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A Numerical Study of a Premixed Flame on a Slit Burner

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ABSTRACT—A numerical study of a premixed methane/air flame on a 4 mm slit burner is presented. A local grid refinement technique is used to deal with large gradients and curvature of all variables encountered in the flame, keeping the number of grid points within reasonable bounds. The method used here leads to a large reduction in the number of mesh points, compared to global or line-by-line refinement techniques.

The procedure to obtain the initial guess for the detailed model simulation, needed for the Newton-like solution method, is discussed. The method uses the result of a one-step global model simulation of the same geometry and an appropriate one-dimensional detailed model simulation. The method works fine for the computations presented here. The results of the detailed model are compared to those of the one-step global reaction model computation. Furthermore, using a direct photograph of the luminescence, the flame-tip height and the general flame shape of the detailed simulation are verified with the corresponding experimental flame. Although only a qualitative comparison can be made, both the height and the flame shape compare well.

Key Words: Premixed laminar flames, modelling, elementary reactions, reacting flows

INTRODUCTION

The numerical simulation of laminar flames with the use of detailed chemical models has received a widespread interest in the past two decades. The major part of the studies concerns zero- and one-dimensional systems (see e.g. Dixon-Lewis, 1968), where the latter may be subdivided in diffusion- and premixed flame configurations. The modelling of two-dimensional flame configurations with detailed chemical models has come within our grasp only recently (see e.g. Smooke *et al.*, 1992). This is mainly caused by the stiffness that evolves in the equations if detailed chemical models are incorporated in combination with the size of the system in more-dimensional flame modelling. The algorithms used to solve the discretized combustion equations have to take this property into account. The computing time is mainly determined by the quality of the initial guess for the solution and the gridding strategy, although the algorithm, reaction scheme and transport model also are of influence.

In the present work a Newton technique is used to solve the combustion problem (e.g. Smooke, 1983, Dixon-Lewis, 1968). The leading dimension of the resulting Jacobian matrix is roughly proportional to $N_s \times N_p$, where N_s is the number of species and N_p the number of points in the computational mesh. With a given number of species the number of points N_p has to be as small as possible, to keep the storage within reasonable bounds because the storage space of the Jacobian is of the order of $N_s^2 \times N_p$. However, the chemical reactions generally occur only in a small region of the flame

($\mathcal{O}$(0.1 mm) in a premixed flame), thus yielding very small mesh spacings, whereas the complete burner will have a typical length scale as large as $\mathcal{O}$(1 cm). Clearly, this implies the use of a local refinement technique. Here, we use a local refinement technique, which creates meshes that are essentially different from structured tensor meshes used in the studies of most other authors dealing with multi-dimensional flame phenomena (see e.g. Behrendt *et al.*, 1992).

Although the mesh strategy is important, the success of solving the flame equations is closely related to the availability of an appropriate initial guess. Many numerical studies of multi-dimensional flames are, therefore, concerned with diffusion flames (Smooke *et al.*, 1992). A good initial guess for the flow and main species concentrations, in these flames, can be obtained from a single-step reaction model simulation with infinitely fast chemistry (flame-sheet appoximation). Simultaneously, a fairly accurate guess of the flame sheet location is obtained which is then used to construct an appropriate refined mesh. For premixed flames the construction of an accurate initial guess is not so easy. The application of infinitely fast chemistry, for instance, is not possible. In this paper we present a method to obtain an accurate initial guess for premixed flames. In the following section the physical model will be presented. The governing equations are treated and the chemical models are introduced. Furthermore, the numerical method is discussed briefly. The method is used to simulate the cross-section of a stoichiometric premixed methane/air flame on a 4 mm wide slit burner (see Fig. (1)) with a detailed chemical model. The results of this simulation are presented in the third section and compared with one-step chemistry results and experiments. Finally, the results are discussed in the fourth section of this paper.

