M2AN. MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
- MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

M. GHILANI
B. LARROUTUROU

Upwind computation of steady planar flames with complex chemistry

M2AN. Mathematical modelling and numerical analysis - Modélisation mathématique et analyse numérique, tome 25, n° 1 (1991), p. 67-91

<http://www.numdam.org/item?id=M2AN_1991__25_1_67_0>

MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
MODÉLISATION MATHÉMATIQUE ET ANALYSE NUMÉRIQUE

(Vol. 25, n° 1, 1991, p. 67 à 92)

UPWIND COMPUTATION OF STEADY PLANAR FLAMES WITH COMPLEX CHEMISTRY (*)

M. GHILANI (1), B. LARROUTUROU (2)

Communicated by R. TEMAM

Abstract. — *We consider the problem of simulating a steady planar premixed flame with a complex chemical mechanism and realistic transport models, and examine how upwind schemes derived from the Petrov-Galerkin finite-element method can be useful in this context. The resulting upwind scheme is shown to preserve the positivity of the mass fractions of all species and to give non oscillatory results for any values of the local cell Reynolds number and of the time step, while remaining second-order accurate. This results in a numerical algorithm which is as accurate as but more robust than the centered methods which are usually employed for this class of problems.*

Résumé. — *Nous nous intéressons au problème de la simulation numérique d'une flamme plane prémélangée stationnaire avec chimie complexe, et examinons l'apport des méthodes d'éléments finis décentrés de type Petrov-Galerkin dans ce contexte. Le schéma décentré proposé préserve la positivité des fractions massiques de toutes les espèces et donne des résultats sans oscillations, quelles que soient les valeurs du nombre de Reynolds de maille et du pas de temps, tout en étant précis au deuxième ordre.*

1. INTRODUCTION

The study reported in this paper aims at designing an upwind scheme of the finite-element Petrov-Galerkin type for the simulation of planar steady premixed flames with complex chemistry.

The phenomenon is described by a system of non linear convection-diffusion-reaction equations. But, outside the thin reaction zone inside the flame front (see e.g. [3]), the reaction term is exponentially small ; in particular, in the pre-heat zone ahead of the flame, the problem behaves as

(*) Received in October 1989.

(1) Present address : Faculté des Sciences, Département de Mathématiques, BP 4010, Beni M'hamed, Meknes, Maroc.

(2) Present address : CERMICS, INRIA, Sophia-Antipolis, 06560 Valbonne, France.

M²AN Modélisation mathématique et Analyse numérique 0764-583X/91/01/67/25/$ 4.50

a system of convection-diffusion equations, with a thin region of sharp gradients (which acts as a boundary layer for the cold zone, see e g [3], [9]) Thus, we are faced with the classical difficulties of the numerical discretization of convection-diffusion equations for this type of problems, a centered approximation may cause unphysical instabilities (see e g [4], [6]) This is our motivation for using an uncentered scheme

In Section 2, we consider a class of schemes where the approximation of the first-order derivative is written as a combination of the classical centered second-order accurate and of the fully uncentered first-order accurate formulas, for a single convection-diffusion equation Although most of the presented facts are classical, we find it useful to recall the complete analysis of this class of schemes, from both viewpoints of the finite-element Petrov-Galerkin method and of the finite-difference method The aim of the analysis for this simple model problem is to determine the optimal value of the so-called « upwind parameter » involved in these schemes

Next, we consider in Section 3 a fully implicit scheme which uses the optimized upwind approximation derived in Section 2 for a system of time-dependent convection-diffusion-reaction equations with stiff nonlinear source terms, and we prove in particular the unconditional stability of this scheme in the maximum norm

This scheme is used in Section 4 for the simulation of steady premixed hydrogen-air planar flames, with complex chemistry and realistic transport models It is shown there that this scheme, which preserves the positivity of the species mass fractions, is more robust and at least as accurate as the second-order centered scheme commonly used in the literature for this type of applications

2. A LINEAR MODEL PROBLEM

We consider in this section the model convection-diffusion problem

$$\begin{cases} cu_x = du_{xx} & \text{for} \quad x \in (0,1)\,, \\ u(0) = 0\,, \quad u(1) = 1\,, \end{cases} \tag{1}$$

whose exact solution is

$$u(x) = \frac{\exp\left(\frac{cx}{d}\right) - 1}{\exp\left(\frac{c}{d}\right) - 1} \tag{2}$$

We assume that c and d are positive constants The numerical solution of (1) is of course classical, and has been the subject of several investigations (see the references below) It is our goal in this section to summarize in a unified

presentation the results of theses analyses, in both contexts of finite elements and finite differences.

For the numerical solution of (1), we will consider schemes of the form :

$$c\left(\alpha\frac{u_i-u_{i-1}}{h}+(1-\alpha)\frac{u_{i+1}-u_{i-1}}{2h}\right)=d\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}$$
$$\text{for}\quad 1\leqslant i\leqslant N\,, \quad (3)$$

with :

$$u_0=0\,,\quad u_{N+1}=1\,, \quad (4)$$

where $h=\dfrac{1}{N+1}$ and where the constant α is an upwind parameter to be appropriately chosen later. We will first analyse the scheme (3)-(4) in the context of the Petrov-Galerkin finite-element method, and then from the point of view of the finite-difference method.

2.1. Finite-element analysis

2.1.1. *Background*

The variational formulation of problem (1) is classical; setting $u(x)=x+\hat{u}(x)$, one wants to find $\hat{u}\in H_0^1(0,1)$ such that :

$$\int_0^1 \hat{u}'(dw'+cw)\,dx=-c\int_0^1 w\,dx\quad \forall w\in H_0^1(0,1)\,. \quad (5)$$

The Petrov-Galerkin approximation of (5) consists in searching an approximate solution $\hat{u}_h$ in some finite-dimensional subspace $\Phi_h\subset H_0^1(0,1)$ while using test functions w_h chosen in a different subspace $\Psi_h\subset H_0^1(0,1)$ (with $\dim\Phi_h=\dim\Psi_h<+\infty$). Setting $a(v,w)=\displaystyle\int_0^1 v'(dw'+cw)\,dx$ and $L(w)=-c\displaystyle\int_0^1 w\,dx$ for $v,\ w\in H_0^1(0,1)$, we consider the problem :

$$\text{Find}\ \hat{u}_h\in\Phi_h\quad\text{such that}\quad a(\hat{u}_h,w_h)=L(w_h)\quad\forall w_h\in\Psi_h\,. \quad (6)$$

The next result, due to Babuska and Aziz (see [1]), plays in the present context the role of Cea's lemma for the classical finite-element Galerkin approximation (see e.g. [2]) :

THEOREM 1 : *Assume that a is a continuous bilinear mapping from $H_0^1(0,1)\times H_0^1(0,1)$ into $\mathbb{R}$, and let C_a be a positive constant such that, for all $v,\ w\in H_0^1(0,1)$:*

$$|a(v,w)|\leqslant C_a\|v\|_{H^1}\|w\|_{H^1}\,. \quad (7)$$

Assume that :

$$C_h = \inf_{v \in \Phi_h - \{0\}} \sup_{w \in \Psi_h - \{0\}} \frac{a(v, w)}{\|v\|_{H^1} \|w\|_{H^1}} > 0 , \tag{8}$$

and that, for all $w \in \Psi_h - \{0\}$:

$$\sup_{v \in \Phi_h} a(v, w) > 0 . \tag{9}$$

Lastly, assume that L is a continuous linear mapping from $H_0^1(0, 1)$ *into* $\mathbb{R}$. *Then, problem* (6) *has a unique solution* $\hat{u}_h$, *which satisfies* ($\hat{u}$ *stands for the unique solution of* (5)) :

$$\|\hat{u} - \hat{u}_h\|_{H^1} \leq \left(1 + \frac{C_a}{C_h}\right) \min_{v_h \in \Phi_h} \|\hat{u} - v_h\|_{H^1} . \quad \blacksquare \tag{10}$$

Following Griffiths and Lorenz [6], we will now consider two different choices for the spaces Φ_h and Ψ_h, and therefore obtain two distinct Petrov-Galerkin schemes.

