Mathematical and numerical aspects of one-dimensional laminar flame simulation

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Abstract :

The aim of this paper is to solve several mathematical and numerical questions related to the simulation of stationary and unstationary premixed flat flames. Most of the results are obtained in the general context of complex chemical and diffusion mechanisms. The main mathematical results concern : (i) the a priori positivity of the mass fractions, (ii) the sensitivity of the flame speed to the computational domain. The numerical method that I propose for solving the stationary problem is a new combination of the pseudo-unstationary approach, the Newton iterations and the adaptive gridding. The computation of H_2-O_2-N_2 flames with various initial concentrations (including the chemical extinction zone) shows the efficiency of this method.

Résumé :

Le but de ce papier est de résoudre plusieurs questions mathématiques et numériques liées à la simulation des flammes planes prémélangées stationnaires et instationnaires. La plupart des résultats sont obtenus dans le contexte général de mécanismes chimiques et diffusifs complexes. Les résultats mathématiques principaux concernent : (i) la positivité a priori des fractions massiques, (ii) la sensibilité de la vitesse de flamme au domaine de calcul. La méthode numérique que je propose pour résoudre le problème stationnaire est une combinaison originale de l'approche pseudo-instationnaire, des itérations de Newton et du maillage adaptatif. Le calcul de flammes H_2-O_2-N_2 avec différentes concentrations initiales (y compris la zone d'extinction chimique) montre l'efficacité de cette méthode.

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0. INTRODUCTION

The question of propagation (or no propagation) of a planar flame in a premixed gazeous mixture covers a great variety of situations for the following reasons :

(i) each different composition of the fresh mixture gives rise to a different physical phenomenon ;

(ii) the diffusion and chemical mechanisms can be described by a rather realistic or simplified model.

As an example of (ii), the hydrogen-air flame

$$2H_2 + O_2 \longrightarrow 2H_2O$$

can be modelled by eleven elementary chemical reactions and eight species (cf. J. WARNATZ [42]) or by a more complex or a less complex chemical mechanism.

When the flame model is chosen, the computation of planar travelling waves present the following difficulties : (i) existence of a continuum of solutions (in relation with the so-called "cold boundary difficulty"), (ii) the partial differential equations are strongly nonlinear, (iii) the partial differential equations are stiff with disparate length scales, (iv) the system can be very large (depending on the degree of simplification).

Various methods have been proposed for solving these difficulties in a given chemical context. Most of these methods use an unstationary approach (see for instance [6] [8] [9] [17] [23] [24] [32] [36] [37] [39] [45]). A more recent approach is to solve directly the boundary value problem([35] [46]). In the GAMM Workshop (1981) "Numerical methods in laminar flame", some of these methods have been compared on the same chemical mechanism describing the hydrogen-air flame (cf. J. WARNATZ [42]). The participating groups were : DIXON-LEWIS, HEIMERL, JINNO & FUKUTANI, REITZ, SMOOKE, THIES & PETERS, WARNATZ, ORAN.

The aim of the present paper is to solve several mathematical and numerical questions related to stationary and unstationary flames. Most of the results are obtained in the general context of complex chemical and transport models. The corresponding equations are described in Sec. 1.

In Sec. 2, I give some mathematical properties of the unstationary problem. The main result is the a priori positivity of the mass fractions. This property was known only for a simplified combustion model (cf. CHUEH-CONLEY-SMOLLER [4]). This a priori positivity of solutions is important being a first step for obtaining the stability of numerical pseudo-unstationary methods.

Sec. 3 is devoted to the mathematical study of the stationary problem. The main result concerns the sensitivity of the flame speed to the computational domain.

Sec. 4 contains a detailled description of a new numerical method for solving the stationary problem. This method combines the use of the pseudo-unstationary approach, the global Newton method and the mesh adaptation.

The efficiency of this method is illustrated in Sec. 5 by the computation of H_2-O_2-N_2 flames with complex diffusion and chemical mechanisms. First, I have carried out the test of the GAMM Workshop [42] (stoichiometric case). The method of Sec. 4 seems faster compared to the other methods and as robust and accurate. Secondly, I present new numerical results concerning the chemical extinction of the H_2-O_2-N_2 flame by increase of the inert concentration (this last study was suggested to me by P. CLAVIN).

The results presented in this paper were announced in [33][34] .

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1. Problem formulation

1.1. Combustion equations in one-dimensional space

Let us consider a mixture of M species in one-dimensional space ; conservations equations for total mass, enthalpy and masses of each species may be written (see [3] [12] [39] [47] [48]):

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \tag{1.1}$$

$$\rho\Big(\sum_{i=1}^{M} h_i' Y_i\Big)\Big(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x}\Big) - \Big(\sum_{i=1}^{M} h_i' U_i\Big)\frac{\partial T}{\partial x} - \frac{\partial}{\partial x}\Big(\lambda \frac{\partial T}{\partial x}\Big) + \tag{1.2}$$
$$+ \sum_{i=1}^{M} h_i r_i = 0$$

$$\rho\Big(\frac{\partial Y_i}{\partial t} + u \frac{\partial Y_i}{\partial x}\Big) - \frac{\partial}{\partial x} U_i - r_i = 0, \quad 1 \le i \le M. \tag{1.3}$$

The independant variables are the flow velocity u, the temperature T and the mass fractions Y_i of each species ($1 \le i \le M$).

We shall consider that the diffusion fluxes U_i are given by one of the following models :

1) Model recommended by Coffee-Heimerl [6] (see also [7] [16] [40] [41])

$$U_i = Y_i \rho d_i \frac{1}{X_i} \frac{\partial X_i}{\partial x} + Y_i \rho d_{T,i} \frac{1}{T} \frac{\partial}{\partial x} T - Y_i U_c$$

where

$$X_i = \frac{Y_i/m_i}{\sum_{i=1}^{M} Y_i/m_i}, \tag{1.4}_1$$

$$U_c = \sum_{i=1}^{M} \Big(Y_i \rho d_i \frac{1}{X_i} \frac{\partial X_i}{\partial x} + Y_i \rho d_{T,i} \frac{1}{T} \frac{\partial T}{\partial x}\Big)$$

2) Approximation of 1) when $\sum_{j=1}^{M} Y_j/m_j \simeq$ cte :

$$U_i = \rho\, d_i \frac{\partial Y_i}{\partial x} + Y_i\, \rho\, d_{T,i} \frac{1}{T} \frac{\partial T}{\partial x} - Y_i\, U_c \qquad (1.4)_2$$

where $U_c = \sum_{i=1}^{M} (\rho\, d_i \frac{\partial Y_i}{\partial x} + Y_i\, \rho\, d_{T,i} \frac{1}{T} \frac{\partial T}{\partial x})$

3) The Mth species is in excess :

$$U_i = \rho\, d_i \frac{\partial Y_i}{\partial x} + Y_i\, \rho\, d_{T,i} \frac{1}{T} \frac{\partial T}{\partial x} \qquad 1 \le i \le M-1$$
$$U_M = - \sum_{i=1}^{M-1} U_i \qquad (1.4)_3$$

Sometimes, we shall take for U_i the more general expression :

$$U_i = \sum_{j=1}^{M} \mu_{ij}(T,Y) \frac{\partial Y_j}{\partial x} + \mu_i(T,Y) \frac{\partial T}{\partial x} \qquad (\widehat{1.4})'$$

In the previous equations, ρ denotes the mass density of the mixture ; λ , the thermal conductivity of the mixture ; h_i, the specific enthalpy of the ith species ; $h_i' = \frac{dh_i}{dT}$ $(= C_{pi})$, the constant pressure heat capacity of the ith species ; d_i, $d_{T,i}$, the diffusion coefficients of the ith species in the mixture ; r_i, the mass rate of production of the ith species per unit volume ; m_i, the molar mass of the ith species.