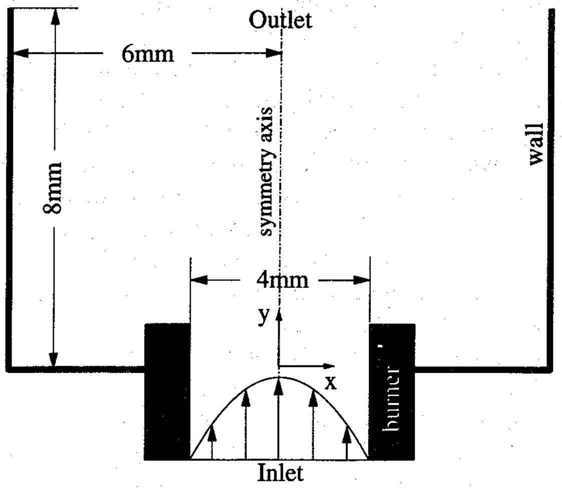

FIGURE 1 Cross-section of the experimental burner geometry. The slit is 4 mm wide, burner wall is 0.8 mm thick and extends over a distance of 1.0 mm in the computational domain.

SYSTEM EQUATIONS

Physical Model

In any application using detailed chemical models it is necessary to model the transport of the many species involved. Here a Fick-like model is used for the diffusive transport (see e.g. Dixon-Lewis, 1968). Furthermore, we are only interested in stationary phenomena thus the species transport equation is written as,

$$\rho\vec{v}\cdot\vec{\nabla}Y_i-\vec{\nabla}\cdot(\rho D_{im}\vec{\nabla}Y_i)=M_i\sum_{j=1}^{N_r}v_{ij}q_j \tag{1}$$

where $\vec{v}=(u,v)$ is the velocity vector, ρ the density of the mixture and D_{im} is the so-called mixture-averaged diffusion coefficient (Kee *et al.*, 1985) computed from the Lewis numbers. The constant Lewis number assumption given by Smooke and Giovangigli (1991) has proven to be very successful in the computation in 1D flames. The symbol $Y_i=\rho_i/\rho$ is introduced for the mass fraction of speciec i in the mixture, with its molar mass M_i. The q_j is the molar reaction rate of the elementary reaction j, N_r is the number of reactions and the v_{ij} symbolize the stoichiometric coefficients.

For isobaric steady flows a similar equation can be derived for the temperature T of the mixture (e.g. Somers, 1994),

$$\rho c_p\vec{v}\cdot\vec{\nabla}T-\vec{\nabla}\cdot(\lambda'\vec{\nabla}T)=-\sum_{i=1}^{N_s}\left(h_iM_i\sum_{j=1}^{N_r}v_{ij}q_j\right)-\sum_{i=1}^{N_s}\rho Y_ic_{p_i}\vec{V}_i\cdot\vec{\nabla}T \tag{2}$$

where the mixture heat capacity is given by $c_p=\sum_{i=1}^{N_s}Y_ic_{p_i}$ and λ' denotes the thermal conductivity of the mixture. The molar enthalpies and specific heat capacities of the species are given by h_i and c_{p_i}, respectively. The last term, which involves a sum over the diffusion velocities $\vec{V}_i$, can be neglected for methane/air flames as shown by e.g. Smooke and Giovangigli (1991) and Somers (1994) for planar flames.

For modelling the flow, various choices for the remaining set of equations are possible. Mainly, these can be subdivided in a primitive variable approach (e.g. Xu and Smooke, 1993) a vorticity/stream function formulation (e.g. de Lange and de Goey, 1993) or mixed approaches, such as vorticity/velocity models (e.g. Gatski *et al.*, 1982, Ern and Smooke, 1993). We use the vorticity/stream function formulation, which has proven to be very appropriate for numerical studies on reactive steady 2D isobaric flows (de Lange and de Goey, 1993). In 2D systems the vorticity vector $(\vec{\omega}\equiv\vec{\nabla}\times\vec{v})$ reduces to a scalar $\omega=\partial v/\partial x-\partial u/\partial y$, which in the absence of external forces (e.g. gravity) obeys a convection-diffusion equation,

$$\rho\vec{v}\cdot\vec{\nabla}\omega-\vec{\nabla}\cdot\eta\vec{\nabla}\omega=-S_\omega \tag{3}$$

where S_ω is given by e.g. Smooke *et al.* (1989) or Somers (1994). The terms associated with partial derivatives of the viscosity in S_ω are neglected for the time being.

