and Lipschitz-continuous on } \mathbb{R}_+ , \\ \exists T_i^0 \in (T_u^0, T_b^0) , \ f_{0\epsilon} \equiv 0 \text{ on } [T_u^0, T_i^0] , \ f_{0\epsilon} > 0 \text{ on } (T_i^0, +\infty) , \end{cases}$$

where T_i^0 is an ignition temperature, and look for $T(x)$, $Y(x)$ and $c \in \mathbb{R}$ satisfying (compare with (3.1))

$$(3.18) \qquad \begin{cases} cT_x = Y f_{0\epsilon}(T) + T_{xx} , \\ cY_x = -Y f_{0\epsilon}(T) + \dfrac{1}{\mathcal{L}} Y_{xx} , \end{cases}$$

$$(3.19) \qquad \begin{cases} T(-\infty) = T_u^0 , \ Y(-\infty) = Y_u^0 , \\ T(+\infty) = T_b^0 , \ Y(+\infty) = Y_b^0 . \end{cases}$$

In agreement with Section 2, we assume here that the boundary values T_u^0, T_b^0, Y_u^0, and Y_b^0 satisfy

$$(3.20) \qquad T_b^0 = T_u^0 + Y_u^0 , \ Y_u^0 > 0 , \ Y_b^0 = 0 ,$$

the first relation in (3.20) being the normalized analogue of (2.7).

About problem (3.18)-(3.19), we will simply state below the simplest existence and uniqueness problem: in the equidiffusional case, that is when $\mathcal{L} = 1$, (3.18)-(3.19) imply that $T + Y \equiv T_b^0$. The problem therefore reduces to a single ordinary differential equation; it remains to find a C^2 function $\mathcal{T}(x)$ and a real c satisfying

$$(3.21) \qquad \begin{cases} c(\mathcal{T})_x = g_{0\epsilon}(\mathcal{T}) + (\mathcal{T})_{xx} , \\ \mathcal{T}(-\infty) = T_u^0 , \ \mathcal{T}(+\infty) = T_b^0 , \end{cases}$$

(we have set $g_{0\epsilon}(T) = (T_b^0 - T) f_{0\epsilon}(T)$). The result, proved in e.g. [4], [6], is the following (its proof essentially relies on a shooting argument):

THEOREM 2. *Under the hypotheses (3.17), there exists a solution $(\mathcal{T}, c)$ of (3.21), with $c > 0$. Moreover, this solution is unique up to a translation of the origin.* •

4. Long-time behaviour. In this section, we consider the long-time behaviour of the time-dependent solutions of (3.1)-(3.4).

We will consider two basically different situations, depending on the assumptions on the reaction term. On one hand, we consider problem (3.1)-(3.4), where the nonlinear term f_ϵ corresponds to the actual Arrhenius reaction term; we will call this problem $(\mathcal{P}_\epsilon)$. On the other hand, we will consider the similar problem with $f_{0\epsilon}$ instead of f_ϵ, that is with the assumption of an ignition temperature: we will call this second problem $(\mathcal{P}_{0\epsilon})$.

For problem $(\mathcal{P}_\epsilon)$, we have the following result:

THEOREM 3. *Assume that the hypotheses (3.9)-(3.11) hold, and that f_ϵ satisfies*

$$\min_{T \geq T_{min}} f_\epsilon(T) > 0 \ . \tag{4.1}$$

Let (T,Y) be the unique solution of problem $(\mathcal{P}_\epsilon)$. Then, for any $x \in I\!R$, we have

$$\lim_{t \to +\infty} T(x,t) = \frac{T_u^\infty + T_b^\infty}{2} \ , \tag{4.2}$$

$$\lim_{t \to +\infty} Y(x,t) = 0 \ . \ \bullet \tag{4.3}$$

The proof of Theorem 3 is sketched in Section 4.2 below; the reader is referred to [23] for the detailed proof. Let us also add here that the limit (4.3) is uniform in $I\!R$: one shows indeed that $\|Y(.,t)\|_\infty$ exponentially decays to 0 as t tends to $+\infty$. On the other hand, the limit (4.2) is uniform on every compact subset of $I\!R$; in the particular case where $T_u^\infty = T_b^\infty$, this limit is uniform in all of $I\!R$.

Let us now turn to problem $(\mathcal{P}_{0\epsilon})$. We will simply consider the equidiffusional case, where there exists a unique traveling-wave solution $\mathcal{T}$ from Theorem 2; moreover, we will assume that the initial conditions (3.2) satisfy

$$T^0 + Y^0 \equiv T_b^0 \text{ on } I\!R \ . \tag{4.4}$$

Then problem $(\mathcal{P}_{0\epsilon})$ reduces to (4.5)-(4.6) below:

$$\begin{cases} T_t = g_{0\epsilon}(T) + T_{xx} \ , \\ T(x,0) = T^0(x) \ , \\ T(-\infty,t) = T_u^0 = T^0(-\infty) \ , \ T(+\infty,t) = T_b^0 = T^0(+\infty) \ , \end{cases} \tag{4.5}$$

$$T(.,t) + Y(.,t) \equiv T_b^0 \ . \tag{4.6}$$

The long-time behaviour of the solutions is then given by the next result, which says that the traveling-wave solution of (4.5) is stable:

THEOREM 4. *Assume that the hypotheses (3.9)-(3.10), (3.17) and (4.4) hold. Let (T,Y) be the unique solution of problem $(\mathcal{P}_{0\epsilon})$ (i.e. (4.5)-(4.6)), and let $(\mathcal{T},c)$ be the unique solution of (3.21). Assume moreover that $T_u^0 \leq T^0(x) \leq T_b^0$ for any $x \in I\!R$, and that $\lim_{x \to -\infty} \dfrac{T^0(x)}{\exp(cx)}$ exists in $I\!R_+^*$. Then there exist a real x_0 and two positive constants K and r such that, for any x and t:*

$$|T(x,t) - \mathcal{T}(x + x_0 + ct)| \leq K e^{-rt} \ . \ \bullet \tag{4.7}$$

The main ideas of the proof of this convergence result are presented in Section 4.2 below; the complete proof can be found in [25].

4.1. Complete asymptotic burning. We sketch here the proof of Theorem 3.

From (3.14) and (4.1), there exists a constant δ such that $f_\epsilon(T(x,t)) \geq \delta > 0$ for all $x \in I\!R$ and $t \geq 0$. Let $Y_\delta(t)$ be the solution of

$$\begin{cases} \dfrac{dY_\delta}{dt} = -\delta Y_\delta(t) \ , \\ \\ Y_\delta(0) = \|Y^0\|_\infty \ , \end{cases} \tag{4.8}$$

that is, $Y_\delta(t) = \|Y^0\|_\infty e^{-\delta t}$. An additional application of the maximum principle yields $Y(t,x) \leq Y_\delta(t)$, which is the desired estimate for Y.

Thus, the reason why the reactant eventually vanishes is clear from a physical point of view: it is a straightforward consequence of the fact that, with the present hypotheses, the reaction term $f_\epsilon(T)$ is always positive and bounded away from 0.

From an heuristic point of view, we can see now why the temperature has the behaviour (4.2). Because of (4.3), one may think that the reaction rate $Yf_\epsilon(T)$ eventually vanishes on all of $I\!R$; moreover, the term $T_u'(t)$ also tends to 0 as t tends to $+\infty$. One therefore expects that the temperature asymptotically behaves like the solution Θ of the linear heat equation $\Theta_t = \Theta_{xx}$ with the boundary conditions $\Theta(-\infty,t) = T_u^\infty$, $\Theta(+\infty,t) = T_b^\infty$. But Θ has the behaviour (4.2): $\lim\limits_{t\to+\infty} \Theta(x,t) = \dfrac{T_u^\infty + T_b^\infty}{2}$).

The rigorous mathematical proof of (4.2) exactly follows these lines, using the semi-group expression of the solution T and some technical but simple arguments (see [23]).

4.2. Stability of the traveling-front solution. The proof of Theorem 4 is based on the same ideas as the one of the stability result of Fife-McLeod [9] for a model arising in biology, with some differences related to the behaviour of the nonlinear function $g_{0\epsilon}$ near the cold boundary T_u^0. In particular, the third step in the proof below, which involves here some local stability results obtained by Sattinger [26] in a general framework, is simpler for the model of [9].

From now on, we assume that $(\mathcal{T}, c)$ is the unique solution of (3.21) such that $\mathcal{T}(0) = T_i^0$. Moreover, examining the solution of (4.5) in the reference frame of the traveling-front solution $\mathcal{T}$, we assume that T now satisfies

$$\begin{cases} T_t + cT_x = g_{0\epsilon}(T) + T_{xx} \ , \\ T(x,0) = T^0(x) \ , \\ T(-\infty,t) = T_u^0 = T^0(-\infty) \ , \ T(+\infty,t) = T_b^0 = T^0(+\infty) \ , \end{cases} \tag{4.9}$$

instead of (4.5) (that is, we change x into $x + ct$). The whole proof will then be given in the reference frame of the traveling wave.

The proof of Theorem 4 is sketched below, in four steps. We refer to [25] for the details.

<u>Step 1</u>: Estimates near $+\infty$ and $-\infty$.

This step consists in proving the following estimates:

PROPOSITION 2. *There exist $t_0 > 0$ and three positive constants k, λ and μ such that, for all $t \geq t_0$:*

$$(4.10) \qquad |T_b^0 - T(x,t)| + |T_x(x,t)| + |T_{xx}(x,t)| \leq K\ (e^{-\lambda x} + e^{-\mu t})\ ,\ \forall x \geq 0\ ,$$

$$(4.11) \qquad |T(x,t) - T_u^0| + |T_x(x,t)| + |T_{xx}(x,t)| \leq K\ e^{cx}\ ,\ \forall x \leq 0\ . \bullet$$

The proof of this proposition relies on the construction of upper and lower solutions; namely one proves from the maximum principle that the following inequalities hold for t large enough:

$$(4.12)\ \mathcal{T}(x-x_1(t))-q_1(t)\Gamma(x-x_1(t)) \leq T(x,t) \leq \mathcal{T}(x+x_2(t))+q_2(t)\Gamma(x+x_2(t))\ ,$$

where

$$(4.13) \qquad q_1(t) = O(e^{-\omega_1 t})\ ,\ q_2(t) = O(e^{-\omega_2 t})\ ,$$

$$(4.14) \qquad x_1(t) = \hat{x}_1 + O(e^{-\omega_1 t})\ ,\ x_2(t) = \hat{x}_2 + O(e^{-\omega_2 t})\ ,$$

for suitably chosen $\hat{x}_1$, $\hat{x}_2$, $\omega_1 > 0$ and $\omega_2 > 0$. The inequalities (4.12) yield the desired estimates for T; the similar estimates for the first and second derivatives are obtained from (4.12) combined with classical Schauder-type estimates. In addition to (4.10)-(4.11), these Schauder estimates show that the functions $T_{xx}(.,t)$ for $t \geq t_0$ are equicontinuous.