2.1.2. *Optimized Petrov-Galerkin scheme for piecewise quadratic test functions*

First, we take for Φ_h the space of piecewise linear functions, having as basis the usual hat functions ϕ_j :

$$\phi_j(x) = \hat{\phi}\left(\frac{x - x_i}{h}\right) , \tag{11}$$

where $x_i = ih$ and :

$$\hat{\phi}(s) = \begin{cases} 1 - |s| & \text{if} \quad |s| \leq 1 , \\ 0 & \text{otherwise} . \end{cases} \tag{12}$$

We adopt for Ψ_h a family of spaces $\Psi_{h,\beta}$ involving a parameter β, whose basis $(\psi_{j,\beta})_{(1 \leq j \leq N)}$ is defined by the relations :

$$\psi_{j,\beta}(x) = \phi_j(x) + \beta \hat{\sigma}\left(\frac{x - x_i}{h}\right) , \tag{13}$$

where :

$$\hat{\sigma}(s) = \begin{cases} 3\, s(|s| - 1) & \text{if} \quad |s| \leq 1 , \\ 0 & \text{otherwise} . \end{cases} \tag{14}$$

One easily sees that the basis functions ϕ_j and $\psi_{j,\beta}$ have the same support,

that the coordinates of any function $\psi \in \Psi_{h,\beta}$ on the basis $(\psi_{j,\beta})$ are simply the nodal values $\left(\psi(x) = \sum_{j=1}^{N} \psi(x_j)\, \psi_{j,\beta}(x)\right)$, and that the integral $\int_0^1 \psi_{j,\beta}(x)\, dx$ is independent of β. The assymmetric basis function $\psi_{j,\beta}$ is shown on figure 1, for different values of β.

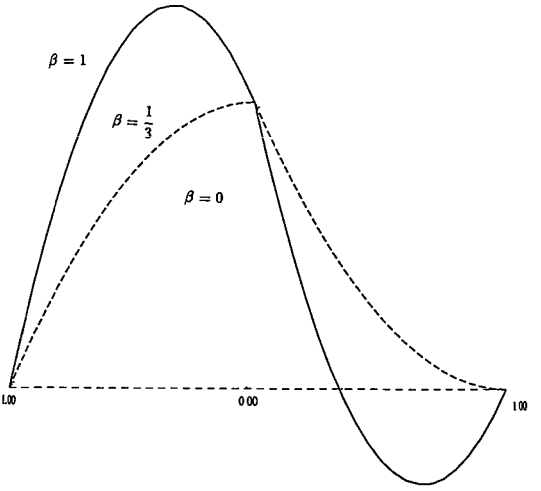

Figure 1. — The basis functions $\psi_{j,\beta}$.

It is shown in [6] that, for any $h > 0$ and $\beta \geq 0$, the inequalities (8)-(9) hold ; moreover, the quantity C_h (which now becomes $C_{h,\beta}$) defined by (8) is shown to satisfy :

$$K_{h,\beta} \leq C_{h,\beta} \leq K_{h,\beta} \cdot \sqrt{1 + h\, \frac{\gamma^2}{(2 + \gamma\beta)^2}}, \tag{15}$$

where γ is the so-called cell Reynolds (or Peclet) number :

$$\gamma = \frac{ch}{d}, \tag{16}$$

and where :

$$K_{h,\beta} = \frac{\left(1 + \frac{\gamma\beta}{2}\right)}{\sqrt{1 + 3\,\beta^2}}. \tag{17}$$

From (15) and (17), we see that $C_{h,\beta}$ is bounded away from 0 as h tends to 0 ; then (10) shows that the approximation error $\|\hat{u} - \hat{u}_h\|$ tends to 0 when the interpolation error $\min_{v_h \in \Phi_h} \|\hat{u} - v_h\|$ tends to 0, which proves the convergence of the present Petrov-Galerkin method.

Let us now come to the choice of β. In view of (10), one may think of choosing β (for h fixed) in order to make $C_{h,\beta}$ as large as possible. Following these lines and in view of (17), Griffiths and Lorenz [6] proposed to choose β in order to make $K_{h,\beta}$ as large as possible ; a straightforward calculation then yields :

$$\beta = \frac{\gamma}{6} = \frac{1}{6}\frac{ch}{d} . \tag{18}$$

This value of β defines our first optimized Petrov-Galerkin approximation, here after denoted « PG1 ».

To end this paragraph, let us write down the developed expression of this PG1 scheme. Writing $\hat{u} = \sum \hat{u}_i \phi_i$, we get :

$$-\frac{1}{h}\int_0^1 \hat{u}' \psi'_{i,\beta} = \frac{\hat{u}_{i+1} - 2\hat{u}_i + \hat{u}_{i-1}}{h^2} , \tag{19}$$

$$\frac{1}{h}\int_0^1 u' \psi_{i,\beta} = \beta\left(\frac{\hat{u}_i - \hat{u}_{i-1}}{h}\right) + (1-\beta)\frac{\hat{u}_{i+1} - \hat{u}_{i-1}}{2h} . \tag{20}$$

The use of the asymmetric test functions $\psi_{i,\beta}$ therefore does not affect the approximation of the second derivative, but introduces an upwind term in the first derivative evaluation. Coming back to the nodal values u_i of u, one readily sees that the PG1 scheme has exactly the form (3), with $\alpha = \beta$, that is :

$$\alpha = \frac{\gamma}{6} . \tag{21}$$

2.1.3. *Optimized Petrov-Galerkin scheme for piecewise exponential trial functions*

A second Petrov-Galerkin approximation is also considered in [6] ; keeping the same space $\Psi_{h,\beta}$ as in the preceding section for the test functions, Griffiths and Lorenz [6] take an approximation space Φ'_h of continuous piecewise exponential functions. A basis $(\lambda_j)_{1 \leq j \leq N}$ of Φ'_h is defined as :

$$\lambda_j(x) = \hat{\lambda}\left(\frac{x - x_i}{h}\right) , \tag{22}$$

$$\hat{\lambda}(s) = \begin{cases} \dfrac{\exp(\gamma s) - \exp(-\gamma)}{1 - \exp(-\gamma)} & \text{if } -1 \leqslant s \leqslant 0\,, \\ \dfrac{\exp(\gamma s) - \exp(\gamma)}{1 - \exp(\gamma)} & \text{if } 0 \leqslant s \leqslant 1\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{23}$$

Obviously, these basis functions again satisfy the relations $\lambda_j(x_i) = \delta_{ij}$, the Kronecker delta. The choice of this approximation space Φ_h' is of course dictated by the fact that, for any real constants A and B, the function $v(x) = A + B\,e^{\frac{cx}{d}}$ satisfies $cv' - dv'' = 0$, or equivalently $a(v, w) = 0$ for any $\mathscr{C}^1$ function w with compact support in (0, 1).