The stream function ψ is introduced so that the stationary continuity equation $\vec{\nabla}\cdot(\rho\vec{v})=0$ is satisfied automatically:

$$\frac{\partial\psi}{\partial y}\equiv\rho u \quad\text{and}\quad -\frac{\partial\psi}{\partial x}\equiv\rho v.$$

An equation for the stream function is derived from the definition of the vorticity yielding a Poisson-like equation,

$$\vec{\nabla}\cdot(\rho^{-1}\vec{\nabla}\psi)=-\omega \tag{4}$$

which together with the equation of state

$$P=nRT \tag{5}$$

closes the set of equation. Here, R is the universal gas constant and n the molar density, which is connected to the density by $\rho=n\bar{M}$, $\bar{M}$ being the average molar mass $\bar{M}=(\sum_{i=1}^{N_s}Y_i/M_i)^{-1}$. Finally, for the boundary conditions, the reader is referred to Smooke *et al.* (1989) and Somers (1994).

Chemical Model

We will use a one-step global reaction model,

$$\text{fuel}+\text{oxigen}\rightarrow\text{products}$$

with an Arrhenius-like reaction rate given by

$$q_f=AT^{\alpha+\beta}[Fu]^{\alpha}[Ox]^{\beta}e^{-E_a/RT} \tag{6}$$

to provide a starting estimate for the flame front position, flow and temperature fields. The parameters A, α, β and E_a are fitted to data obtained from flat flame experiments (van Maaren, 1994). This model has been validated on numerous flames recently and works well to predict the global behavior of the flame in a relatively fast way (e.g. de Lange and de Goey, 1993).

For the detailed chemical model simulations we use a so-called skeletal mechanism which consists of 25 reactions among 15 species as presented by Smooke and Giovangigli (1991). This small chemical scheme has shown to perform well for lean ($\varphi\leq 1.0$) atmospheric flames (e.g. Somers, 1994). However, instead of the original rates for the thermal decomposition of methane, modified values for these rate parameters are used as suggested by Smooke and Giovangigli (1991).

Numerical Approach

To deal with the large differences in length scale encountered in premixed flames, an adapted, locally refined mesh is used. The method, developed by de Lange and de Goey (1993), inserts additional mesh points in areas where the 'solution' exhibits large gradients and/or curvature (see Fig. (2) for a typical example). Note that in contrast to tensor refinement methods not a complete line or row of points is added (see e.g. Behrendt *et al.*, 1992, Smooke *et al.*,1992).

A finite-volume method, developed by Thiart (1990) for convection-diffusion type equations, is used to discretize the combustion equations. With some minor adaptations, this scheme can be applied to the Poisson-like Equation (4) as well, giving a unified approach for all differential equations. The discretized equations are put in a residual form,

$$r_{ij}=s_{ij}\Delta x\,\Delta y-(a_{ij}\gamma_{ijs}+b_{ij}\gamma_{ij}+c_{ij}\gamma_{ijN}+d_{ij}\gamma_{ijw}+e_{ij}\gamma_{ijE}) \tag{7}$$