Step 2: Convergence of a subsequence.

The next result is the following:

PROPOSITION 3. *There exists $x_0 \in I\!R$ and a sequence (t_n) with $\lim_{n\to+\infty} t_n = +\infty$ such that, for any $x \in I\!R$:*

$$(4.15) \qquad \lim_{n\to+\infty} T(x,t_n) = \mathcal{T}(x+x_0)\ . \bullet$$

This result is obtained by classical arguments of dynamical systems theory. One first introduces the following Lyapunov functional:

$$(4.16) \qquad V(t) = \int_{-\infty}^{+\infty} e^{-cx}[\frac{1}{2}T_x^2 - G(T) + G(1)H(x)]dx\ ,$$

where $G(s) = \int_0^s g_{0\epsilon}(s)ds$ and where $H(x)$ denotes the Heaviside step function. Proposition 2 then guarantees that this function of t is well-defined and bounded; it is then easy to see that V is differentiable and that

$$(4.17) \qquad V'(t) = -\int_{-\infty}^{+\infty} e^{-cx}[T_{xx} - cT_x + g_{0\epsilon}(T)]^2 dx \leq 0\ .$$

Thus, there exists a sequence (t_n) with $\lim_{n\to+\infty} t_n = +\infty$ such that

$$\lim_{n\to+\infty} V'(t_n) = 0 \ . \tag{4.18}$$

Since one can show from Step 1 and Ascoli's theorem that the set $\{T(.,t),\ t \geq t_0\}$ is compact in $\mathcal{C}^2(\mathbb{R})$, we can extract a subsequence (t_{n_k}) such that $T(.,t_{n_k})$ converges in $\mathcal{C}^2(\mathbb{R})$. But the limit necessarily satisfies (3.21) from Proposition 2 and (4.17)-(4.18), which concludes the proof of Proposition 3.

Step 3: Uniform convergence.

The next lemma now follows from the previous steps:

LEMMA 1. *There exists a $\mathcal{C}^1$ positive function w_0 such that*

$$\sup_{x\in\mathbb{R}} \exp\left(-\frac{cx}{2}\right) w_0(x) + \sup_{x\in\mathbb{R}} \exp\left(-\frac{cx}{2}\right) |w_0'(x)| < +\infty \ , \tag{4.19}$$

and two sequences (t_n), (δ_n) with $\lim_{n\to+\infty} t_n = +\infty$ and $\lim_{n\to+\infty} \delta_n = 0$ such that, for all n and all $x \in \mathbb{R}$:

$$|T(x,t_n) - \mathcal{T}(x + x_0)| \leq \delta_n w_0(x) \ . \tag{4.20}$$

Now, the local stability theorems of Sattinger [26] apply: they yield the existence of a $\mathcal{C}^1$ function $h(\delta)$ defined in the neighbourhood of 0, and of positive constants k and K such that the solution $\hat{T}$ of the Cauchy problem:

$$\begin{cases} \hat{T}_t + c\hat{T}_x = g_{0\epsilon}(\hat{T}) + \hat{T}_{xx} \ , \\ \hat{T}(x,0) = \mathcal{T}(x+x_0) + \delta w_0(x) \ , \\ \hat{T}(-\infty,t) = T_u^0 \ , \ \hat{T}(+\infty,t) = T_b^0 \ , \end{cases} \tag{4.21}$$

satisfies

$$|\hat{T}(x,t) - \mathcal{T}(x + x_0 + \delta h(\delta))| \leq K e^{-kt} \ , \tag{4.22}$$

for any $x \in \mathbb{R}$ and $t \geq 0$ (the property (4.19) of w_0 is a necessary condition for the local stability result (4.22) to hold). Using now Lemma 1 and the maximum principle, we obtain that, for any n and any $t \geq t_n$

$$\mathcal{T}(x + x_0 - \delta_n h(-\delta_n)) - K e^{-k(t-t_n)} \leq T(x,t) \leq \mathcal{T}(x + x_0 + \delta_n h(\delta_n)) + K e^{-k(t-t_n)} \ . \tag{4.23}$$

This proves the uniform convergence:

$$\lim_{t\to+\infty} \|T(.,t) - \mathcal{T}(.+x_0)\|_\infty = 0 \ . \tag{4.24}$$

Step 4: Exponential convergence.