The physically admissible domain for (T,Y) is

$$S = \{(T,Y) \in \mathbb{R}^{M+1},\ T > 0,\ Y_i \ge 0\ ,\ 1 \le i \le M,\ \sum_{i=1}^{M} Y_i = 1\}\ .$$

The quantities m_i are positive constant ; the quantities ρ, λ , d_i, $d_{T,i}$, r_i are given regular functions of $(T,Y) \in \tilde{S} \supset S$, where

$$\tilde{S} = \{(T,Y) \in \mathbb{R}^{M+1},\ T > 0,\ \sum_{i=1}^{M} Y_i/m_i > 0\}\ ;$$

ρ, λ, d_i are positive functions ; h_i is a function of T alone $(T > 0)$; $h_i' = \frac{dh_i}{dT}$ is positive. The production terms r_i are obtaines as sums of contributions of all elementary chemical reactions. As a consequence, the functions r_i satisfy :

$$\sum_{i=1}^{M} r_i(T,Y) = 0 \quad \forall (T,Y) \in \tilde{S} \quad \text{(mass conservation)} \tag{1.5}$$

$$r_i(T,Y) \geq 0 \quad \forall (T,Y) \in \tilde{S} \quad \text{with } Y \geq 0 \text{ and } Y_i = 0 \tag{1.6}$$

Remark 1.1 :

i) The thermal diffusion terms $\rho\, Y_i\, d_{T,i}\, \frac{1}{T}\, \frac{\partial T}{\partial x}$ which appear in (1.4) are usually negligible, i.e. we can take $d_{T,i} = 0$, possibly except for the light species (cf. J. WARNATZ [41]).

ii) In the special case "$d_{T,i} = 0$, $d_i = d$ $\forall i$", both models $(1.4)_2$ and $(1.4)_3$ are equivalent to

$$U_i = \rho\, d\, \frac{\partial Y_i}{\partial x} \tag{1.4}_4$$

1.2. Evolution problem in lagrangian coordinates

The flow velocity u can be eliminated from (1.1)-(1.3) by introducing the lagrangian coordinates (t,z) defined by $\frac{\partial z}{\partial x} = \rho$, $\frac{\partial z}{\partial t} = -\rho u$. We obtain the following problem $(\mathcal{E}_k)$, where k refers to the choice of the diffusion fluxes model $(1.4)_k$.

$$(\mathcal{E}_k) \begin{cases} \left(\sum_{i=1}^{M} h_i' Y_i\right) \frac{\partial T}{\partial t} - \left(\sum_{i=1}^{M} h_i' U_i\right) \frac{\partial T}{\partial z} - \frac{\partial}{\partial z}\left(\rho \lambda \frac{\partial T}{\partial z}\right) + \sum_{i=1}^{M} \frac{h_i r_i}{\rho} = 0 & (1.7) \\ \frac{\partial Y_i}{\partial t} - \frac{\partial}{\partial z} U_i - \frac{r_i}{\rho} = 0 \ , \ 1 \leq i \leq M & (1.8) \end{cases}$$

1.3. Travelling waves

The travelling waves are the stationary solutions of (1.1)-(1.4) on the spatial domain $(-\infty , +\infty)$; as a result, (c,T,Y) is solution of :

$$(\mathcal{C}_k) \begin{cases} \rho u = c, \text{ unknown constant,} & \\ \left\{c \sum_{i=1}^{M} h_i' Y_i - \sum_{i=1}^{M} h_i' U_i\right\} \frac{dT}{dx} - \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) + \sum_{i=1}^{M} h_i r_i = 0 & (1.9) \\ c \frac{dY_i}{dx} - \frac{d}{dx} U_i - r_i = 0, \ 1 \leq i \leq M \ , & (1.10) \\ \lim_{x \to -\infty} T(x) = T_u, \ \lim_{x \to -\infty} Y_i(x) = Y_{iu} & (1.11) \end{cases}$$

$(\mathcal{C}_k)$ $(T_u, Y_{iu}$ prescribed constants)

$$\lim_{x \to +\infty} T(x) = T_b, \quad \lim_{x \to +\infty} Y_i(x) = Y_{ib} \tag{1.12}$$

$(T_b, Y_{ib}$ unknown constants)

$$\lim_{x \to \pm\infty} \frac{dT}{dx}(x) = \lim_{x \to \pm\infty} \frac{dY_i}{dx}(x) = 0 \tag{1.13}$$

$$T(x_f) = T_f \tag{1.14}$$

where x_f, T_f are prescribed constants which fix the flame with respect to the x-axis (we could also fix Y_{io} instead of T) ; the index k of $(\mathcal{C}_k)$ refers to the choice of the diffusion fluxes model $(1.4)_k$.

2. SOME MATHEMATICAL PROPERTIES OF THE UNSTEADY SOLUTIONS

During Sec. 2, D denotes a bounded interval of $\mathbb{R}$, τ a real positive number, Q is $D \times (0,\tau)$; we call smooth solution of $(\mathcal{E}_k)$ on Q every regular function $(T,Y) : Q \to \tilde{S}$ which satisfies $(\mathcal{E}_k)$ $\forall (z,t) \in Q$.

In Sec. 2.1 and 2.2, we precise the boundary conditions for which we have enthalpy and mass conservation. In Sec. 2.3, we prove that S is an invariant region for $(\mathcal{E}_k)$, i.e. any smooth solution (T,Y) of $(\mathcal{E}_k)$ with initial values in S satisfies $(T,Y)(z,t) \in S$ $\forall (z,t) \in Q$. This result is also important for computing stationary solutions by a pseudo-unstationary approach.

2.1. Enthalpy conservation

Proposition 2.1. Let (T,Y) be a smooth solution of $(\mathcal{E}_k)$, $1 \leq k \leq 3$, on Q. We suppose that

$$\frac{\partial T}{\partial z}(z,t) = \frac{\partial Y_i}{\partial z}(z,t) = 0 \quad \forall (z,t) \in \partial D \times (0,\tau) \tag{2.1}$$

Then

$$\sum_{i=1}^{M} \int_D h_i(T(z,t))Y_i(z,t)dz = \sum_{i=1}^{M} \int_D h_i(T(z,0))Y_i(z,0)dz \quad \forall t \in (0,\tau) \qquad (2.2)$$

Proof : First we observe that

$$h_i'(T(z,t))\frac{\partial T}{\partial t} = \frac{\partial}{\partial t} h_i(T(z,t)),$$

$$h_i'(T(z,t))\frac{\partial T}{\partial z} = \frac{\partial}{\partial z} h_i(T(z,t))$$

We multiply each equation of (1.8) by h_i and we add to (1.7). We obtain

$$\frac{\partial}{\partial t}\Big(\sum_{i=1}^{M} h_i(T)Y_i\Big) - \frac{\partial}{\partial z}\Big(\sum_{i=1}^{M} h_i(T)U_i\Big) - \frac{\partial}{\partial z}\Big(\rho\,\lambda\,\frac{\partial T}{\partial z}\Big) = 0 \qquad (2.3)$$

We integrate (2.3) with respect to z over D. By (2.1), we obtain (2.2)

2.2. Mass conservation

Proposition 2.3. Let (T,Y) be a smooth solution of $(\mathcal{E}_k)$, $1 \le k \le 3$, on Q. We suppose that

$$\sum_{i=1}^{M} Y_i(z,0) = 1 \quad \forall z \in D \ , \qquad (2.4)$$

$$\Big\{\sum_{i=1}^{M} Y_i(z,t) = 1 \text{ or } \sum_{i=1}^{M} U_i(z,t) = 0\Big\} \quad \forall (z,t) \in \partial D \times (0,\tau) \qquad (2.5)$$

Then

$$\sum_{i=1}^{M} Y_i(z,t) = 1 \quad \forall (z,t) \in Q. \qquad (2.6)$$

Proof : We add the equations of (1.8). By (1.5), we obtain

$$\frac{\partial}{\partial t}\Big(\sum_{i=1}^{M} Y_i\Big) - \frac{\partial}{\partial z}\Big(\sum_{i=1}^{M} U_i\Big) = 0 \text{ on } Q.$$

The case $(1.4)_3$ is trivial ; in the other cases, we have

$$\sum_{i=1}^{M} U_i = (1 - \sum_{i=1}^{M} Y_i)U_c$$

The function $\phi = 1 - \sum_{i=1}^{M} Y_i$ satisfies

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial z}(U_c \phi) = 0 \text{ on } Q \ .$$

We multiply by ϕ and we integrate in z. We obtain

$$\frac{1}{2} \frac{d}{dt} \int_D \phi^2 \, dz + \frac{1}{2} \int_D \frac{\partial U_c}{\partial z} \phi^2 \, dz - \frac{1}{2} [U_c \phi^2]_{\partial D} = 0 \ .$$

We have $\phi U_c = \sum_{i=1}^{M} U_i$. By (2.5), we obtain

$$[U_c \phi^2]_{\partial D} = [(\sum_{i=1}^{M} U_i)\phi]_{\partial D} = 0 \ .$$

Hence

$$\frac{1}{2} \frac{d}{dt} \int_D \phi^2 \, dz = - \frac{1}{2} \int_D \frac{\partial U_c}{\partial z} \phi^2 \, dz$$

Since (T,Y) is a regular function from Q in $\tilde{S}$, U_c is regular. Thus, we can write

$$\frac{d}{dt} \int_D \phi^2 \, dz \leq \alpha \int_D \phi^2 \, dz$$

with $\alpha = \sup_{(z,t) \in Q} \left| \frac{\partial}{\partial z} U_c(z,t) \right| < \infty$

From Gronwall lemma, we obtain

$$\int_D \phi^2(z,t) dz \leq \exp(\alpha t) \int_D \phi^2(z,0) dz = 0$$

and Prop. 2.2. is proved.