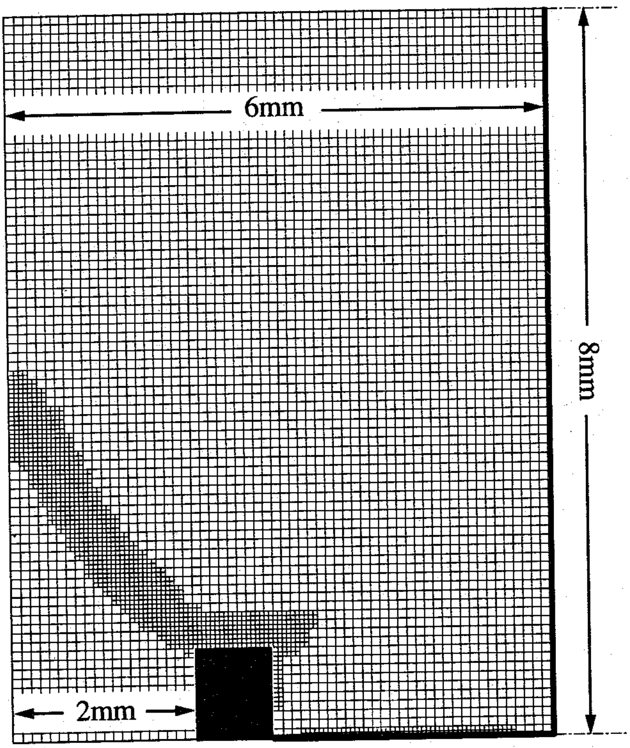

FIGURE 2 The locally refined mesh with one refinement layer.

with s_{ij} the source term at mesh point j and $\Delta x = (x_E - x_W)/2$ and $\Delta y = (y_N - y_S)/2$. All variables are denoted by $y_{ij}(= Y_{ij}, T_j, \omega_j, \psi_j)$. The coefficients $a_{ij} \cdots e_{ij}$ represent the discretization coefficients of the convection-diffusion operator and are specified in (Thiart, 1990). Since the mesh is unstructured, pointers j_k with $(k = E, W, S, N)$ to all four neighbors of the central point j have to be introduced.

Since the discretized equations are non-linear and stiff, we use the often employed Newton-like method, given symbolically by,

$$\mathbf{J}_{(t)} \Delta \vec{y} = -\vec{r}_{(t)} \tag{8}$$

to solve the combustion equations. The $\mathbf{J}$ is the Jacobian-matrix and $\vec{y}$ the vector of unknowns, the subscript $_t$ refers to a "false-transient" approach which is implemented also. If the variables are grouped in a vector per grid point the Jacobian becomes a block tri-diagonal matrix for one-dimensional systems. Then, Equation (8) can be solved with a direct method which does not need much additional storage. A specific block tri-diagonal technique (Fletcher, 1988) equivalent to a block-LU decomposition, or even a regular LU-decomposition (Kee *et al.*, 1985) can be used. For two-dimensional systems a direct method is not feasible, even if structured meshes are used. The bandwidth increases and depending on the discretization used, block penta-, or nona-diagonal matrices evolve. Obviously, an LU-decomposition will lead to fill-in of

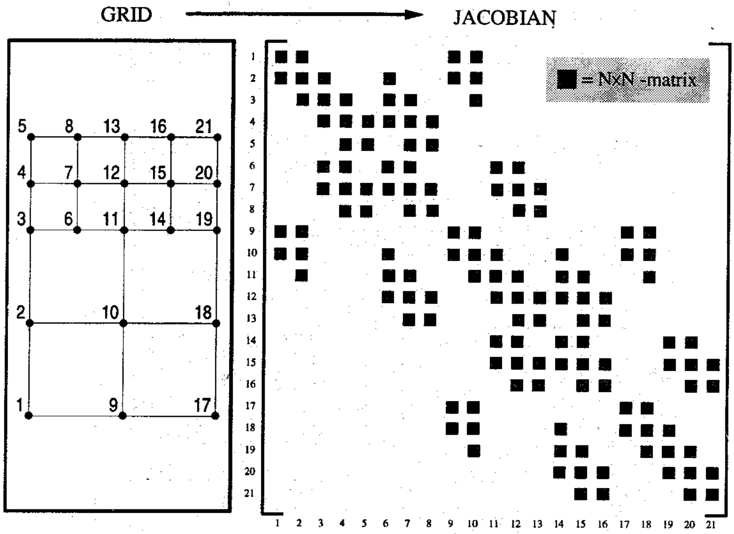

FIGURE 3 Jacobian matrix for a very simple unstructured mesh. The squares symbolize block-matrices ($N \times N$) which contain the inter-variable coupling. N equals the number of physical variables, here equal to $N_s + 3$.

many of the empty diagonals thus leading to large memory requirements due to the increased bandwidth, even for moderately small problems. In our case unstructured block matrices arise as a result of the meshes used (see e.g. Somers, 1994 or Fig. (3) for a typical example) and the bandwidth increases even more. For this reason another approach is used to obtain a solution to the flame problem.