This step is identical to the last step of Fife and McLeod's proof. One now looks for a $\mathcal{C}^1$ function $\alpha(t)$ which, at each time t, minimises a certain distance between $T(.,t)$ and all translations of the traveling-wave solution; namely one looks for $\alpha(t)$ satisfying $F_t(\alpha(t)) = \min_{\beta\in\mathbb{R}} F_t(\beta)$, F_t being defined by

$$F_t(\beta) = \int_{-\infty}^{+\infty} e^{-cx}[T(x,t) - \mathcal{T}(x + x_0 + \beta)]^2 dx \; . \tag{4.25}$$

The Euler equation for the minimum reads

$$\int_{-\infty}^{+\infty} e^{-cx}[T(x,t) - \mathcal{T}(x + x_0 + \alpha(t))]\mathcal{T}'(x + x_0 + \alpha(t))dx = 0 \; . \tag{4.26}$$

Using (4.26) and the implicit function theorem, one can prove that $\alpha(t)$ exists for large t. Then, some technical arguments are needed to prove successively that

$$|T(x,t) - \mathcal{T}(x + x_0 + \alpha(t))| \leq Ce^{-\omega t} \; , \tag{4.27}$$

for some positive constants ω and C, and that $\alpha(t) \leq C'e^{-\omega' t}$ for other positive constants ω' and C'. This ends the proof of Theorem 4.

5. The cold boundary difficulty. The long-time behaviours of the solutions of problems $(\mathcal{P}_\epsilon)$ and $(\mathcal{P}_{0\epsilon})$ therefore appear from Section 4 to be thoroughly different. But in fact, the two situations do not differ so much, just because the activation energies that are involved are large: we will see in this section that Theorems 3 and 4 provide a mathematical answer to the paradox of the cold boundary difficulty.

In view of the expression (2.2) of the Arrhenius term, we make a mathematical "large activation energy analysis". Keeping in mind that f_ϵ is the actual Arrhenius non linear reaction term and that ϵ is proportional to the inverse of the activation energy, we now assume that we have two families of functions (f_ϵ) and $(f_{0\epsilon})$ such that *(i)* for any $\epsilon > 0$, f_ϵ satisfies (3.11), *(ii)* for any $\epsilon > 0$, $f_{0\epsilon}$ satisfies (3.17), and *(iii)* there exists a sequence (δ_ϵ) with $\lim_{\epsilon\to 0} \delta_\epsilon = 0$ and

$$\|f_{0\epsilon} - f_\epsilon\|_\infty \leq \delta_\epsilon \; . \tag{5.1}$$

Comparing the solutions of problems $(\mathcal{P}_\epsilon)$ and $(\mathcal{P}_{0\epsilon})$ is the subject of the next lemma:

LEMMA 2. *Assume that the hypotheses of Theorems 3 and 4 hold, and that (4.1) hold. Let (T_ϵ, Y_ϵ) be the solution of $(\mathcal{P}_\epsilon)$, and let $(T_{0\epsilon}, Y_{0\epsilon})$ be the solution of $(\mathcal{P}_{0\epsilon})$.*

Then there exist two sequences (δ'_ϵ) and (t_ϵ) with $\lim_{\epsilon\to 0} \delta'_\epsilon = 0$ and $\lim_{\epsilon\to 0} t_\epsilon = +\infty$ such that

$$\|T_\epsilon(.,t) - T_{0\epsilon}(.,t)\|_\infty + \|Y_\epsilon(.,t) - Y_{0\epsilon}(.,t)\|_\infty \leq \delta'_\epsilon \; . \tag{5.2}$$

The proof of Lemma 2 relies on an appropriate use of Gronwall's lemma.

Now, this result provides a mathematical answer to the paradox of the cold boundary difficulty. Under the preceding assumptions, Lemma 2 shows that, if ϵ is small enough (that is, if the activation energy is large enough), the time-dependent solution of the Arrhenius model ($\mathcal{P}_\epsilon$) remains close during a long time to the time-dependent solution of the model with an ignition temperature ($\mathcal{P}_{0\epsilon}$; but Theorem 4 then says that the latter solution converges exponentially to the corresponding traveling wave $\mathcal{T}_{0\epsilon}$. Therefore, we have proved that *the solution of the Arrhenius model behaves like a traveling wave during a period of time which is larger and larger as the activation energy increases*, before it has the asymptotic behaviour described in Theorem 3. This is the mathematical answer to the cold boundary difficulty.

6. Numerical illustration. In this last section, we illustrate the preceding analysis by showing a numerical example.

6.1. The numerical method. Before discussing the numerical results, let us briefly present the numerical method used in the calculation. We solve problem (3.1)-(3.4) (that is, problem ($\mathcal{P}_\epsilon$)) on a finite interval $[-L, L]$, using a computational grid which is equally spaced in space and time. In order to avoid too severe restrictions on the time step, while still describing accurately the transient flame evolution, we use an integration scheme which is implicit for the diffusive terms but explicit for the reactive terms (we refer to [3] for a discussion on the choice of the time step). Moreover, we use homogeneous Neumann conditions at both boundaries $-L$ and $+L$. The scheme ($\mathcal{S}$) can therefore be written as

$$(6.1)\quad \frac{T_j^{n+1}-T_j^n}{\Delta t}=\frac{T_{j-1}^{n+1}-2T_j^{n+1}+T_{j+1}^{n+1}}{\Delta x^2}+Y_j^n f_\epsilon(T_j^n)+\frac{\gamma-1}{\gamma}\,\frac{T_u'(t^n)}{T_u(t^n)}T_j^n \text{ for } 1\le j\le N \ ,$$