Once the spaces Φ_h' and $\Psi_{h,\beta}$ are chosen, the analysis follows the same lines as in the previous section. In this new context, (15) becomes (γ is again the cell Reynolds number (16)) :

$$K'_{h,\beta} \leqslant C_{h,\beta} \leqslant K'_{h,\beta} \cdot \sqrt{1 + h \tanh^2\left(\frac{\gamma}{2}\right)}\,, \tag{24}$$

with now :

$$K'_{h,\beta} = \sqrt{\frac{\dfrac{\gamma}{2}\coth\left(\dfrac{\gamma}{2}\right)}{1 + 3\,\beta^2}}\,. \tag{25}$$

These relations prove the convergence of the method, and show that the optimal value of β for this second class of Petrov-Galerkin schemes is $\beta = 0$. There is no difficulty in checking that the resulting optimized scheme is also of the form (3), but now with :

$$\alpha = \coth\left(\frac{\gamma}{2}\right) - \frac{2}{\gamma}\,. \tag{26}$$

2.2. Finite-difference analysis

The preceding finite-element analysis, with two different choices of the pair of spaces (Φ_h, Ψ_h), allowed us to consider two particular schemes of type (3), corresponding to the choices (21) and (26) for the upwind parameter α. We now examine the schemes (3) from the finite-difference point of view ; in particular, we will see how the values (21) and (26) of α again emerge in the finite-difference context.

2.2.1. *Requesting monotone solutions*

Let us first rewrite (3) in two different equivalent forms :

$$c\frac{u_{i+1}-u_{i-1}}{2h}=\left(d+\frac{\alpha hc}{2}\right)\frac{u_{i+1}-2u_i+u_{i-1}}{h^2}, \tag{27}$$

$$(2+\gamma(\alpha-1))u_{i+1}-2(2+\alpha\gamma)u_i+(2+\gamma(\alpha+1))u_{i-1}=0. \tag{28}$$

The form (27) is classically used to explain that the use of an upwind approximation of the first derivative introduces an artificial or numerical diffusion. The form (28) tells us that the nodal values u_i are given by :

$$u_i=Ar_1^i+Br_2^i, \tag{29}$$

where r_1 and r_2 are the roots of the polynomial :

$$(2+\gamma(\alpha-1))r^2-2(2+\alpha\gamma)r+(2+\gamma(\alpha+1))=0, \tag{30}$$

and where A and B are chosen such that :

$$A+B=0, \quad Ar_1^{N+1}+Br_2^{N+1}=1. \tag{31}$$

It follows from the consistency of the scheme (3) that $r_1=1$. Then, we have $r_2=\dfrac{2+\gamma(1+\alpha)}{2+\gamma(1-\alpha)}$ (if the denominator is not zero), and we obtain $u_i=A+Br_2^i$, which implies that for $1\leqslant i\leqslant N$:

$$(u_{i+1}-u_i)(u_i-u_{i-1})=B^2(r_2-1)^2r_2^{2i+1}. \tag{32}$$

This shows that the numerical solution (u_i) does not oscillate (and is therefore monotone increasing) if $r_2>0$, that is if :

$$\alpha>1-\frac{2}{\gamma}. \tag{33}$$

To be precise, let us add that the solution is still monotone ($u_i=1$ for all $i\geqslant 1$!) in the limiting case where $\alpha=1-\dfrac{2}{\gamma}$. When $\alpha<1-\dfrac{2}{\gamma}$, r_2 is negative and even less that -1 since the sum $1+r_2$ of the roots of (30) is then negative : the numerical solution is then oscillating, and the amplitude of these oscillations increases like $|r_2|^i$ as i increases. These conclusions include of course the well-known facts that the fully centered scheme ($\alpha=0$) provides a non oscillating solution if the cell Reynolds number is less than or equal to 2, while the fully upwind scheme ($\alpha=1$) always gives a monotone solution.

2.2.2. *Truncation error analysis*

There are two distinct classical ways of defining the truncation error of the scheme (3), and we find it important, although it has not always been done in the literature, to avoid any confusion between these two definitions.

To make it clear, let us call $\mathscr{L}$ and $\mathscr{L}_h$ the differential and difference operators under consideration. Then the exact solution u and the approximate solution u_h respectively satisfy $\mathscr{L}u = 0$ and $\mathscr{L}_h u_h = 0$. Then the quantities $\mathscr{L}_h u$ and $\mathscr{L}u_h$ are two distinct quantities : $\| \mathscr{L}_h u \|$ measures how much the exact solution fails to satisfy the approximate problem, while $\| \mathscr{L}u_h \|$ measures how much the approximate solution fails to satisfy the exact equation.

Let us first use $\| \mathscr{L}_h u \|$ as a measure of the error. Following Richtmyer and Morton [11], we define the truncation error as :

$$TE = \varepsilon = \| (\varepsilon_i)_{1 \leqslant i \leqslant N} \| , \tag{34}$$

where ε_i is defined by :

$$\begin{aligned} \varepsilon_i = c \left(\alpha \frac{u(x_i) - u(x_{i-1})}{h} + (1-\alpha) \frac{u(x_{i+1}) - u(x_{i-1})}{2h} \right) \\ - d \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} \end{aligned} \tag{35}$$

where the $u(x_j)$ are the nodal values of the exact solution. Using an infinite Taylor expansion for the $\mathscr{C}^\infty$ function u, we get :

$$\begin{aligned} \varepsilon_i = & - \frac{\alpha\gamma d}{2} u''(x_i) - 2d \left(1 + \frac{\alpha\gamma}{2} \right) \sum_{n=2}^{\infty} \frac{h^{2n-2}}{(2n)!} u^{(2n)}(x_i) \\ & + d\gamma \sum_{n=1}^{\infty} \frac{h^{2n-1}}{(2n+1)!} u^{(2n+1)}(x_i) . \end{aligned} \tag{36}$$

Since u is the *exact* solution (2), we have, for all $1 \leqslant i \leqslant N$ and $n \geqslant 2$:

$$u^{(n)}(x_i) = \left(\frac{c}{d} \right)^{n-2} u''(x_i) . \tag{37}$$

We then get :

$$\varepsilon_i = du''(x_i) \left[- \frac{\alpha\gamma}{2} - 2 \left(1 + \frac{\alpha\gamma}{2} \right) \sum_{n=2}^{\infty} \frac{\gamma^{2n-2}}{(2n)!} + \gamma \sum_{n=1}^{\infty} \frac{\gamma^{2n-1}}{(2n+1)!} \right] . \tag{38}$$

Since γ is proportional to h, this shows that the scheme is at least first-order accurate (provided that α remains bounded when $h \to 0$). Furthermore, the scheme is exactly first-order accurate if α as independent of h.

If now, in a first step, we simply keep the first terms in the expansion (38), we obtain :

$$\varepsilon_i = du''(x_i) \left[- \frac{\alpha\gamma}{2} + \frac{\gamma^2}{12} - \frac{\alpha\gamma^3}{24} + O(h^4) \right] , \tag{39}$$

and we see that $\varepsilon_i = O(h^4)$ if we choose $\alpha = \frac{\gamma}{6} = \frac{ch}{6d}$, i.e. the choice (21). Thus we come to the conclusion (already reached in [6], [7]), that the scheme (3) with the upwind parameter α chosen according to (21) is fourth-order accurate.

Let us now come back to (38), which can be rewritten as :

$$\varepsilon_i = -du''(x_i)\left[\frac{\alpha\gamma}{2} + \frac{2}{\gamma^2}\left(1 + \frac{\alpha\gamma}{2}\right)\left(\cosh\gamma - \frac{\gamma^2}{2} - 1\right) - \frac{1}{\gamma}(\sinh\gamma - \gamma)\right], \tag{40}$$

whence :

$$\varepsilon_i = -2\,du''(x_i)\sinh^2\left(\frac{\gamma}{2}\right)\frac{\alpha - \left(\coth\left(\frac{\gamma}{2}\right) - \frac{2}{\gamma}\right)}{\gamma}. \tag{41}$$

Therefore, $\varepsilon_i = 0$ for all i if α is given by (26) : the scheme (3), with α given by (26), is of infinite order of accuracy ! In other words, the equalities $u_i = u(x_i)$ hold for all i.