The general structure of the Jacobian consists of a block tri-diagonal matrix (with some 'empty' blocks), as for the one-dimensional flame and irregularly spaced 'off-diagonal' blocks (e.g. see Fig. (3)). If these off-diagonal blocks are discarded, the direct solver developed for the one-dimensional case can be used without any modification. For all resuls presented here this feature is used explicitly to solve the flame problem. To minimize the computation time the Jacobian is kept fixed for several iterations. The numbering direction is switched from x to y or vice versa typically every five sweeps and the solution is updated for several iterations again. This ADI-like approach is used until convergence is reached:

$$C = \max(|r_{ij}|/R) < \varepsilon, \quad \forall (i, j) \in (N_s + 3, N_p). \tag{9}$$

where R is used to scale the residual and ε a given maximum value for the convergence factor C. For R, the maximum value of the source term $|s_{ij}\Delta x \Delta y|$ and the discretized flux term $|a_{ij}Y_{ijS} + b_{ij}Y_{ij} + c_{ij}Y_{ijN} + d_{ij}Y_{ijW} + e_{ij}Y_{ijE}|$ of Equation (7) is taken.

RESULTS

Results of the simulation of a stoichiometric premixed methane/air flame on a 4 mm slit burner are presented in this section. A cross-section of the burner is given in Figure (1).

The inlet conditions are specified by a parabolic velocity profile with a maximum of 1.1 m/s on the symmetry axis. Then the velocity gradient is equal to $1100\,\mathrm{s}^{-1}$ which is much larger than the flash-back gradient of about $400\,\mathrm{s}^{-1}$ and much smaller than $4000\,\mathrm{s}^{-1}$ for the critical blow-off gradient. The fresh stoichiometric methane/air mixture has a uniform temperature of 298 K, equal to the temperature of the walls and burner. During the computation, the temperature of the wall and the burner are kept at their initial value.

The starting estimate for the temperature, the vorticity and stream function for the detailed model simulation is obtained from an unrefined one-step global chemical model solution. For the species concentrations an interpolation of the solution of a one-dimensional burner-stabilized flame is used. This one-dimensional flame is computed with the same average mass-flow rate and equivalence ratio. The composition of the one-dimensional simulation is parameterized using the corresponding temperature, $Y_i(T)$. The temperature of the one-step two-dimensional simulation is used to interpolate this one-dimensional solution on the unrefined mesh. This initial guess is updated for several iterations, until the norm C is reduced to 0.01. Subsequently, the solution is interpolated on the refined mesh and the computation is continued until convergence is reached. For this specific case the number of points increases from 4500 for the unrefined mesh to 5500 for the refined mesh.

In Figure (4) the computed temperature fields of the one-step model simulation and the detailed model simulation are compared. The flow, temperature field and flame shape show remarkable resemblance. However, there are also some clear differences. The temperature gradient of the global model simulation as well as the curvature of the flame front are larger. This may be attributed to the fact that the one-step model yields a higher adiabatic burning velocity than the detailed model ($S_L \approx 42\,\mathrm{cm/s}$ and $S_L \approx 37\,\mathrm{cm/s}$, respctively).