$$(6.2)\quad \frac{T_0^{n+1}-T_0^n}{\Delta t}=\frac{T_1^{n+1}-T_0^{n+1}}{\Delta x^2}+Y_0^n f_\epsilon(T_0^n)+\frac{\gamma-1}{\gamma}\,\frac{T_u'(t^n)}{T_u(t^n)}T_0^n \text{ for } j=0 \ ,$$

$$(6.3)\quad \frac{T_{N+1}^{n+1}-T_{N+1}^n}{\Delta t}=\frac{T_N^{n+1}-T_{N+1}^{n+1}}{\Delta x^2}+Y_{N+1}^n f_\epsilon(T_{N+1}^n)+\frac{\gamma-1}{\gamma}\,\frac{T_u'(t^n)}{T_u(t^n)}T_{N+1}^n \text{ for } j=N+1 \ ,$$

with the similar equations for Y. The terms $T_u(t^n)$ and $T_u'(t^n)$ are evaluated and stored in a preliminary step using an explicit Runge-Kutta scheme. In (6.1)-(6.3), Δt is the time step, and N is the number of interior mesh points and $\Delta x = \dfrac{2L}{N+1}$ is the mesh spacing. For $0 \le j \le N+1$, we set $x_j = j\Delta x - L$.

Since we want to observe the time-dependent behaviour of the solution to (3.1)-(3.4), it is of interest to know that the above scheme ($\mathcal{S}$) converges, in the following sense:

PROPOSITION 4. *Assume in addition to (3.9)-(3.11) that there exist two positive constants A and α such that the initial data (3.2) satisfy*

$$(6.4)\quad \begin{cases} |T^0(x)-T_u^0|+|Y^0(x)-Y_u^0| \le A\exp(\alpha x)\ \forall x<0 \ , \\ |T^0(x)-T_b^0|+|Y^0(x)-Y_b^0| \le A\exp(-\alpha x)\ \forall x>0 \ . \end{cases}$$

Let (T, Y) be the unique solution of (3.1)-(3.4). Lastly, let (T_j^n, Y_j^n) be the numerical solution of the scheme $(\mathcal{S})$, and assume that the time step Δt satisfies

$$\Delta t \leq \|f_\epsilon\|_\infty^{-1} \ . \tag{6.5}$$

Then, for any $t_0 > 0$, there exists a positive constant $K = K(t_0)$ such that, for any j and n with $0 \leq j \leq N+1$, $0 \leq n\Delta t \leq t_0$:

$$|T(x_j, n\Delta t) - T_j^n| + |Y(x_j, n\Delta t) - Y_j^n| \leq K \left(\Delta t + \Delta x + \frac{\exp(-\alpha L)}{\Delta x}\right) \ . \tag{6.6}$$

We refer to [23] for the proof of this convergence result (see also [2] where a similar result is proved for a two-dimensional explicit scheme).

6.2. Numerical results. We will now use the scheme $(\mathcal{S})$ to solve the normalized problem (3.1)-(3.4)), with the following non linear function:

$$f_\epsilon(T) = \exp\left(-\frac{9}{T}\right) \ , \tag{6.7}$$

and the following initial boundary values:

$$\begin{cases} T_u^0 = 1 \ , \ T_b^0 = 11 \ , \\ Y_u^0 = 1 \ , \ Y_b^0 = 0 \ , \end{cases} \tag{6.8}$$

and with a unit Lewis number.

Of course, these values are not realistic, since we want to observe the long-time behaviour described at the end of Section 5: with realistic parameters, we should have to perform the calculation during an extremely long time before the fresh gases temperature increases substantially above its initial value (see e.g. [16], [22], where the steady solution $\mathcal{T}$ is approached by solving numerically the problem $(\mathcal{P}_\epsilon)$ with the actual Arrhenius term (and not $(\mathcal{P}_{0\epsilon})$), because the "very-long-time behaviour" (complete burning) described in Theorem 3 occurs only extremely far after the "convergence" to steady-state).

We have taken $L = 100$, and used the following initial data (which are inspired from the planar steady-state temperature and mass fraction profiles obtained using high activation energy asymptotics; see e.g., [21]):

$$Y^0(x) = \begin{cases} 1 - \exp(60 - x) & \text{if } -100 \leq x \leq 60 \ , \\ 0 & \text{if } 60 \leq x \leq 100 \ , \end{cases} \tag{6.9}$$

$$T^0(x) = T_b^0 - 10Y^0(x) \text{ for } -100 \leq x \leq 100 \ . \tag{6.10}$$

The results are shown for 12 successive (inequally spaced) time levels. Notice, that the variable $\Theta = \dfrac{T - T_u^0}{T_b^0 - T_u^0}$ is plotted instead of T, and that the scale on the Θ axis changes at time t_9 (Figure 5).