Prop.2.2 shows that $(\mathcal{E}_k)$, $1 \leq k \leq 3$, is equivalent with the following problem $(\tilde{\mathcal{E}}_k)$:

$$(\tilde{\mathcal{E}}_k) \begin{cases} \text{equation (1.7)} \\ \text{equations of (1.8) for } 1 \leq i \leq M-1 \\ Y_M = 1 - \sum_{i=1}^{M-1} Y_i \end{cases}$$

It is easy to prove that $(\tilde{\mathcal{E}}_k)$ is elliptic in z, i.e. the diffusion matrix of $(\tilde{\mathcal{E}}_k)$ is regular, whereas $(\mathcal{E}_k)$ is not elliptic.

Remark 2.1. Without more hypotheses on the coefficients d_i, the diffusion matrix of $(\tilde{\mathcal{E}}_k)$, k = 1,2, is not always positive definite ; for this reason, the existence of smooth solution of $(\mathcal{E}_k)$ or $(\tilde{\mathcal{E}}_k)$ is not always guaranteed. In the case k = 3, the diffusion matrix is positive definite (and diagonal) and the existence of solution is proved (cf. B. LARROUTUROU [20]).

2.3. Invariant regions

We put

$$I_k = \{1,\ldots,M\} \quad \text{for } 1 \le k \le 2$$

$$I_3 = \{1,\ldots,M-1\}$$

The main result of this section is

Theorem 2.1. Let (T,Y) be a smooth solution of $(\mathcal{E}_k)$ on Q, $1 \le k \le 3$. We suppose that

$$Y_i(z,0) > 0 \quad \forall z \in D, \forall i \in I_k , \tag{2.7}$$

$$\{Y_i(z,t) > 0 \quad \text{or} \quad \frac{\partial Y_i}{\partial \nu}(z,t) \ge 0\} \quad \forall (z,t) \in \partial D \times (0,\tau), \forall i \in I_k \tag{2.8}$$

Then

$$Y_i(z,t) > 0 \quad \forall (z,t) \in Q, \forall i \in I_k \tag{2.9}$$

Several authors (WEINBERGER [44], CHUEH-CONLEY-SMOLLER [4]) have given necessar and sufficient conditions for determining the invariant regions of weakly coupled [1] parabolic or elliptic systems. The system $(\mathcal{E}_k)$ is not weakly coupled ; nevertheless, we can adapt the method of proof used by WEINBERGER in [44].

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(1) A system of m partial differential equations in m unknown functions is said "weakly coupled" if the ith equation only contains derivatives of the ith function.

Proof : Each definition $(1.4)_k$ can be rewritten as

$$U_i = \tilde{d}_i(T,Y) \frac{\partial Y_i}{\partial z} + Y_i F_i(T,Y, \frac{\partial Y}{\partial z}, \frac{\partial T}{\partial z}) \quad i \in I_k$$

where $\tilde{d}_i$ and F are smooth functions (we observe that, for $Y_i = 0$, the system is weakly coupled).

As a consequence, for $i \in I_k$, Y_i is solution of

$$\frac{\partial Y_i}{\partial t} - a_i(z,t) \frac{\partial^2 Y_i}{\partial z^2} + b_i(z,t) \frac{\partial Y_i}{\partial z} + c_i(z,t) Y_i = f_i(z,t,Y_i)$$

where a_i, b_i, c_i are regular functions on Q ; f_i is defined by

$$f_i(z,t,s) = r_i(T(z,t),Y_1(z,t),\ldots,Y_{i-1}(z,t),s,Y_{i+1}(z,t),\ldots,Y_M(z,t)).$$
$$.\rho(T(z,t),Y(z,t))^{-1}$$

We proceed now by contradiction. Let $t^* > 0$ such that

$$\begin{cases} Y_i(z^*,t^*) = 0 & \text{for some } z^* \in \bar{D} \text{ and some } i \\ Y_j(z,t) > 0 & \forall (z,t) \times D \times (0,t^*) \ , \ \forall j \end{cases} \tag{2.10}$$

From (2.10), (1.6), we have

$$f_i(z,t,0) \geq 0 \quad \forall (z,t) \in D \times (0,t^*)$$

Hence

$$\frac{\partial Y_i}{\partial t} - a_i(z,t) \frac{\partial^2 Y_i}{\partial z^2} + b_i(z,t) \frac{\partial Y_i}{\partial z} + c_i(z,t) Y_i \geq f_i(z,t,Y_i) - f(z,t,0)$$

We introduce

$$\mu(z,t) = \begin{cases} \dfrac{f_i(z,t,Y_i(z,t)) - f_i(z,t,0)}{Y_i(z,t)} & \text{if } Y_i(z,t) \neq 0 \ , \\ 0 & \text{otherwise} \end{cases}$$

Since r_i is a smooth function, μ is bounded on $D \times (0,\tau)$.

We finally obtain that Y_i satisfies

$$\frac{\partial Y_i}{\partial t} - a_i(z,t)\frac{\partial^2 Y_i}{\partial z^2} + b_i(z,t)\frac{\partial Y_i}{\partial z} + (c_i-\mu)(z,t)Y_i \geq 0 \quad \forall (z,t) \in D \times (0,t^*)$$

where a_i, b_i, c_i are smooth, a_i is positive, μ is bounded on $D \times (0,t^*)$. It follows from the maximum principle (cf. PROTTER-WEINBERGER [31] th. 3.5-3.6) that : (i) if $z^* \in D$, then $Y_i = 0$ on $D \times (0,t^*)$, (ii) if $z^* \in \partial D$, then $\frac{\partial}{\partial \nu} Y_i < 0$. Both cases i) and ii) contradicts (2.7) or (2.8), which proves Theorem 2.1.

Remarks 2.2.

i) In the case k = 3 (but not k = 1 or 2), theorem 2.1 is also valid with all strict inequalities replaced by large inequalities (cf.Remark 2.1).

ii) Proposition 2.1 and Theorem 2.1 yield the following a priori bound

$$\begin{cases} 0 \leq Y_i(z,t) \leq 1 \quad \forall (z,t) \in Q, \ i \in I_k \\ \int_D T(z,t)dz \leq c \end{cases} \tag{2.11}$$

But we have not $L^\infty(Q)$ bound on the temperature, except in the case $d_{T,i} = 0$ and Lewis numbers = 1, i.e. $d_i \equiv d \equiv \frac{\rho\lambda}{c_{p\,i}}$ $\forall i$.

3. SOME MATHEMATICAL PROPERTIES OF THE TRAVELLING WAVES

In Sec. 3.1, we recall the classical enthalpy conservation for travelling waves. We intend to solve $(\mathcal{C}_k)$ by a finite-difference method, so we need to formulate an approximate problem on a bounded domain. In Sec. 3.2, we present an heuristic method for choosing the boundary conditions on a bounded domain and we show that the enthalpy is still conserved. In Sec. 3.3, we give an upper bound of the error due to the truncation of the domain in the case of a single one-step chemical reaction.

3.1. Enthalpy conservation

Proposition 3.1. Let (c,T,Y) be a smooth solution of $(\mathcal{C}_k)$, $1 \leq k \leq 3$, with $c \neq 0$. Then

$$\sum_{i=1}^{M} h_i(T_u)\, Y_{iu} = \sum_{i=1}^{M} h_i(T_b) Y_{ib} \tag{3.1}$$

Proof : We multiply each equation of (1.10) by h_i and we add to (1.9). We obtain

$$c\frac{d}{dx}\Big(\sum_{i=1}^{M} h_i Y_i\Big) - \frac{d}{dx}\Big(\sum_{i=1}^{M} h_i U_i\Big) - \frac{d}{dx}\Big(\lambda \frac{dT}{dx}\Big) = 0 \qquad (3.2)$$

We integrate in x. By (1.13), we obtain (3.1).