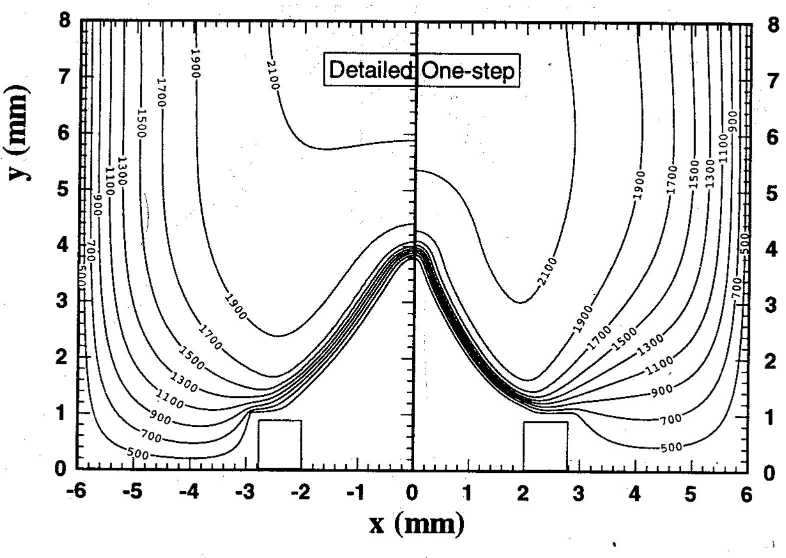

FIGURE 4 Temperature contours of the solution of the detailed chemistry simulation (left) and the solution of the one-step simulation on the same mesh (right).

To determine the effect of the refinement procedure, the temperature fields obtained on the unrefined and refined mesh of the detailed chemical model simulations are compared in Figure (5). The isotherms of the refined computation are smoother near the symmetry axis especially near the tip where the curvature is largest. It should be noted that the differences are not large, which is mainly attributed to the fact that the mesh is adapted to the one-step model results and is fixed during the detailed model simulation for the time being. The grid will be adapted to complex chemistry solution in the future. Therefore, the refined mesh is not optimally adapted to the detailed model simulation. This is illustrated in the false-color plot in Figure (6). As can be seen in the enlarged section, the maxima of the HCO mole fraction are located just outside the refined region. The small peak of HCO near the burner rim edge, is caused by diffusion of C_1-intermediates (CH_3, CH_2O mainly) from the reaction front to the burner rim. Mainly at the edge of the burner rim, these species convert back to CH_4 and HCO causing the small peak observed in Figure (6). Since reaction rates are very small due to the low temperatures, the concentration of HCO is not very high, approximately 20% of the maximum.

Still, the advantages of the local refinement technique are obvious. While the spatial resolution in the reaction layer is doubled in both directions with respect to the unrefined mesh, only 1000 extra mesh points are needed. If the same spatial resolution had to be achieved using a uniformly refined mesh, the number of points would increase dramatically to $N_p \approx 18000 = (4 \times 4500)$. Even if lines or rows of points would be added, the number of points would still increase to $N_p \approx 10000$ which is almost a factor of two larger than $N_p \approx 5500$ found for te locally refined mesh. Note that in this simulation only one refinement layer is added. Without any problems a two or more layer mesh can be used, which increases the spatial resolution even more (de Lange

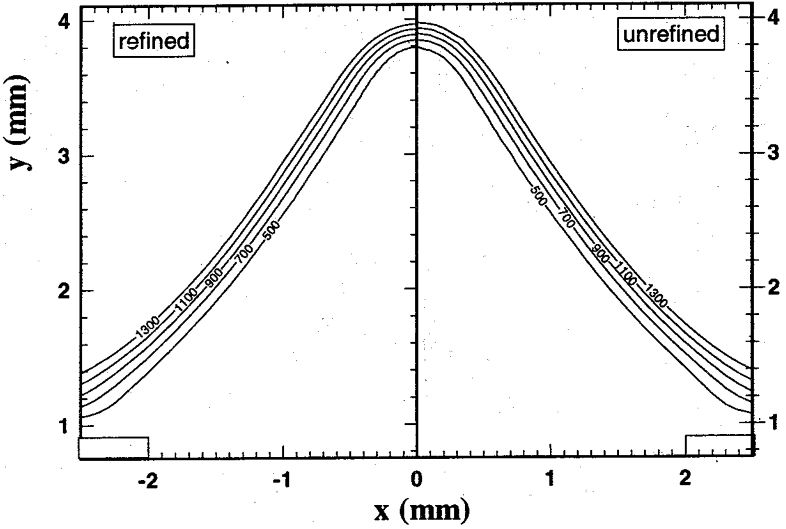

FIGURE 5 Temperature contours for the detailed chemistry calculation. Left part: the solution found on the refined mesh of Figure (2) (≈ 5500 mesh points). Right: solution on the unrefined base mesh (≈ 4500 mesh points).