Before commenting further these results, let us examine the second way of defining the truncation error. Following now the point of view of Warming and Hyett [15], we define, for any $\mathscr{C}^\infty$ function w which interpolates the numerical solution (that is, such that $w(x_i) = u_i$ for all i), the quantities :

$$\hat{\varepsilon}_i^w = cw'(x_i) - dw''(x_i)\,; \tag{42}$$

the scheme is said to be of order p if $\|(\hat{\varepsilon}_i^w)\|$ *formally* tends to 0 like $O(h^p)$ when $h \to 0$ (this measure of the truncation error is nothing but $\|\mathscr{L}u_h\|$ with the notations of the beginning of this section).

Using again Taylor expansions, one sees that :

$$\hat{\varepsilon}_i^w = -\frac{\alpha ch}{2}w''(x_i) + O(h^2). \tag{43}$$

The conclusions here are (i) that the scheme is first-order accurate if α is independent of h, and (ii) that the scheme is second-order accurate if $\alpha = 0$ or if α tends to 0 as $O(h)$ when $h \to 0$.

2.3. Conclusions

Let us now try to get some clear lessons from all these different analyses.

From the different conclusions reached in the previous section about the accuracy of the scheme (3), it is clear that only the last ones (obtained with the error $\hat{\varepsilon}_i^w$) are problem-independent. Therefore, we will say that the

scheme (3) is second-order accurate, provided that α tends to 0 as $O(h)$ when $h \to 0$ (which is of course true when α is chosen according to (21) or (26); it follows indeed from the previous analyses that $\coth\left(\frac{\gamma}{2}\right) - \frac{2}{\gamma}$ behaves as $\frac{\gamma}{6}$ when $\gamma \to 0$).

On the opposite we do not find reasonable to say that the scheme (3) is fourth-order accurate, or « infinitely accurate ». The fact that the error ε_i vanishes when (26) holds is only true for the particular problem (1), and would not be true in general for the problem :

$$\begin{cases} cu' - du'' = f(x, u) \\ + \text{ boundary conditions} . \end{cases} \tag{44}$$

Nevertheless, we can retain from the analysis (35)-(41) some informations that are not given by the latter analysis (42)-(43) : when α is evaluated from (26), and when the right-hand side of (44) vanishes, the scheme gives the node values of the exact solution (we do not say « the scheme becomes of a higher-order of accuracy »). Since moreover, it is easy to see that :

$$\coth\frac{\gamma}{2} - \frac{2}{\gamma} > 1 - \frac{2}{\gamma}, \tag{45}$$

for all $\gamma > 0$, we know from Section 2.2.1 that the value (26) of α guarantees the monotonicity of the solution (and therefore the L^∞ stability of the scheme). For all these reasons, we will use the scheme (3)-(26) in the sequel : for problems like (44), we will approximate $cu' - du''$ by :

$$c\left(\alpha\frac{u_i - u_{i-1}}{h} + (1-\alpha)\frac{u_{i+1} - u_{i-1}}{2h}\right) - d\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}, \tag{46}$$

with :

$$\alpha = \coth\left(\frac{ch}{2d}\right) - \frac{2d}{ch}. \tag{47}$$

In this way, we will have a second-order accurate scheme, which remains L^∞ stable for any value of the cell Reynolds number.

3. A NONLINEAR MODEL PROBLEM

As an intermediate step before we consider the simulation of planar steady flames in the next section, we now apply the conclusions of Section 2 to the study of a system of time-dependent nonlinear convection-reaction-diffusion equations.

3.1. The model problem

To simplify the analysis in this section, we will consider a system which only contains equations for the mass fractions. In comparison with the actual flame problem addressed in Section 4, this simplification amounts to assuming here that the temperature profile and the mass flux $c > 0$ are known. Again for the sake of simplicity, we also assume that all species have the same diffusion coefficient d, and we will use an equally spaced grid and Dirichlet boundary conditions ; but the analysis presented in this section could also be carried out with variable diffusion coefficients, with a non uniform grid, and with mixed Neumann-Dirichlet conditions, as we will have in Section 4 (see [5]).

We therefore consider the next system, where the unknowns are the mass fractions Y_k, $1 \leqslant k \leqslant K$ for a mixture made of K reactive species :

$$(Y_k)_t + c(Y_k)_x = d(Y_k)_{xx} + R_k(\bar{Y}, x)\,, \tag{48}$$

for $0 \leqslant x \leqslant L$, $t \geqslant 0$, $1 \leqslant k \leqslant K$, with the Dirichlet boundary conditions :

$$Y_k(0) = Y_k^u\,, \quad Y_k(L) = Y_k^b \tag{49}$$

for $1 \leqslant k \leqslant K$ (the supscripts u and b refer to an unburnt and a burnt state respectively).

In (48), the source term $R_k(\bar{Y}, x)$ is the rate of formation of species k, and $\bar{Y}$ is the vector $\bar{Y} = (Y_{k'}) \in \mathbb{R}^K$. Considering a general situation with a complex set of chemical reactions, we write :

$$R_k(\bar{Y}, x) = \sum_{r \in \mathscr{P}_k} \mathscr{A}_{r,k}(x) \prod_{k'=1}^{K} Y_{k'}^{\nu_{r,k'}} - \sum_{r \in \mathscr{C}_k} \mathscr{B}_{r,k}(x) \prod_{k'=1}^{K} Y_{k'}^{\nu_{r,k'}}\,, \tag{50}$$

where the $\mathscr{A}_{r,k}$'s and $\mathscr{B}_{r,k}$'s are positive reals, the $\nu_{r,k'}$'s are non negative integers, and where $\mathscr{P}_k$ (resp. : $\mathscr{C}_k$) represents the set of those chemical reactions which produce (resp. : consume) the k-th species (see [16]). In fact, the law of mass action implies that :

$$\nu_{r,k} > 0 \quad \text{if} \quad r \in \mathscr{C}_k\,; \tag{51}$$

in other words, the rate of comsumption of species k in a reaction is proportional to some positive power of Y_k (see e.g. [16]).

Moreover, we will use in the sequel the fact that :

$$\sum_{k=1}^{K} R_k(\bar{Y}, x) \equiv 0\,, \tag{52}$$

which simply says that the chemical reactions do not create mass.

In fact, we will need to slightly modify the expression of the reaction rates. Let $g : \mathbb{R} \to \mathbb{R}$ be defined by :

$$g(x) = \begin{cases} 0 & \text{if} \quad x \leqslant 0 , \\ x & \text{if} \quad 0 \leqslant x \leqslant 1 , \\ 1 & \text{if} \quad 1 \leqslant x . \end{cases} \tag{53}$$

For $\bar{Y} = (Y_{k'}) \in \mathbb{R}^K$ and $1 \leqslant k \leqslant K$, we define $\bar{g}(\bar{Y}) = (g(Y_{k'})) \in \mathbb{R}^K$ and :

$$S_k(\bar{Y}, x) = R_k(\bar{g}(\bar{Y}, x)) . \tag{54}$$

3.2. Numerical analysis

For the numerical solution of system (48)-(49), we will consider a fully implicit scheme, which uses the modified source terms (54) and the « optimized » upwind approximation of Section 2 for the convection-diffusion terms. Using again the notation h for $\Delta x = \dfrac{L}{N+1}$ and setting $\tau = \Delta t$, we consider the discrete system :

$$\frac{Y_{k,i}^{n+1} - Y_{k,i}^{n}}{\tau} + c \left(\alpha \frac{Y_{k,i}^{n+1} - Y_{k,i-1}^{n+1}}{h} + (1-\alpha) \frac{Y_{k,i+1}^{n+1} - Y_{k,i-1}^{n+1}}{2h} \right) = d \frac{Y_{k,i+1}^{n+1} - 2\, Y_{k,i}^{n+1} + Y_{k,i-1}^{n+1}}{h^2} + S_k(\bar{Y}_i^{n+1}, x_i), \tag{55}$$

for $1 \leqslant k \leqslant K$ and $1 \leqslant i \leqslant N$, with :

$$Y_{k,0}^{n+1} = Y_k^u , \quad Y_{k,N+1}^{n+1} = Y_k^b , \tag{56}$$

and an initial condition :

$$Y_{k,i}^{0} = Y_k^0(x_i) . \tag{57}$$

In (55), the upwind parameter α is given by (47).