In full agreement with the preceding analysis, we observe that the flame initially "converges" towards a traveling wave (in the interval $[t_1, t_2]$) and propagates at constant speed (in the interval $[t_1, t_4]$). At time t_4, the fresh mixture temperature has just begun to increase over its initial value T_u^0 (as explained above, the induction time t_4 would be extremely larger if realistic values of the parameters were used). In the interval $[t_4, t_{10}]$, the temperature increases on the whole domain: as it is well-known from the study of homogeneous combustion, there is a rather sudden transition where the fresh gas tenperature $T_u(t)$ increases to its final value (notice that the time lag between two consecutive figures has been reduced in this interval). Again here, one should add that this transition would be much more sudden with more realistic parameter values. Lastly, after t_{10}, complete burning has occured, and heat diffusion very slowly conducts the temperature to its final value

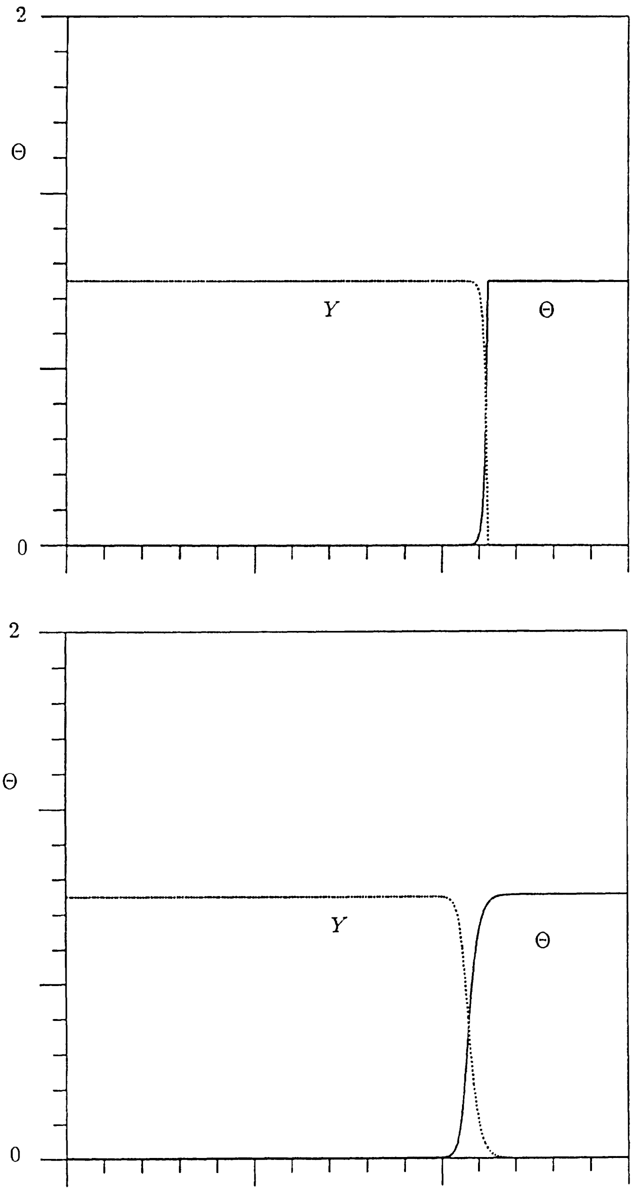

Figure 1. Temperature and mass fraction profiles at $t_1 = 0$ and $t_2 = 10$.

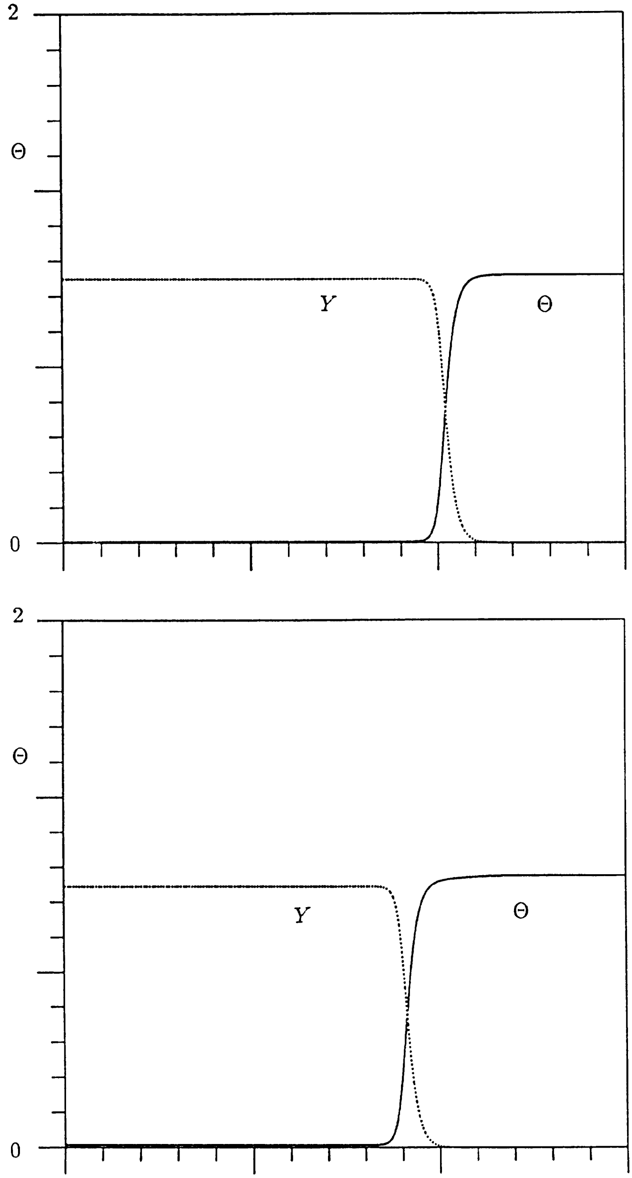

Figure 2. Temperature and mass fraction profiles at $t_3 = 20$ and $t_4 = 40$.