Remark 3.1. Since h_i are strictly increasing functions, it turns out that (3.1) gives a unique value $T_b = T_b(T_u, Y_{iu}, Y_{ib})$, which is called the adiabatic flame temperature.

3.2. Heuristic choice of the boundary conditions

Let $[a,b]$ a bounded domain of $\mathbb{R}$ which contains x_f.
Let (c,T,Y) be a smooth solution of $(\mathcal{C}_k)$, $1 \le k \le 3$. We integrate (3.2) and (1.10) over $(-\infty, a)$; we obtain

$$\lambda(a)\frac{dT}{dx}(a) + \sum_{i=1}^{M} h_i(T(a))U_i(a) = c\sum_{i=1}^{M}(h_i(T(a))Y_i(a) - h_i(T_u)Y_{iu}), \qquad (3.3)$$

$$U_i(a) = c(Y_i(a) - Y_{iu}) - \int_{-\infty}^{a} r_i(T(x),Y(x))dx \qquad (3.4)$$

The combination of (3.3), (3.4) gives

$$\lambda(a)\frac{dT}{dx}(a) = c\sum_{i=1}^{M}(h_i(T(a)) - h_i(T_u))Y_{iu} + \sum_{i=1}^{M} h_i(T(a))\int_{-\infty}^{a} r_i(T(x),Y(x))dx \qquad (3.5)$$

If we suppose now that the reactions terms are negligible on the region $(-\infty, a)$, we obtain

$$\lambda(a)\frac{dT}{dx}(a) = c\sum_{i=1}^{M}(h_i(T(a)) - h_i(T_u))Y_{iu} \qquad (3.6)$$

$$U_i(a) = c(Y_i(a) - Y_{iu}) \qquad (3.7)$$

As a result, we shall consider the following problem $(\mathcal{C}_k^*)$ on a given bounded domain $[a,b]$ which contains x_f and which is large enough :

$$(\mathcal{C}_k^*)\begin{cases} \text{equations (1.9), (1.10) on } (a,b), \\ \text{boundary conditions (3.6), (3.7) for } x = a, \\ \dfrac{dT}{dx}(b) = \dfrac{dY_i}{dx}(b) = 0 \\ T(x_f) = T_f \end{cases} \tag{3.8}$$

The boundary conditions (3.7), (3.8) (but not (3.6)) are those used by Smooke-Miller-Kee in [35] (cf. also [21]). Otherwise the reason for which we don't use similar left and right boundary conditions is that unburnt quantities T_u, Y_{iu} are prescribed, whereas burnt quantities T_b, Y_{ib} are unknown.

Proposition 3.2. Let (c,T,Y) be a smooth solution of $(\mathcal{C}_k^*)$, $1 \le k \le 3$, with $c \neq 0$. Then

$$\sum_{i=1}^{M} h_i(T_u)Y_{iu} = \sum_{i=1}^{M} h_i(T(b))Y_i(b) \tag{3.9}$$

Proof. We integrate (3.2) over (a,b) ; we obtain

$$c \sum_{i=1}^{M} h_i(T(b))Y_i(b) = c \sum_{i=1}^{M} h_i(T(a))Y_i(a) - \sum_{i=1}^{M} h_i(T(a))U_i(a) - \lambda(a)\frac{dT}{dx}(0) .$$

By (3.6), (3.7), we obtain (3.9).

3.3. Estimation of the error due to the truncation of the domain

3.3.1. One-step reaction with Le = 1.

In the case of a single one-step reaction with Le = 1, the problem $(\mathcal{C})$ reduces to the following scalar equation :

$$\begin{cases} -(d(u)u')' + cu' = g(u) \\ u(-\infty) = 0,\ u(+\infty) = 1,\ u(0) = 0.5 \end{cases} \tag{3.10}$$

The function $g : [0,1] \to [0, \infty)$ is supposed to be lipschitzian, differentiable at 0, and to satisfy $g(0) = g(1) = 0$, $g(s) \neq 0$ for $s \in (0,1)$; the function $d : [0,1] \to (0,\infty)$ is supposed to be continuously differentiable.

It has been proved that there exist a positive real number c_o such that (3.10) has a unique solution for every $c \geq c_o$ and no solution for c in the interval $0 < c < c_o$ (cf. [1] [14] [15] [38] for $d \equiv 1$ and [25] for any d). We shall denote u_o the solution corresponding to c_o. This solution seems to be the only physical one.

Let (a,b) a given bounded domain of $\mathbb{R}$ containing 0 ; the problem ($\mathcal{P}^*$) (with Dirichlet condition for x = b) reduces to

$$\begin{cases} -(d(u)u')' + cu' = g(u) \\ d(u(a))u'(a) = cu(a),\ u(b) = 1 \end{cases} \tag{3.11}$$

Let a = -b. Problem (3.11) has a unique solution (c_b,u_b) satisfying $u_b(0) = 0.5$ (cf. BERESTYCKI et al. [2]) and this solution satisfies (cf. M. MARION [25])

$$(c_b,\ u_b) \to (c_o,u_o) \text{ for } b \to +\infty .$$

We have obtained the following new result concerning the system (3.11).

Theorem 3.1. Let (c,u) be a solution of (3.11) with $b = +\infty$. We suppose that

$$d(0)g'(0) < \alpha \equiv \sup_{0<s<u(a)} \frac{d(s)g(s)}{s} < \int_0^1 d(s)g(s)ds \tag{3.12}$$

Then

$$\frac{1}{2}(c_o + (c_o^2 - 4\alpha)^{1/2}) \leq c < c_o \tag{3.13}$$

Proof. The basic tool is the comparison of ODE's.

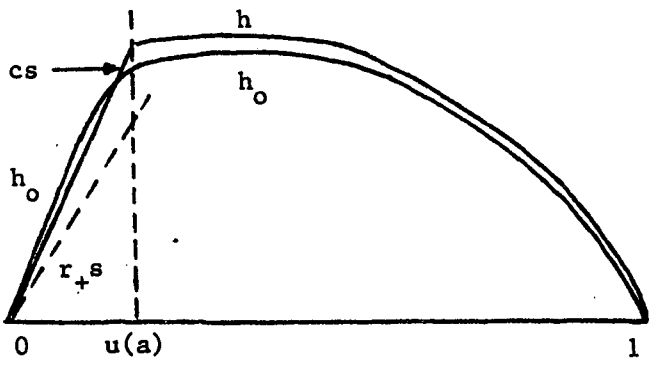


Fig. 3.1.

The function $h_o(s) \equiv d(s)u_o'(u_o^{-1}(s))$ is continuous from $[0,1]$ in $[0,+\infty)$ and satisfies (cf. M. MARION [25]) :

$$h_o'(s) = c_o - \frac{d(s)g(s)}{h_o(s)}, \qquad (3.14)$$

$$h_o(0) = h_o(1) = 0,\ h_o'(0) = \frac{1}{2}(c_o + (c_o^2 - 4d(0)g'(0))^{1/2})$$

Let α' be any real number in the interval $\alpha < \alpha' < \int_0^1 d(s)g(s)ds$

i) On one hand, $h_o'(s) > F(s,h_o(s))$ for every s in the interval $0 < s \leq u(a)$ where $F(s,y) \equiv c_o - \alpha' s/y$. We solve the differential equation $y'(s) = F(s,y(s))$ with the initial condition $y(0) = 0$. Since $c_o \geq (2\int_0^1 k(s)g(s)ds)^{1/2}$ (cf. [25]), we obtain the two following solutions

$$y_\pm(s) = r_\pm s, \text{ with } r_\pm = \frac{1}{2}(c_o \pm (c_o^2 - 4\alpha')^{1/2}).$$

Since $h_o'(0) = \frac{1}{2}(c_o + (c_o^2 - 4d(0)g'(0))^{1/2}) > y_\pm'(0)$, the comparison theorem for ODE gives that

$$h_o(s) > r_+ s \text{ for } 0 < s \leq u(a) \qquad (3.15)$$

ii) On the other hand, we know (cf [25]) that $c < c_o$ and that the function $h(s) = d(s)u'(u^{-1}(s))$ satisfies

$$h(s) > h_o(s) \text{ for } u(a) \leq s < 1 \qquad (3.16)$$

By (3.15), (3.16), we obtain (cf. Fig. 3.1)

$$h(u(a)) = cu(a) > h_o(u(a)) > r_+ u(a)$$

We take $\alpha' \to \alpha$ and we obtain (3.13).