Evaluating the new values $Y_{k,i}^{n+1}$ using the scheme (55) requires to solve at each time step a nonlinear discrete problem. The two next propositions say that (i) this nonlinear discrete problem (55) has a unique solution provided that τ is small enough, and (ii) for any $\tau > 0$ such that (55) has a solution, then this solution satisfies $0 \leqslant Y_{k,i}^{n+1} \leqslant 1$ for all k and i (and therefore $S_k = R_k$) : in other words, the nonlinear scheme (55) is unconditionnally stable.

Let $n \geqslant 0$ be fixed. We will always assume in the following analysis that the values $Y_{k,i}^{n}$ are given and satisfy, for all k $(1 \leqslant k \leqslant K)$ and i $(1 \leqslant i \leqslant N)$:

$$0 \leq Y_{k,i}^n , \quad \sum_{k=1}^{K} Y_{k,i}^n = 1 . \tag{58}$$

Also, we assume that :

$$Y_k^u \geq 0 , \quad Y_k^b \geq 0 , \quad \sum_{k=1}^{K} Y_k^u = \sum_{k=1}^{K} Y_k^b = 1 . \tag{59}$$

PROPOSITION 1 : *There exists* $\tau_0 > 0$ *such that, for any* $\tau \in]0, \tau_0[$, *the nonlinear discrete problem* (55) *has a unique solution* $(Y_{k,i}^{n+1})$. ■

PROPOSITION 2 : *Let* $\tau > 0$ *be such that* (55) *has a solution* $(Y_{k,i}^{n+1})$. *Then, for all* k $(1 \leq k \leq K)$ *and* $i (1 \leq i \leq N)$, *the following holds .*

$$0 \leq Y_{k,i}^{n+1} , \quad \sum_{k=1}^{K} Y_{k,i}^{n+1} = 1 . \tag{60}$$

In particular, $S_k(\bar{Y}_i^{n+1}, x_i) = R_k(\bar{Y}_i^{n+1}, x_i)$ *for all* k *and* i. ■

Proof of Proposition 1 : Let us first write the scheme in developed form as :

$$\begin{aligned} Y_{k,i}^{n+1} + \tau \sum_{j=1}^{N} a_{i,j} \, Y_{k,j}^{n+1} = {} & Y_{k,i}^n + \tau S_k(\bar{Y}_i^{n+1}, x_i) \\ & - \tau \, \delta_{i,1} \, a_{1,0} \, Y_k^u - \tau \, \delta_{i,N} \, a_{N,N+1} \, Y_k^b . \end{aligned} \tag{61}$$

The coefficients $a_{i,j}$ stand for the convection-diffusion operator :

$$a_{i,j} = \frac{2\,d}{h^2} + c\,\frac{\alpha}{h} , \quad a_{i,i-1} = \frac{-d}{h^2} - c\,\frac{1+\alpha}{2\,h} , \quad a_{i,i+1} = \frac{-d}{h^2} + c\,\frac{1-\alpha}{2\,h} , \tag{62}$$

with $a_{i,j} = 0$ if $|i-j| > 1$. In (61), δ is the Kronecker delta.

In matricial form, considering the vector $Y^{n+1} = (Y_{k,i}^{n+1}) \in \mathbb{R}^{NK}$, we write the scheme as :

$$Y^{n+1} + \tau A Y^{n+1} = Y^n + \tau S(Y^{n+1}) + \tau X , \tag{63}$$

where the vectors $S \in \mathbb{R}^{NK}$ and $X \in \mathbb{R}^{NK}$ stand for the reaction terms and the boundary terms respectively ; the $NK \times NK$ matrix A represents the discrete convection-diffusion operator.

a) It is classical to check that A is a definite positive matrix in the sense that :

$$^t Y A Y > 0 \quad \forall Y \in \mathbb{R}^{NK} - \{0\} . \tag{64}$$

The proof of (64) relies on a « discrete integration by parts ». Let $V = (v_1, ..., v_N) \in \mathbb{R}^N$, and define (to simplify the writing) $v_0 = 0$, $v_{N+1} = 0$. Then, a straightforward calculation shows that :

$$- d \sum_{i=1}^{N} v_i \left(\frac{v_{i+1} - 2 v_i + v_{i-1}}{h^2} \right) = d \frac{v_1^2}{h^2} + d \sum_{i=1}^{N-1} \frac{(v_{i+1} - v_i)^2}{h^2} + d \frac{v_N^2}{h^2}, \quad (65)$$

and :

$$c \sum_{i=1}^{N} v_i \left[\alpha \frac{v_i - v_{i-1}}{h} + (1 - \alpha) \frac{v_{i+1} - v_{i-1}}{2h} \right] =$$

$$= - \frac{\alpha h c}{2} \sum_{i=1}^{N} v_i \left(\frac{v_{i+1} - 2 v_i + v_{i-1}}{h^2} \right) + c \sum_{i=1}^{N} v_i \left(\frac{v_{i+1} - v_{i-1}}{2h} \right)$$

$$= - \frac{\alpha h c}{2} \sum_{i=1}^{N} v_i \left(\frac{v_{i+1} - 2 v_i + v_{i-1}}{h^2} \right), \quad (66)$$

which proves (64).

b) Let now Id be the identity matrix in $\mathbb{R}^{NK}$, and let $\tau > 0$. From *a*) above we know that the matrix $\mathrm{Id} + \tau A$ is non singular. Furthermore, if $Z_1, Z_2 \in \mathbb{R}^{NK}$ satisfy $Z_2 = (\mathrm{Id} + \tau A) Z_1$, then :

$$\| Z_1 \|^2 = {}^t Z_1 Z_1 \leq {}^t Z_1 (\mathrm{Id} + \tau A) Z_1 \leq {}^t Z_1 Z_2 \leq \| Z_1 \| \| Z_2 \|, \quad (67)$$

whence $\| Z_1 \| \leq \| Z_2 \|$. This shows that :

$$\| (\mathrm{Id} + \tau A)^{-1} \| \leq 1, \quad (68)$$

for any $\tau > 0$.

c) For $Y \in \mathbb{R}^{NK}$, let us now set $Q_\tau(Y) = Y^n + \tau X + \tau S(Y)$. From our definition (53)-(54) of S_k, it appears that S is a Lipschitz-continuous mapping (whereas R_k is not Lipschitz-continuous !) : let $L_S > 0$ be a positive constant such that :

$$\| S(Y_1) - S(Y_2) \| \leq L_S \| Y_1 - Y_2 \| \quad (69)$$

for all $Y_1, Y_2 \in \mathbb{R}^{NK}$. Now Q_τ is also Lipschitz-continuous. If $\tau > 0$ is chosen such that $\tau L_S < 1$, then the mapping :

$$Y \in \mathbb{R}^{NK} \to (\mathrm{Id} + \tau A)^{-1} Q_\tau(Y) \quad (70)$$

is strictly contractant, and therefore has a unique fixed point, which is the unique solution of (63). This proves Proposition 1. ■

Proof of Proposition 2 : *a*) It is easy to check that, for all i $(1 \leq i \leq N)$:

$$a_{i,i} > 0\,, \quad a_{i,i+1} < 0\,, \quad a_{i,i-1} < 0\,, \tag{71}$$

$$\sum_{j=i-1}^{i+1} a_{i,j} = 0\,. \tag{72}$$

Notice here that checking the inequality $a_{i,i+1} < 0$ requires to use the value (47) of α and the property (45).

b) Let now $\tau > 0$, and assume that (63) has a solution Y^{n+1}. Assuming further that Y^{n+1} has a negative component, we set : $Y^{n+1}_{k,i} = \min_{k',j} Y^{n+1}_{k',j} < 0$.