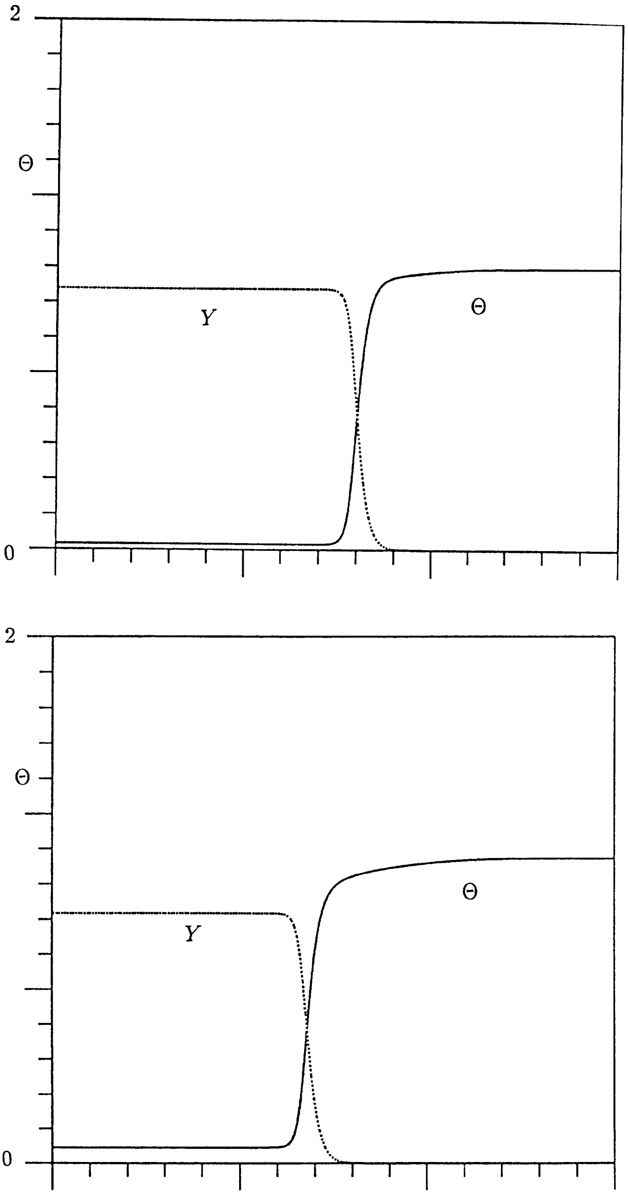

Figure 3. Temperature and mass fraction profiles at $t_5 = 60$ and $t_6 = 80$.

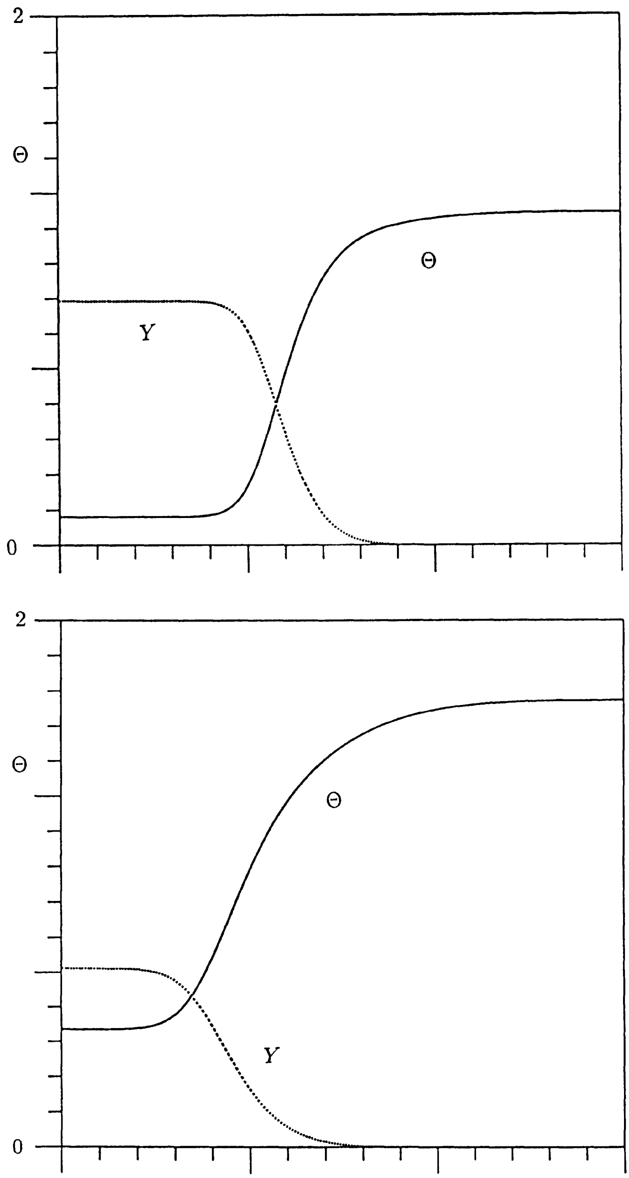

Figure 4. Temperature and mass fraction profiles at $t_7 = 80.5$ and $t_8 = 81$.