Remark 3.2.

i) In the case $g'(0) = 0$, the first inequality of (3.12) is always satisfied and the second one is satisfied when $u(a)$ is small enough. Moreover, the left term of (3.13) converges to c_o when $u(a) \to 0$.

ii) The case $k(s) \equiv$ cte, $g(s) < sg'(0)$, studied by KOLMOGOROFF-PETROVSKY-PISCOUNOFF [18], never satisfies (3.12).

3.3.2. One step reaction with Le ≥ 1 .

In the case of one-step reaction with Le ≥ 1, the problem ($\mathcal{C}$) reduces to the following system ($\lambda = 1/Le$)

$$\begin{cases} -u'' + cu' = f(u)v \\ -\lambda v'' + cv' = -f(u)v \\ u(-\infty) = 0 \ , \ u(+\infty) = 1 \\ v(-\infty) = 1 \ , \ v(+\infty) = 0 \end{cases} \tag{3.17}$$

where f is a C^1 function : $[0,1] \to [0,\infty)$ with $f(0) = 0$ and $f(s) \neq 0$ for $s \neq 0$.

We consider the following problem on the half-line $(0,\infty)$:

$$\begin{cases} -u'' + cu' = f(u)v \\ -\lambda v'' + cv' = -f(u)v \\ -u'(0) + cu(0) = 0 \ , \ u(+\infty) = 1 \\ -\lambda v'(0) + c(v(0)-1) = 0 \ , \ v(+\infty) = 1 \end{cases} \tag{3.18}$$

As in the scalar case, there exists $c_o > 0$ such that (3.17) has a solution if and only if $c \geq c_o$ (cf. [22] [26]).

We obtain the following new result

Theorem 3.2. Let (c,u,v) be a solution of (3.18). We suppose that

$$f'(0) < \alpha \equiv \frac{1}{\lambda} \sup_{0<s<u(a)} \frac{f(s)(1-s)}{s} < \int_0^1 f(s)(1-s)ds \tag{3.19}$$

Then

$$\frac{1}{2}(c_o + (c_o^2 - 4\alpha)^{1/2}) \leq c < c_o \quad . \tag{3.20}$$

Proof : The function $h_o(s) = u_o'(u_o^{-1}(s))$ satisfies (cf. [26])

$$\begin{aligned} h_o'(s) &= c_o - \frac{v_o(u_o^{-1}(s))f(s)}{h_o(s)} \ , \\ h_o(0) &= h_o(1) = 0, \ h_o'(0) = \frac{1}{2}(c_o + (c_o - 4f'(0))^{1/2}) \end{aligned} \tag{3.21}$$

Let α' be any real number in the interval $\alpha < \alpha' < \int_0^1 f(s)(1-s)ds$.

i) On one hand, the function v_o satisfies (cf. [2] [26])

$$1-u_o(x) \le v_o(x) \le \frac{1}{\lambda}(1-u_o(x)).$$

As a consequence, $h_o'(s) > F(s,h_o(s))$ where $F(s,y) = c_o - \alpha' s/y$.
We obtain as in Theorem 3.1 that

$$h_o(s) > r_+ s \quad \text{for} \quad 0 < s \le u(a) \tag{3.22}$$

where $r_+ = \frac{1}{2}(c_o + (c_o^2 - 4\alpha')^{1/2})$

ii) On the other hand, since $0 < \lambda < 1$, we still have (cf. [26]) $c < c_o$ and

$$h(s) = u'(u^{-1}(s)) > h_o(s) \quad \text{for} \quad u(a) \le s < 1 \tag{3.23}$$

By (3.22), (3.23), we obtain (3.21).

4. NUMERICAL METHOD FOR COMPUTING TRAVELLING WAVES

We describe the main aspects of our method : use of a pseudo-unstationary approach (Sec. 4.1) and use of adaptive gridding (Sec. 4.2).

4.1. Pseudo-unstationary approach

The solution of $(\mathcal{C}_k^*)$ on a given interval [a,b] will be computed by the pseudo-unstationary scheme :

$$(\mathcal{C}_k)\begin{cases} \rho^n C_p^n \dfrac{T^{n+1}-T^n}{k} + \{c^{n+1} C_p^n - \sum_{i=1}^M h_i'(T^n) U_i^n\} \dfrac{dT^{n+1}}{dx} \\ \qquad - \dfrac{d}{dx}(\lambda^n \dfrac{dT^{n+1}}{dx}) + \sum_{i=1}^M h_i(T^n) r_i^{n+1} = 0 , \\ \rho^n \dfrac{Y_i^{n+1} - Y_i^n}{k} + c^{n+1} \dfrac{dY_i^{n+1}}{dx} - \dfrac{d}{dx}(\mu_i^n \dfrac{dT^{n+1}}{dx} + \sum_{i=1}^M \mu_{ij}^n \dfrac{dY^{n+1}}{dx}) - r_i^{n+1} = 0 \\ \lambda^n T'^{,n+1}(a) = c^{n+1}(T^{n+1}(a)-T_u)\{\sum_{i=1}^M (h_i(T^n(a))-h_i(T_u))Y_{iu}\}/(T^n(a)-T_u) \\ \mu_i^n \dfrac{dT^{n+1}}{dx}(a) + \sum_{i=1}^M \mu_{ij}^n \dfrac{dY_j^{n+1}}{dx}(a) = c^{n+1}(Y_i^{n+1}(a) - Y_{iu}), \\ T'^{,n+1}(b) = Y_i'^{,n+1}(b) = 0, \\ T^{n+1}(x_f) = T_f , \end{cases}$$

where

$$C_p^n = \sum_{i=1}^{M} h_i'(T^n) Y_i^n ,$$

$$U_i^n = \mu_i^n \frac{dT^n}{dx} + \sum_{j=1}^{M} \mu_{ij}^n \frac{dY_j^n}{dx} ,$$

$$r_i^{n+1} = r_i(T^{n+1}, Y^{n+1}),\ \lambda^n = \lambda(T^n, Y^n),\ \mu_{ij}^n = \mu_{ij}(T^n, Y^n).$$

Remark 4.1. The system of partial differential equations derived from $(\mathcal{R})$ by substituting $(\frac{T^{n+1}-T^n}{k}, \frac{Y_i^{n+1}-Y_i^n}{k})$ by $(\frac{\partial T}{\partial t}, \frac{\partial Y_i}{\partial t})$ is a variant reading of problem $(\mathcal{E})$. It can be shown, by the method of proof of Theorem 3.1, that the region $Y_i > 0$ is invariant for this system.

Space discretization

Let $\mathcal{S} = \{a = x_0 < x_1 < \ldots < x_N = b\}$ be a mesh of $[a,b]$. Let P_1 be the space of polynomials of one variable of degree less or equal to one and let $V(\mathcal{S})$ be the space

$$V(\mathcal{S}) = \{\phi \in C^0([a,b]) ; \phi|_{[x_j, x_{j+1}]} \in P_1,\ 0 \le j \le N-1\}$$

The computations presented in this paper are obtained by looking for a solution (c,T,Y) in the space $\mathbb{R} \times V(\mathcal{S})^{M+1}$ and by making use of the central differences both for second and first order derivatives. The functions $h_i'(T(x))$ is approximated by the piecewise constant function δh_i given on each interval $[x_j, x_{j+1}]$ by

$$\delta h_i(T(x)) = \begin{cases} \dfrac{h_i(T(x_{j+1}) - h_i(T(x_j))}{T(x_{j+1}) - T(x_j)} & \text{if } T(x_j) \neq T(x_{j+1}), \\ h_i'(T(x_j)) & \text{otherwise.} \end{cases}$$