Then, we see from (51) and (54) that $S_k(Y^{n+1}_{\cdot,i}, x_i) \geq 0$ (here appears the second reason why we consider the modified nonlinear term S_k instead of R_k). Then (59), (61) and (71) show that :

$$Y^{n+1}_{k,i} + \tau \sum_j a_{i,j}\, Y^{n+1}_{k,j} \geq 0\,. \tag{73}$$

Since $Y^{n+1}_{k,j} \geq Y^{n+1}_{k,i}$ for all j, we have :

$$\sum_{j \neq i} a_{i,j}\, Y^{n+1}_{k,j} \leq \sum_{j \neq i} a_{i,j}\, Y^{n+1}_{k,i}\,, \tag{74}$$

from (71), whence :

$$\sum_j a_{i,j}\, Y^{n+1}_{k,j} \leq \sum_j a_{i,j}\, Y^{n+1}_{k,i} = 0 \tag{75}$$

from (72). This proves that the left-hand side of (73) is the sum of a negative term and of a non positive term, whence a contradiction. Therefore, we have proved that $Y^{n+1}_{k,i} \geq 0$ for all k and i.

c) Let us lastly show the second property in (60). Denoting $Z^{n+1}_i = \sum_{k=1}^{K} Y^{n+1}_{k,i}$, we have :

$$Z^{n+1}_i + \tau \sum_{j=1}^{N} a_{i,j}\, Z^{n+1}_j = 1 - \tau\, \delta_{i,1}\, a_{1,0} - \tau\, \delta_{i,N}\, a_{N,N+1}\,. \tag{76}$$

We have used the fact that $\sum_k S_k(\bar{Y}^{n+1}_i, x_i) = 0$ (which follows from (52) and (54)) and the assumptions (58), (59). Since the matrix $(\mathrm{Id} + \tau A)$ is non singular, it is easy to deduce from (76) that $Z^{n+1}_i = 1$ for all i (that is, the scheme preserves the identity $\sum Y_k = 1$), which ends the proof. ■

Remark 1 : Proposition 2 is of much greater practical interest that Proposition 1. Indeed, the time-step τ_0 below which the nonlinear problem (63) is shown to have a unique solution is simply the time-step one would use with an explicit integration of the source term. But, although we cannot prove it with the preceding fixed point arguments, problem (63) is expected to have a solution Y^{n+1} for much larger values of τ. Proposition 2 then says that this solution is always physically admissible (i.e. satisfies (60)), whatever the value of the time-step τ. ■

In fact, examining in detail the proof of Proposition 2, we can show a more precise result. Before stating it, let us define the set $\mathscr{S}$ of « the species which can be created from Y^u, Y^b and Y^0» : this set contains all species which are actually present in the prescribed states Y^u and Y^b or in the initial condition Y^0 (that is, the k-th species is in the set $\mathscr{S}$ as soon as $Y^u_k > 0$ or $Y^b_k > 0$ or $Y^0_{k,i} > 0$ *for some* i) ; but it also contains all species which can be produced from the previous ones using one of the considered chemical reactions.

To make it clear, let us consider some examples, with the chemical mechanism of Table 1 below. If only the species O_2 is present in the states Y^u, Y^b, Y^0 (that is, if $Y^u_{O_2} = Y^b_{O_2} = Y^0_{O_2,i} = 1$ for all i), then $\mathscr{S} = \{O_2\}$ since no other species can be created from O_2 alone. If only the species O and N_2 are present in Y^u, Y^b and Y^0, then $\mathscr{S} = \{O, N_2\}$ because no third species

TABLE 1

Reaction mechanism for the hydrogen-air flame

$([M] = [H_2] + 0.4\,[O_2] + 0.4\,[N_2] + 6.5\,[H_2O])$.

Number	Reaction
(1)	$H + O_2 \rightarrow OH + O$
(2)	$O + OH \rightarrow H + O_2$
(3)	$O + H_2 \rightarrow OH + H$
(4)	$H + OH \rightarrow O + H_2$
(5)	$OH + H_2 \rightarrow H_2O + H$
(6)	$H + H_2O \rightarrow OH + H_2$
(7)	$OH + OH \rightarrow H_2O + O$
(8)	$H_2O + O \rightarrow OH + OH$
(9)	$H + H + M \rightarrow H_2 + M$
(10)	$H + OH + M \rightarrow H_2O + M$
(11)	$H + O_2 + M \rightarrow HO_2 + M$
(12)	$HO_2 + M \rightarrow H + O_2 + M$
(13)	$H + HO_2 \rightarrow OH + OH$
(14)	$H + HO_2 \rightarrow H_2 + O_2$
(15)	$O + HO_2 \rightarrow OH + O_2$
(16)	$OH + HO_2 \rightarrow H_2O + O_2$

can be created from O and N_2. Lastly, if O, H and N_2 are present in Y^u, Y^b and Y^0 then $\mathscr{S}$ contains every species of Table 1 (H_2 can be produced by reaction (9), then OH can be produced by reaction (3) and so on).

Having defined this set $\mathscr{S}$, we can state :

PROPOSITION 3 : *For any species k belonging to the set $\mathscr{S}$, one has $Y^n_{k,i} > 0$ for any $n > 0$ and $1 \leqslant i \leqslant N$.* ■

Proof : Let us assume that $Y^n_{k,i} = 0$, for some $n > 0$, $1 \leqslant k \leqslant K$, $1 \leqslant i \leqslant N$. Then (61) writes :

$$\tau a_{i,i-1}\, Y^n_{k,i-1} + \tau a_{i,i+1}\, Y^n_{k,i+1} = Y^{n-1}_{k,i} + \tau R_k(\bar{Y}^n_i, x_i) - \tau\, \delta_{i,1}\, a_{1,0}\, Y^u_k - \tau\, \delta_{i,N}\, a_{N,N+1}\, Y^b_k . \tag{77}$$

We have already noticed that $S_k(\bar{Y}^n_i, x_i) \geqslant 0$ since $Y^n_{k,i} \leqslant 0$. Then all terms in the left-hand side of (77) are non positive from (71), while all terms in the right-hand side are non negative. All these terms must therefore vanish. Thus, under the assumption that $Y^n_{k,i} = 0$, we have proved that :

$$\begin{cases} Y^n_{k,i+1} = Y^n_{k,i-1} = 0 , \\ R_k(\bar{Y}^n_i, x_i) = 0 , \\ Y^{n-1}_i = 0 , \\ Y^u_k = 0 \quad \text{if} \quad i = 1 , \\ Y^b_k = 0 \quad \text{if} \quad i = N . \end{cases} \tag{78}$$

This implies in turn that :

$$\begin{cases} Y^n_{k,j} = 0, R_k(\bar{Y}^n_j, x_j) = 0, Y^{n-1}_{k,j} = 0 \quad \text{for all} \quad j, 1 \leqslant j \leqslant N , \\ Y^u_{k,j} = Y^b_k = 0 , \end{cases} \tag{79}$$

and Proposition 3 easily follows. ■

Remark 2 : This result may be found rather surprising : from a physical point of view, one may expect that the mass fraction of some species in the set $\mathscr{S}$ vanishes in some parts of the computational domain. In fact, this result is just related to the implicit integration of the diffusive terms. Indeed, the implicit scheme :