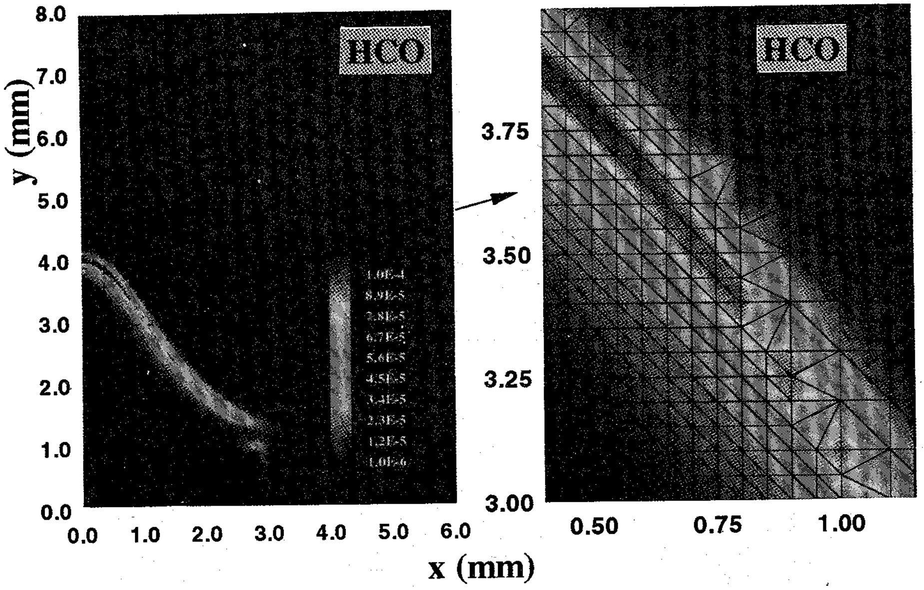

FIGURE 6 False-color plot of the HCO contours on the complete domain. On the right the dashed box is enlarged and the finite element mesh used by the plotting code is shown. Note that this is not the same mesh as the computational mesh given in Figure (2). See COLOR PLATE IV.

and de Goey, 1993), obviously leading to larger differences between the number of points obtained by the different refinement methods.

An attempt has been made to make a comparison with an experimental flame in Figure (7). For that reason a luminescence plot of a cross-section of a flame is compared with the magnitude of the CO to CO_2 conversion reaction, which is believed to be responsible for the faint broad-band luminescence of the flame (Gaydon, 1957; Diatto *et al.*, 1994). Figure (7) shows that both the flame height and the global flame shape compare reasonably well. However, the experimental flame shows a larger curvature, which might indicate that the detailed model used here, yields a burning velocity which is too small. Still, although no quantitative comparison has been made, the resemblance between the photograph and the computation is remarkable. It's worth mentioning that such a direct comparison can not be made from the one-step global model simulation.

DISCUSSION

With the method presented here, we are able to compute two-dimensional premixed flames with detailed chemical models. The problem of obtaining an appropriate initial guess is solved by using a one-step global reaction model. It is found that the initial guess for all chemical components can be obtained from an interpolation of the solution of a one-dimensional simulation with the same equivalence ratio and average