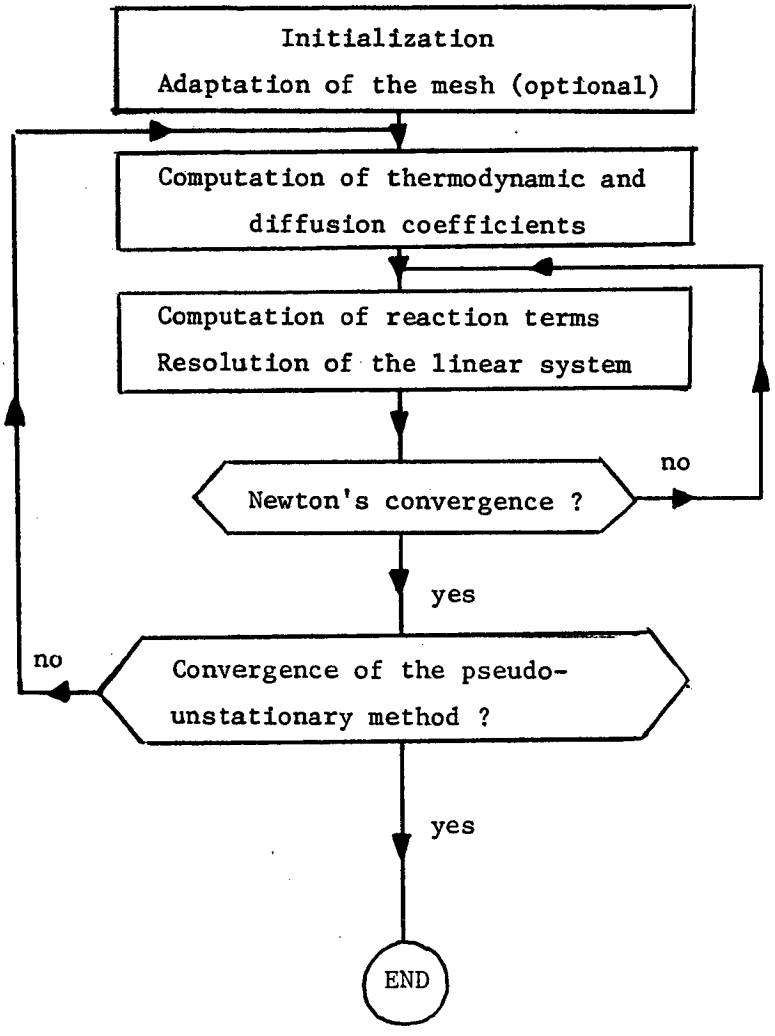
With this choice of approximation, every approximate stationary solution (c,T,Y) satisfies the enthalpy equality :

$$\sum_{i=1}^{M} h_i(T(b)) Y_i(b) = \sum_{i=1}^{M} h_i(T_u) Y_{iu}$$

Numerical comparisons between centered and various uncentered first differences are in progress and will be reported by GHILANI (thesis in preparation).

Solution of the discrete problem

The solution $(c^{n+1}, T^{n+1}, Y^{n+1})$ of $(\mathcal{H})$ is computed by a global Newton method, which gives the following organigram :



The pseudo-unstationary loop is the external loop ; the Newton's loop is the inner loop. The thermodynamic and diffusion coefficients, which are costly to compute and not strongly nonlinear, are explicit in time, so that they are computed only once in an external loop. Since reaction terms are strongly nonlinear, they are computed implicitly.

Adaptation of the time-step k

The time-step k is automatically adjusted according to the rate of convergence of Newton's method :
if convergence in less than ITMIN iterations, k is multiplied by 2
if no convergence after ITMAX iteration, k is multiplied by 0.3 and we restart Newton's iterations.
Typical values for ITMIN, ITMAX are ITMIN = 4, ITMAX = 6.

Linear algebra

Each Newton's iteration consists in solving a linear system which has the following structure :

$$\begin{aligned} K\,Z + c\,b_1 &= b_2 \\ Z_{i_f} &= T_f \end{aligned} \qquad (4.1)$$

where K is a block-tridiagonal matrix, b_1, b_2 two vectors.
The global matrix for (4.1) is no more block-tridiagonal. In order to keep the block-tridiagonal structure (which is useful for the vectorization), we solve (4.1) as

$$Z = K^{-1}\,b_2 + c\,K^{-1}\,b_1 \;,\; Z_{i_f} = T_f \;,$$

i.e. we factorize K by Gauss method , we solve two linear systems $K\,Z_1 = b_1$, $K\,Z_2 = b_2$ (negligible cost) and finally we determine $Z = Z_1 + c\,Z_2$ by the condition $Z_{i_f} = T_f$.

Initialization

Two kinds of computations are done : (i) computation of a solution of ($\mathcal{C}$) with given values of all the (physical and numerical) parameters

(ii) the study of the variation of the solution of ($\mathcal{C}$) as a function of some parameter.

In the case (i), we use the following initialization :

$$T_o(x) = \begin{cases} T_u + (T^* - T_u)\exp(x-x^*) & a \le x \le x^* \\ T_b + (T^* - T_b)\exp(x^* - x) & x^* \le x \le b \end{cases}$$

$$Y_i(x) = \begin{cases} Y_{iu} + (Y_i^* - Y_{iu})\exp(x-x^*) & a \le x \le x^* \\ Y_{ib} + (Y_i^* - Y_{ib})\exp(x^* - x) & x^* \le x \le b \end{cases}$$

where T^* , T_b, Y_i^*, Y_{ib} are initial values that have to be given ; the position x^* is determined by

$$T(x_f) = T_f \quad .$$

In the case (ii), we use a previously computed solution as initial guess for the next computation, i.e. we use a continuation method.

4.2. Adaptive mesh generation

When using the continuation method, we adapt the mesh to the initialization. The method for doing this is to equidistribute some weight-function (see for instance [10] [11] [13] [17] [19] [28]). Hereafter, we give the function that we have used.

Let $\{x_o,\ldots,x_N\}$ be any subdivision of $[a,b]$ and let $U \in V(\mathcal{P})^M$, $M \ge 1$. We put $I = \{i,\ 1 \le i \le M,\ \text{s.t. } U_i' \not\equiv 0\}$. We suppose that $I \neq \emptyset$.

We define a function Φ_U that we call (absolute) total variation of U on (a,t) :

$$\Phi_U(t) = \int_a^t \max_{i\in I} \frac{|U_i'(s)|}{\max\limits_{\tau\in(a,b)} U_i(\tau) - \min\limits_{\tau\in(a,b)} U_i(\tau)}\, ds$$

For M = 1, Φ_U is the classical total variation of U/(max U - min U).

We observe that $\Phi_U \in V(\mathcal{S})$ and Φ_U is nondecreasing. As a consequence, we can define an equidistributed mesh $\{\tilde{x}\}$ of $\tilde{N}+1$ points, $\tilde{N}$ arbitrary, by

$$\begin{cases} \tilde{x}_o = a \\ \Phi_U(\tilde{x}_{j+1}) = \Phi_U(\tilde{x}_j) + \dfrac{\Phi_U(b)}{\tilde{N}} , \quad 0 \le j \le \tilde{N} \end{cases} \tag{4.2}$$

The new function $\tilde{U}$ is defined by linear interpolation of U on the new mesh.

Since $\Phi_U \in V(\mathcal{S})$, the effective computation of $\{\tilde{x}\}$ by (4.2) is very easy. The number of elementary operations for computing $(\tilde{x},\tilde{U})$ from (x,U) is $O(\max(MN,M\tilde{N}))$.

The number $\Phi_U(b)$ is an indication of the complexity of the vector function U. It's easy to prove that :

Proposition 4.1. For every $\mathcal{S}$ and $U \in V(\mathcal{S})$ (with $I \neq \emptyset$), we have

i) $1 \le \Phi_U(b) \le N$

ii) $\Phi_U(b) = 1 \iff U_i$ are monotone and $U_i(t)-U_i(a)$ are proportional for every i, $1 \le i \le M$.

We can also define a relative total variation of U by computing Φ_V with $V = (\text{Log } U_1,\ldots,\text{Log } U_M)$. In the present computations, we take the total variation Φ_W corresponding to

$$W = (T,Y_1,\ldots,Y_M, \text{ Log } T, \text{ Log } Y_1,\ldots,\text{Log } Y_M).$$

5. NUMERICAL RESULTS

We have tested the algorithm discussed above on several typical problems. One of them is the case of the scalar equation (3.10) with such a choice of the function g that the exact solution is known (example : $g(s) = 2s^2(1-s)$) ; the corresponding numerical results will be reported by M. GHILANI in his thesis. In this section, we test the method on the determination of hydrogen-oxygen-nitrogen flames with a complete reaction mechanism and a realistic transport model. First results concern the stoichiometric hydrogen-air case (test problem B

of GAMM Workshop [42]) ; then we present a calculation which displays a chemical extinction when the concentration of inert is increased.