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \sigma \frac{u_{i+1}^{n+1} - 2\, u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} \tag{80}$$

applied to the heat equation $u_t = \sigma u_{xx}$ has the property that :

$$\left.\begin{array}{l} u_j^n \geqslant 0 \quad \text{for all } j \\ u_j^n > 0 \quad \text{for some } j \end{array}\right\} \Rightarrow u_j^{n+1} > 0 \quad \text{for all } j \,. \tag{81}$$

Moreover, one should keep in mind here that the mass fraction of a species which is consumed by the reactions is expected to vanish only asymptotically as $t \to +\infty$. ■

Remark 3 : When the diffusion coefficient d varies with x or with the species, or when the mesh is no longer uniform, then the upwind parameter α must vary as a function of the *local* cell Reynolds number. For instance, (62) becomes, for the k-th species :

$$a_{i,i}^k = \left[2\frac{d_i^k}{h_i} + 2\frac{d_{i-1}^k}{h_{i-1}} + c(\alpha_i^k + \alpha_{i-1}^k) \right] . \, (h_i + h_{i-1})^{-1} , \tag{82}$$

$$a_{i,i-1}^k = \left[-\frac{2\, d_{i-1}^k}{h_{i-1}} - c(\alpha_{i-1}^k + 1) \right] . \, (h_i + h_{i-1})^{-1} , \tag{83}$$

$$a_{i,i+1}^k = \left[-\frac{2\, d_i^k}{h_i} + c(1 - \alpha_i^k) \right] . \, (h_i + h_{i+1})^{-1} , \tag{84}$$

where $d_i^k = d^k(\bar{Y}_i, x_i)$ is the diffusion coefficient of species k, $h_i = x_{i+1} - x_i$, and :

$$\alpha_i^k = \coth\left(\frac{\gamma_i^k}{2}\right) - \frac{2}{\gamma_i^k} , \tag{85}$$

γ_i^k being the local cell Reynolds number for the k-th species :

$$\gamma_i^k = \frac{c h_i}{d_i^k} . \tag{86}$$

The expressions (82)-(86) are used in the method presented in the next section for the simulation of flames with variable diffusion coefficients. ■

4. APPLICATION TO THE SIMULATION OF STEADY PLANAR FLAMES

After having checked in Section 3 that the upwind scheme designed in Section 2 is unconditionnally stable when applied to the nonlinear model system (48), we now turn to the simulation of planar premixed flames.

4.1. A sketch of the method

The method we are going to employ for flame simulation is essentially the one used by Sermange [12] (and shares many features with the algorithms used by other authors ; see e.g. [13], [14]), but with the « optimized » upwind approximation defined above.

Let us first recall from [12] the equations which we will consider in the truncated computational domain $[0, a]$:

$$\begin{cases} \left(c \sum_k C_{pk} Y_k - \sum_k C_{pk} U_k \right) T_x - (\lambda T_x)_x + \sum_k h_k r_k = 0 , \\ c Y_{k,x} - U_{k,x} - r_k = 0 , \end{cases} \tag{87}$$

$$\begin{cases} \lambda[T(0), Y(0)] T_x(0) = c \sum_k [h_k(T(0)) - h_k(T_u)] Y_k^u , \\ U_k(0) = c[Y_k(0) - Y_k^u] , \end{cases} \tag{88}$$

$$\begin{cases} T_x(a) = 0 , \\ Y_{k,x}(a) = 0 , \end{cases} \tag{89}$$

$$T(x_f) = T_f . \tag{90}$$

In these equations, c is the (unknown) mass flux accross the flame, $C_{pk} = \dfrac{dh_k}{dT}$ is the specific heat of the k-th species, U_k is the diffusive mass flux of species k, $\lambda = \lambda(T, Y)$ is the thermal conductivity of the mixture, h_k is the specific enthalpy of the k-th species, r_k its mass rate production by the chemical reactions. The diffusive fluxes U_k are assumed to be given by expressions of the form :

$$U_k = \sum_{k'} \mu_{kk'}(T, Y) Y_{k',x} + \mu_k(T, Y) T_x . \tag{91}$$

We refer to [5], [12] for the derivation of the boundary conditions (88) : they are obtained by integrating the governing equations (87) in the interval $(-\infty, 0)$ and assuming that the reaction rates are negligible in this interval. In (88), T^u and Y_k^u are given and refer to the state of the fresh mixture (at $-\infty$). Zero flux conditions (89) are assumed at the right boundary $x = a$. The additional condition (90), which fixes the flame with respect to the x-axis, allows us to keep c unknown in (87) ; here x_f is fixed ($x_f \in [0, a]$), and T_f is also chosen fixed.

We will not precisely describe all features of the method used to solve problem (87)-(90), since it closely follows the method of [12]. Let us simply make precise that we use a pseudo-unsteady approach : instead of solving

the steady equations (87), we introduce time derivatives and consider the partially discretized system :

$$\begin{cases} \rho^n \left(\sum_k C_{pk}^n \, Y_k^n \right) \dfrac{T^{n+1} - T^n}{\Delta t} + \left(c^{n+1} \sum_k C_{pk}^n \, Y_k^n - \sum_k C_{pk}^n \, U_k^n \right) T_x^{n+1} - \\ \qquad - (\lambda^n \, T_x^{n+1})_x + \sum_k h_k(T^n) \, r_k^{n+1} = 0 \, , \\ \rho^n \dfrac{Y_k^{n+1} - Y_k^n}{\Delta t} + c^{n+1} \, Y_{k,x}^{n+1} - \left(\mu_i^n \, T_x^{n+1} + \sum_{k'} \mu_{kk'} \, Y_{k',x}^{n+1} \right)_x - r_{0k}^{n+1} = 0 \, . \end{cases} \tag{92}$$

In (92), ρ^n is given as a function of T^n by an isobaric equation of state (see [8]) ; we call this a *pseudo*-unsteady approach because system (92), which allows us to use an iterative approach to the steady solutions of (87), does not describe the true transient behaviour of the flame (ρu is no longer constant in space in the true unsteady solution ; see [8]).

The solution of (92) essentially follows the lines of the previous section : we use the « optimized » upwind scheme, with a fully implicit pseudo-time integration. One noticeable difference is that we now use a non uniform adaptive grid, which is constructed by equidistributing a mesh function based on the variation of the solution (see [5], [12] for the details). The nonlinear discrete problem to be solved at each time step is solved using Newton's method, and a variable time step is used.

4.2. Numerical results

Without detailing more the method, we now examine how the use of the « optimized » upwind approximation improves the numerical results in comparison with those obtained using a fully centered or a fully uncentered approximation.

4.2.1. *A model problem*

Again, we first consider a model problem, which now includes a nonlinear reaction term chosen so that an exact steady solution is explicitly known. We consider the system :

$$\begin{cases} - T_{xx} + cT_x = 2 \, YT^2 , \\ - Y_{xx} + cY_x = - 2 \, YT^2 , \end{cases} \tag{93}$$

with the conditions :

$$\begin{aligned} Y(-\infty) &= Y^u = 1 \, , \quad T(-\infty) = T^u = 0 \, , \\ Y(+\infty) &= Y^k = 0 \, , \quad T(+\infty) = T^k = 1 \, . \end{aligned} \tag{94}$$

The solution of (93)-(94) is :

$$c = 1\,, \quad T(x) = \frac{e^{x - x_0}}{1 + e^{x - x_0}}\,, \quad Y(x) = 1 - T(x)\,, \tag{95}$$

for some $x_0 \in \mathbb{R}$.