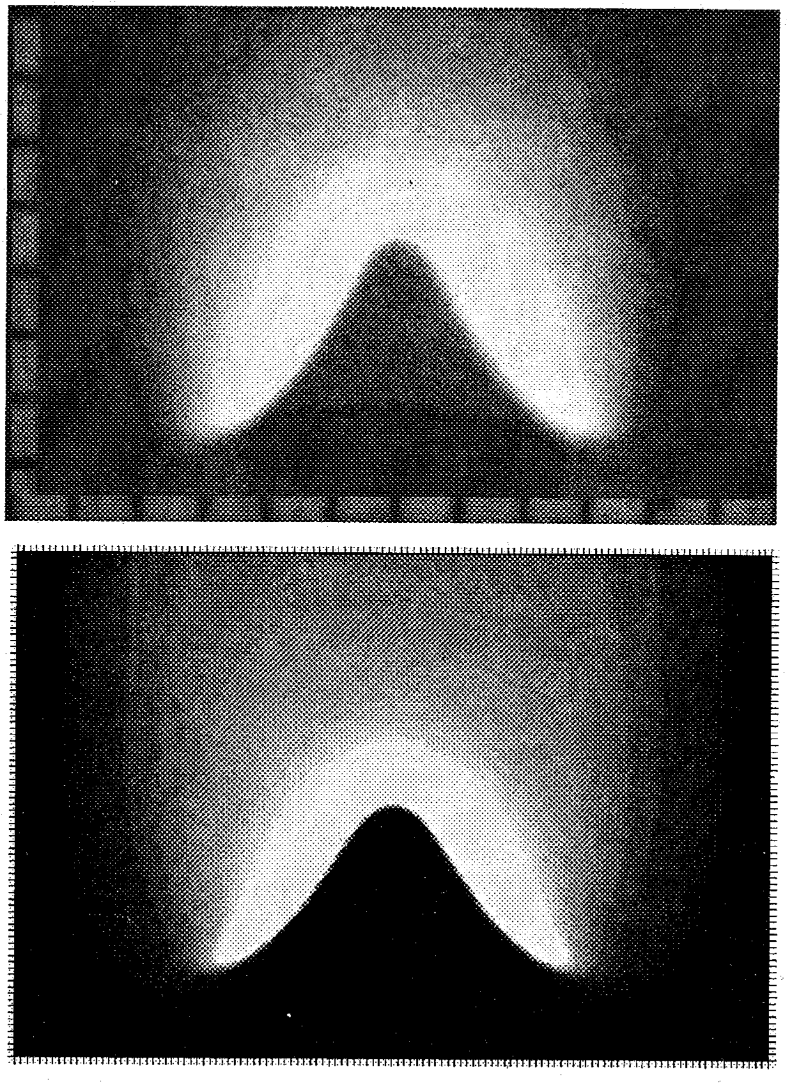

FIGURE 7 Top: Luminescence plot of the experimental flame. Bottom: False color plot of the computed magnitude of the reaction rate of $CO + OH \rightarrow CO_2 + H$. See COLOR PLATE V.

mass-flow rate. The simulation with a locally refined mesh yields good results, which shows the applicability of the approach. Compared to a uniform refinement of the mesh or a tensor refinement technique, significantly less discretization points are needed. A drawback of the local refinement technique is the data structure, which is much more complicated. As a result, the penta- or nona-diagonal structure of the matrix equation is lost as well. However, for the ADI-like approach used here, this fact does not complicate the solution procedure for the Jacobian equations.

The ADI-like approach used here to solve the discretized combustion equations is not optimal yet. After a fast decrease of the initial norm (≈ 0.05 within 1 hour on a MIPS R4400), the global convergence rate slows down. Although, $C \leq 10^{-3}$ near the flame front, there exist randomly scattered areas where $C \approx 10^{-2}$. The fast initial decrease may be due to the fact that the flame moves to its steady-state position which is mainly determined by the chemistry. With our discretization method and data structure, chemical effects are represented by the block matrices on the main diagonal in the Jacobian equations. The ADI method always takes the central block matrix into account in either direction, and thus captures this effect properly. However, the slow final decrease of the norm is caused by small diffusive and convective controlled corrections to the final solution, which are determined by the three diagonal blocks as well as by the 'off-diagonal' blocks. The ADI approach does not treat both directions simultaneously and the solution shows oscillatory convergence.

In the future a Bi-CGSTAB with preconditioning will be implemented to solve the full Jacobian equations. With this method both directions are treated similarly and it is believed that the oscillatory convergence will disappear. The mesh refinement technique will be improved such that the meshes are adapted to the detailed model solution. Furthermore, a more sophisticated measurement techniques (LIF, CARS) will be used to provide data for a more quantitative comparison between computation and measurement.

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