5.1. Chemical and transport models

5.1.1. Reaction mechanism

For the computation 5.2, we use the reaction mechanism of the test problem B (table II) of [42] ; for the computation 5.3, we use the following reaction mechanism (for reference, see [42] [43]).

No.	Reaction	A $(cm^3/mol)^{n-1}s^{-1}$	b	E kJ/mol
(1)	$H + O_2 \rightarrow OH + O$	$2.2 \cdot 10^{14}$	0	70.3
(2)	$O + OH \rightarrow H + O_2$	$1.8 \cdot 10^{13}$	0	0
(3)	$O + H_2 \rightarrow OH + H$	$1.5 \cdot 10^{7}$	2.00	31.6
(4)	$H + OH \rightarrow O + H_2$	$6.7 \cdot 10^{6}$	2.00	23.3
(5)	$OH + H_2 \rightarrow H_2O + H$	$1.0 \cdot 10^{8}$	1.60	13.8
(6)	$H + H_2O \rightarrow OH + H_2$	$4.6 \cdot 10^{8}$	1.60	77.6
(7)	$OH + OH \rightarrow H_2O + O$	$1.5 \cdot 10^{9}$	1.14	0
(8)	$H_2O + O \rightarrow OH + OH$	$1.5 \cdot 10^{10}$	1.14	72.1
(9)	$H + H+M \rightarrow H_2 + M$	$9.7 \cdot 10^{16}$	-0.60	0
(10)	$H + OH+M \rightarrow H_2O + M$	$2.2 \cdot 10^{22}$	-2.00	0
(11)	$H + O_2+M \rightarrow HO_2 + M$	$2.0 \cdot 10^{18}$	-0.80	0
(12)	$HO_2 + M \rightarrow H + O_2+M$	$7.0 \cdot 10^{15}$	0	192.1
(13)	$H + HO_2 \rightarrow OH + OH$	$1.5 \cdot 10^{14}$	0	4.2
(14)	$H + HO_2 \rightarrow H_2 + O_2$	$2.5 \cdot 10^{13}$	0	2.9
(15)	$O + HO_2 \rightarrow OH + O_2$	$2.0 \cdot 10^{13}$	0	0
(16)	$OH + HO_2 \rightarrow H_2O + O_2$	$2.0 \cdot 10^{13}$	0	0

$k = A(T/K)^b \exp(-E/RT)$, n = reaction order

$[M] = [H_2] + 0.4[O_2] + 0.4[N_2] + 6.5[H_2O]$

Table I

5.1.2. Transport model

The diffusion coefficient of the species i in the mixture is determined by the formula (cf. [6] [7] [16])

$$D_i(T,Y) = \frac{1-Y_i}{\sum_{j \neq i} X_i / D_{ij}(T)}$$

where the binary diffusion coefficients $D_{ij}(T)$ are given in terms of pressure, temperature and thermodynamic parameters of the species (cf. [16]). We take the thermal diffusion coefficients $d_{T,i} \equiv 0$. Two options are used for the diffusion flux : either $(1.4)_2$ or $(1.4)_3$. The conductivity of the mixture is computed by (cf. [16] [27])

$$\lambda(T,Y) = \frac{1}{2}\left(\sum_{i=1}^{M} X_i \lambda_i(T) + \frac{1}{\sum_{i=1}^{M} X_i/\lambda_i(T)} \right)$$

5.2. Numerical results for stoichiometric hydrogen-air mixture

First numerical results concern the stoichiometric hydrogen-air flame, i.e.

$$T_u = 298 \text{ K}, \quad [H_2]_u = 2\ [O_2]_u \ , \quad [N_2]_u = 4\ [O_2]_u \ ,$$

$$[OH]_u = [H]_u = [HO_2]_u = [H_2]_u = 0 \ .$$

The computation is performed with the following parameters : the length of the domain is L = 500 mm ; $x_f = 0$ and $T_f = 299$ K ; $k_o = 10^{-3}$ ms ; the values for the initialization are listed in Table II ; the mesh has 70 points, given in Table III.

Some computed values are given in Table IV and Fig. 5.1. These results are in good agreement with those reported in [42] and the CPU time seems shorter.

species	H_2	O_2	H_2O	H	OH	HO_2	O	Temperature
T^* , Y_i^*	1.E-5	1.E-5	0.2	1.E-4	1.E-4	1.E-4	1.E-4	2298
T_b, T_{ib}	0	0	0.2	0	0	0	0	2298

Table II

Values for the initialization

0.	0.005	0.01	0.02	0.03	0.04	0.05
0.06	0.07	0.08	0.09	0.10	0.11	0.12
0.13	0.14	0.15	0.16	0.17	0.18	0.19
0.20	0.21	0.22	0.23	0.245	0.26	0.28
0.30	0.32	0.35	0.36	0.38	0.40	0.42
0.44	0.46	0.48	0.50	0.52	0.54	0.56
0.58	0.60	0.62	0.64	0.66	0.68	0.70
0.75	0.80	0.85	0.90	1.0	1.2	1.4
1.6	1.8	2	2.5	3	4	5
8	15	30	50	100	200	500

Table III

Mesh (x in mm)

	Diffusion flux $(1.4)_2$	Diffusion flux $(1.4)_3$
Number of pseudo-time iterations	39	39
Number of Jacobians	121	121
Flame velocity v_u (m/s)	1.95	1.96
10^3 max Y_H	2.77	2.77
10^3 max Y_O	9.14	9.15
10^4 max Y_{HO_2}	6.34	6.36
h_{max} (J/g)	345	344
h_{min} (J/g)	- 83.0	-82.7
total variation	4.75	4.75
total CPU time (CRAY1)	18 s	18 s

Table IV

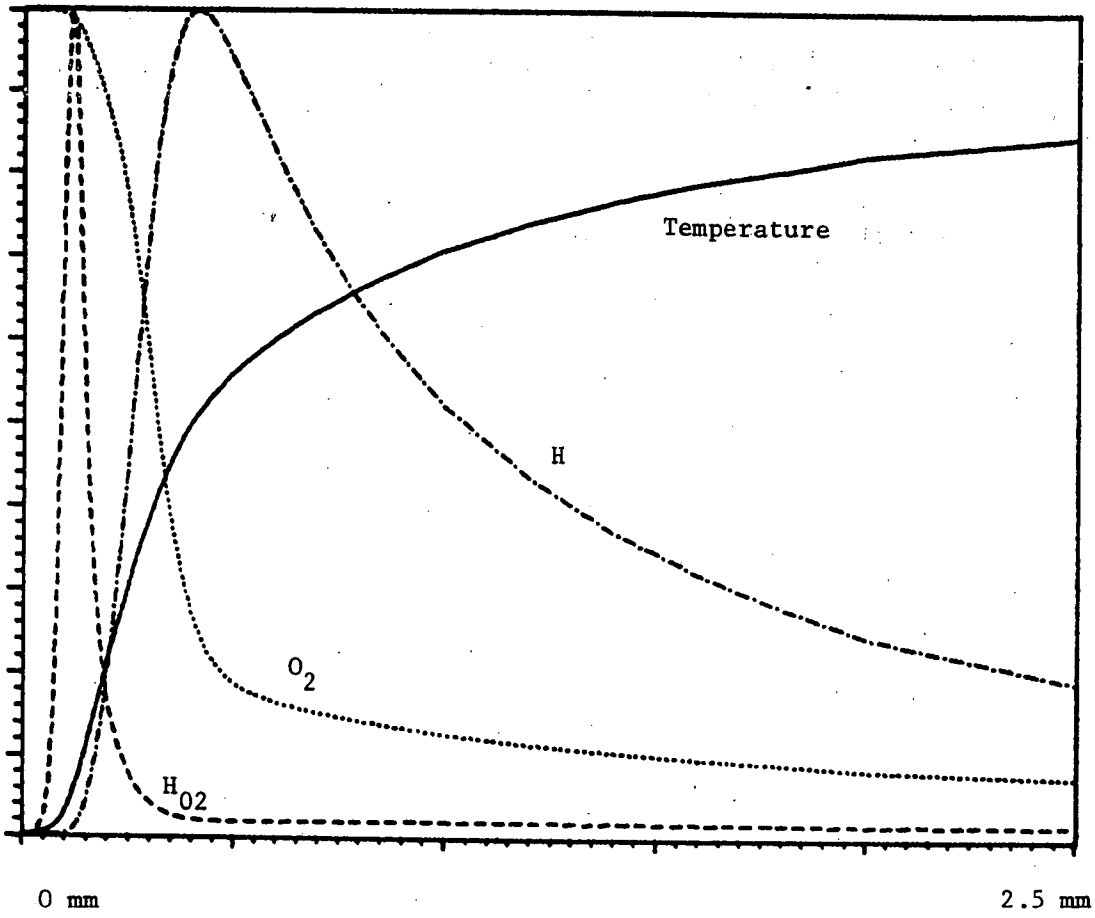


Figure 5.1.