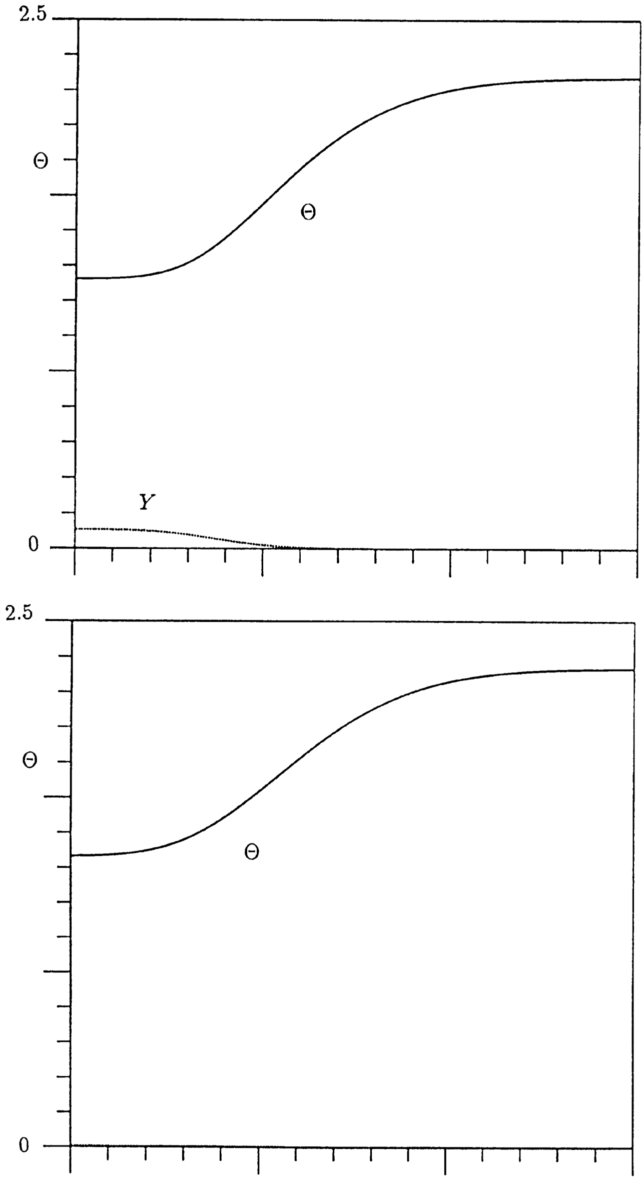

Figure 5. Temperature and mass fraction profiles at $t_9 = 81.5$ and $t_{10} = 82$.

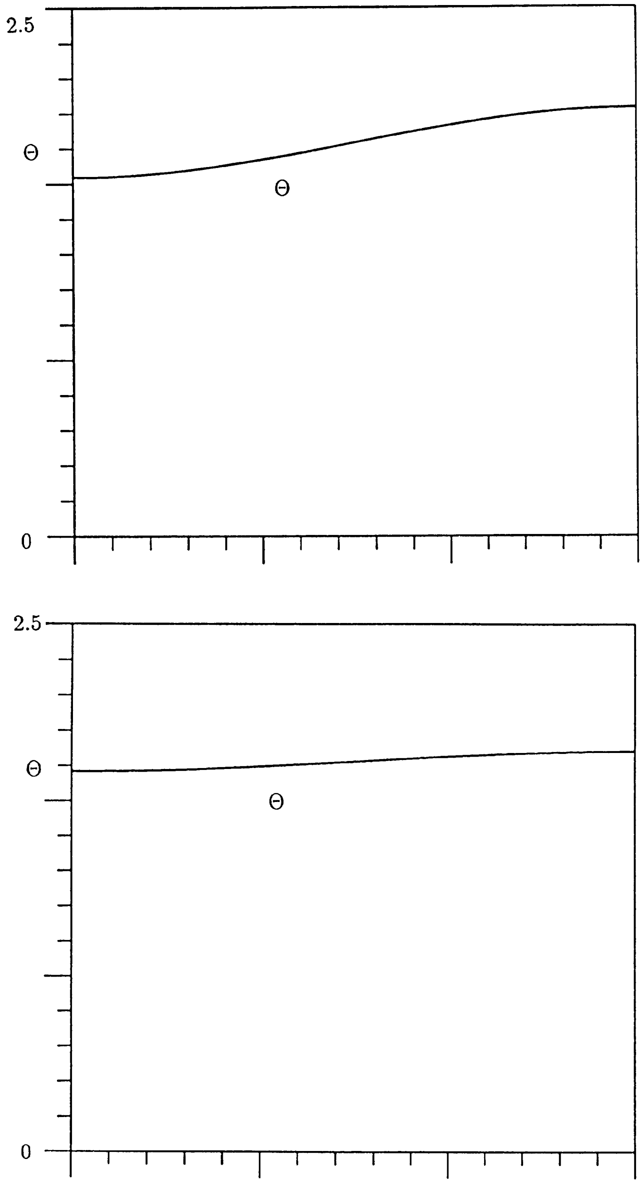

Figure 6. Temperature and mass fraction profiles at $t_{11} = 5,000$ and $t_{12} = 10,000$.

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