We have solved this problem in the interval $[0, a] = [0, 10]$ with different uniformly spaced grids using three different methods : the « optimized » upwind method, the first-order fully uncentered method ($\alpha = 1$) and the second-order fully centered method ($\alpha = 0$). The comparisons of the numerical results with the exact solution shows that the « optimized » upwind method behaves better than the centered method, and that both of them are far superior to the first-order method :

4.2.2. *The hydrogen-air flame*

We now turn to an actual flame with a complex chemical mechanism. We will use the set of chemical reactions shown in Table 1 for the simulation of an hydrogen-air premixed flame (the precise data concerning this reaction can be found in e.g. [12], [10]).

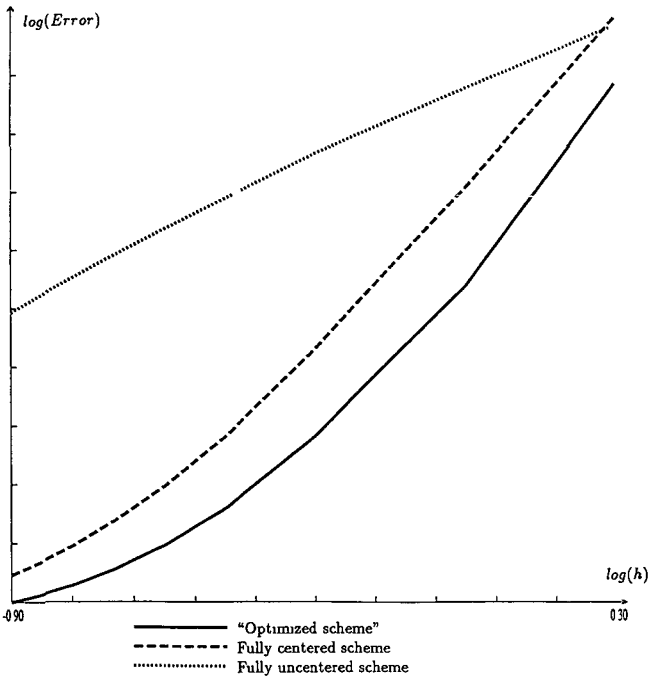

Figure 2. — Discrete errors in sup-norm as a function of the mesh size.

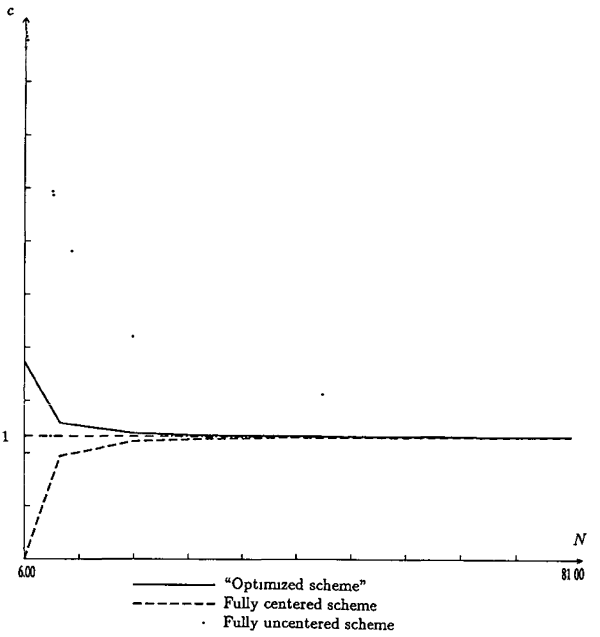

Figure 3. — Variation of the computed flame speed c as a function of the number of nodes.

We consider the case of a stoechiometric flame, where the overall reaction writes :

$$2\,H_2 + O_2 + 4\,N_2 \rightarrow 2\,H_2O + 4\,N_2\,. \qquad (96)$$

Again, we compare the « optimized » upwind scheme, the fully uncentered scheme and the second-order centered scheme. The computed flame speeds presented in Table 2 for the « optimized » upwind scheme and the centered scheme are very close to the most accurate results found in the literature for this case. When less than 31 mesh points are used with the centered approximation, the calculation becomes unstable (because the spatial resolution is too poor : the local cell Reynolds number is greater than 2, oscillations appear and lead to nonlinear numerical instabilities). In comparison, the « optimized » upwind scheme appears to be more robust, and solves the problem even with only 11 nodes. Lastly, as one could expect, it appears that the flame speed is substantially over-estimated when the first-order uncentered scheme is used, since an important amount of numerical diffusion is then added to the physical diffusion.

TABLE 2

Computed flame speeds for the three methods and different numbers of adaptive nodes

Number of nodes	Fully centered scheme	Fully uncentered scheme	"Optimized" scheme
11	**	3 00	2 14
21	**	2 41	2 10
31	2 08	2 27	2 08
41	2 07	2 21	2 08
51	2 07	2 18	2 07
61	2 07	2 16	2 07
71	2 07	2 15	2 07

The « optimized » upwind scheme has also been used to compute the extinction of a rich hydrogen-oxygen-nitrogen flame by excess of nitrogen (see [5])

5 CONCLUSIONS

The upwind scheme presented in this paper presents several interesting advantages for planar premixed flame simulations this scheme preserves the positivity of the mass fractions of all species and gives non oscillatory results for any values of the local cell Reynolds number and of the time step, while remaining second-order accurate This results in an algorithm which is as accurate as but more robust than the centered methods which are usually employed for this class of problems

REFERENCES

[1] A K AZIZ ed , *The mathematical foundations of the finite-element method with applications to partial differential equations,* Academic Press, New York (1972)

[2] P G CIARLET, *The finite-element method for elliptic problems,* Studies in Math and Appl , North-Holland, New York (1978)

[3] P CLAVIN, *Dynamic behavior of premixed flame fronts in laminar and turbulent flows,* Prog Energ Comb Sci , *11,* pp 1-59 (1985)

[4] J DONEA, *Recent advances in computational methods for steady and transient transport problems,* Nuclear Eng Design, *80,* pp 141-162 (1984)

[5] M GHILANI, *Simulation numerique de flammes planes stationnaires avec chimie complexe,* Thesis, Universite Paris-Sud (1987)

[6] D F GRIFFITHS & J LORENZ, *An analysis of the Petrov-Galerkin finite-element method,* Comp Meth Appl Mech Eng , *14,* pp 39-64 (1978)

[7] T. J. R. HUGHES, *A simple scheme for developing upwind finite elements,* Int. J. Num. Meth. Eng., *12,* pp. 1359-1365 (1978).

[8] B. LARROUTUROU, *The equations of one-dimensional unsteady flame propagation : existence and uniqueness,* SIAM J. Math. Anal., *19* (1), pp. 32-59 (1988).

[9] B. LARROUTUROU, *Introduction to combustion modelling,* Springer Series in Computational Physics, to appear.

[10] N. PETERS & J. WARNATZ eds., *Numerical methods in laminar flame propagation,* Notes in Numerical Fluid Mechanics, *6,* Vieweg, Braunschweig (1982).

[11] R. D. RICHTMYER & K. W. MORTON, *Difference methods for initial value problems,* Wiley, New York (1967).

[12] M. SERMANGE, *Mathematical and numerical aspects of one-dimensional laminar flame simulation,* Appl. Math. Opt., *14* (2), pp. 131-154 (1986).

[13] M. D. SMOOKE, *Solution of burner stabilized premixed laminar flames by boundary values methods,* J. Comp. Phys., *48,* pp. 72-105 (1982).

[14] M. D. SMOOKE, J. A. MILLER & R. J. KEE, *Determination of adiabatic flames speeds by boundary value methods,* Comb. Sci. Tech., *34,* pp. 79-90 (1983).

[15] R. F. WARMING & F. HYETT, *The modified equation approach to the stability and accuracy analysis of finite-difference methods,* J. Comp. Phys., *14* (2), p. 159 (1974).

[16] F. A. WILLIAMS, *Combustion theory,* second edition, Benjamin Cummings, Menlo Park (1985).