Computed temperature and species profiles
in the stoichiometric case.

Remarks 5.1.

i) The computing time can be reduced by using the same Jacobian for p iterations (modified Newton method). For p = 3, which seems the best value for the case studied here, we obtain the convergence with : Number of pseudo-time iterations = 25, Number of jacobians = 59, CPU time = 13 s.

ii) A sufficient accuracy can be obtained with only half the mesh points. The corresponding computing time is divided by two.

5.3. Chemical extinction by increase of the nitrogen concentration

The chemical extinction of the H_2-O_2-N_2 flame by increase of the inert concentration has been established analytically by several authors (LINAN ; PETERS ; CLAVIN, NICOLI & PELCE) (cf. [5] [29] [30]), in the context of a simplified chemical mechanism. Hereafter, we present a numerical study of this question for the realistic chemical mechanism given in Sec. 5.1. (this study was suggested to me by P. CLAVIN).
The composition of the fresh mixture is now $[H_2] / [O_2] = 3$, $[N_2] / [O_2] = \lambda$, where λ is a parameter ≥ 4.

We use a continuation procedure (with respect to λ) : the solution of the governing equations for a given value of λ is used as initialization for the next value of λ ; at the beginning of each computation, the mesh is automatically adapted according to the method described in Sec.4.2 In proportion as λ is increased, the flame speed decreases towards zero and the choice of (x_f, T_f) becomes crucial.

Results of these computations are reported in Fig. 5.2 - Fig. 5.3. They show a chemical extinction for $[N_2] / [O_2] \simeq 21$, $T_b \simeq 947$ K.

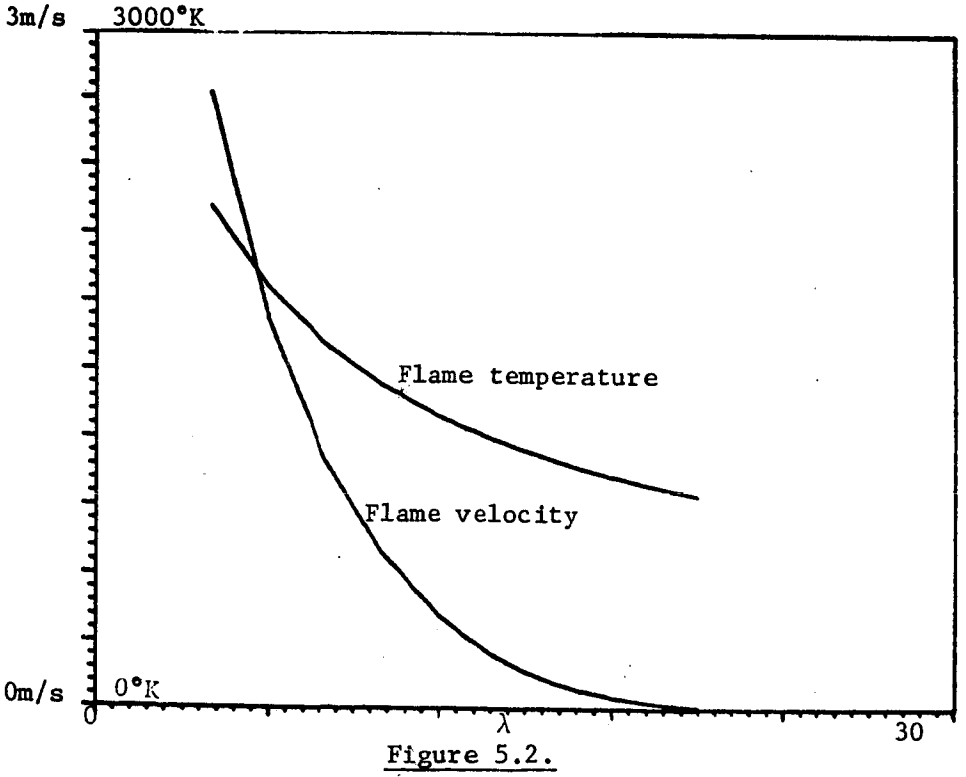


Figure 5.2.

Computed flame velocity and flame temperature as functions of $\lambda = [N_2] / [O_2]$.

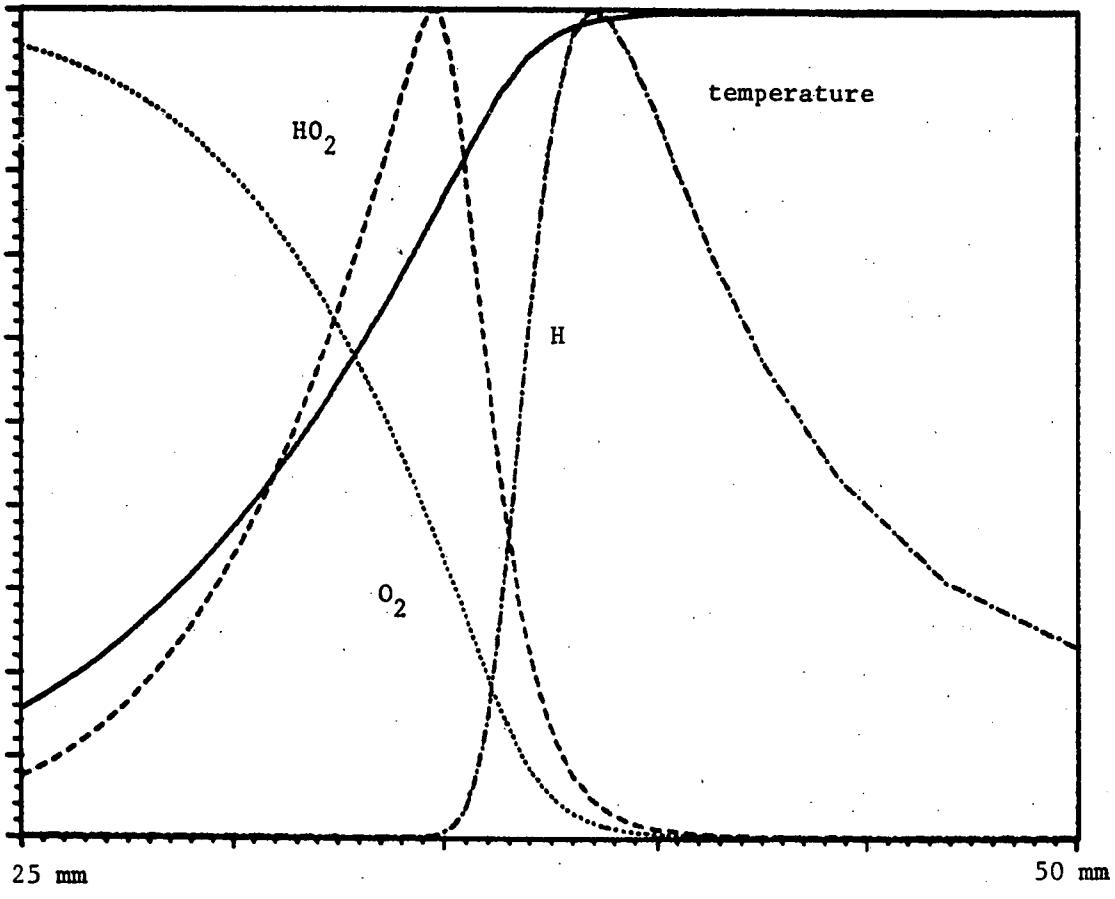


Figure 5.3.

Computed temperature and species profile near extinction ; in this calculation $\lambda = 21$, $x_f = 37.5$ mm, $T_f = 928K$; the computed flame velocity and flame temperature are $v_u = 7mm/s$, $T_b = 947K$; the domain of computation is (0,500 mm).

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