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A Study on Premixed Laminar Flames

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Abstract

This work has been done in the period March–November 2006 as a collaboration between the Department of Computer Science, University of Verona, and the Research & Development Department, Riello Burners, in order to develop a numerical approach for the study of premixed laminar flames.

Keywords: premixed laminar flames, combustion, fluid mechanics, finite differences

Contents

1 Introduction to premixed laminar flames

Combustion may take place in many different forms and circumstances. Depending on the type of flow (laminar or turbulent) and the type of premixing (premixed or not), it is possible to distinguish different flame structures, each of which features its own characteristics. All gaseous combustion processes, however, are based on the same equations, namely the conservation of mass, species mass fraction, momentum and energy.

Many practical combustors, such as burners or internal combustion engines, rely on premixed flame propagation. Moreover, burner-stabilized laminar premixed flames are very often used to study chemical kinetics in a combustion environment. Such flames are effectively one dimensional and can be made very steady, thus facilitating detailed experimental measurements of temperature and species profiles. Also, laminar flame speed is often used to characterize the combustion of various fuel-oxidizer combinations. Therefore, the ability to model chemical kinetics and transport processes in these flames is critical to interpreting flame experiments and to understanding the combustion process itself.

Among the gaseous flames (premixed or non-premixed, laminar or turbulent), here we concentrate on premixed laminar flames only.

Several laminar flame theories have been proposed in the past, starting from the end of the nineteenth century [4], with the objective of determining the fundamental flame attributes. These theories have been based on the degree of realism associated with their assumptions and are carefully described by classical textbooks [3, 8, 1].

2 Governing equations

We consider a steady, two-dimensional, premixed laminar flame governed by the following set of partial differential equations

$$(\rho u)_x + (\rho v)_y = 0 \tag{1}$$

$$(\rho uu)_x + (\rho uv)_y = -\overline{R}(\rho T)_x \tag{2}$$

$$(\rho uv)_x + (\rho vv)_y = -\overline{R}(\rho T)_y \tag{3}$$

$$(\rho(u+u_k)Y_k)_x + (\rho(v+v_k)Y_k)_y = Ae^{-\frac{E}{RT}} \tag{4}$$

$$u_k Y_k = -D_k (Y_k)_x \tag{5}$$

$$v_k Y_k = -D_k (Y_k)_y \tag{6}$$

$$c_p((\rho u T)_x + (\rho v T)_y) - \lambda(T_{xx} + T_{yy}) + \rho \sum_{k=1}^{K} Y_k c_{p_k}(u_k T_x + v_k T_y) = -\sum_{k=1}^{K} h_k A e^{-\frac{E}{\overline{R}T}} \tag{7}$$

where symbols denote the following quantities

- x spatial coordinate
- y spatial coordinate
- ρ density of fluid mixture
- u x-component of the fluid mixture velocity field $\mathbf{U}$
- v y-component of the fluid mixture velocity field $\mathbf{U}$
- T temperature of fluid mixture
- $\overline{R}$ normalized gas mixture constant $\overline{R} = \dfrac{R}{W}$ with
- R universal gas constant
- W mean molecular weight of the mixture
- u_k x-component of the diffusion velocity field $\mathbf{V}_k$ of k-th species
- v_k y-component of the diffusion velocity field $\mathbf{V}_k$ of k-th species
- Y_k mass fraction of the k-th species
- A reaction factor in the Arrhenius expression
- E activation energy in the Arrhenius expression
- D_k diffusion coefficient of the k-th species
- c_p specific heat of gas mixture at constant pressure
- c_{p_k} specific heat of the k-th species at constant pressure
- λ thermal conductivity of the gas mixture

h_k specific enthalpy coefficient of the k-th species

K total number of species

k species index

It should be noted that pressure does not appear in the equations because it has been replaced by employing the state equation for the mixture, $p = \rho\overline{R}T$. The number of unknowns, therefore, reduces to $4 + K \times 3$, where the three unknowns that depend on the k-th species are u_k, v_k and Y_k. On the other hand, the number of equations are $4+K\times 3$, where the three equations that depend on the k-th species are (4) (5) and (6).

3 Discretization

Second-order, centered, uneven finite differences are employed in the fashion shown in figure 1.

In order to avoid the typical problems of Navier-Stokes equations when finite differences are used, a staggered grid in both x and y is introduced (cf. [6, 5]). More specifically, density ρ, temperature T and mass fraction of the k-th species Y_k are known at the grid points ($\bullet$), x-velocity components u and u_k are known at the "staggered" points in x ($\times$), and y-velocity components v and v_k are known at the "staggered" points in y ($\Box$).

Equations are collocated accordingly. Continuity (1), production of k-th species (4) and energy (7) equations are satisfied at the grid points ($\bullet$), x-momentum (2) and x-Fick-law (5) equations are satisfied at the "staggered" points in x ($\times$), and y-momentum (3) and x-Fick-law (6) equations are satisfied at the "staggered" points in y ($\Box$).

By doing so, the following residue is obtained (in vector notation).

$$\mathbf{h}(\mathbf{u}) = 0 \tag{8}$$

with

$$\mathbf{u} = \left\{ \begin{array}{c} \vdots \\ \rho_l \\ T_l \\ u_l \\ v_l \\ u_{kl} \\ v_{kl} \\ Y_{kl} \\ \vdots \end{array} \right\}, \quad l = i + J(j-1), \quad i = 1\dots I, \quad j = 1\dots J. \tag{9}$$

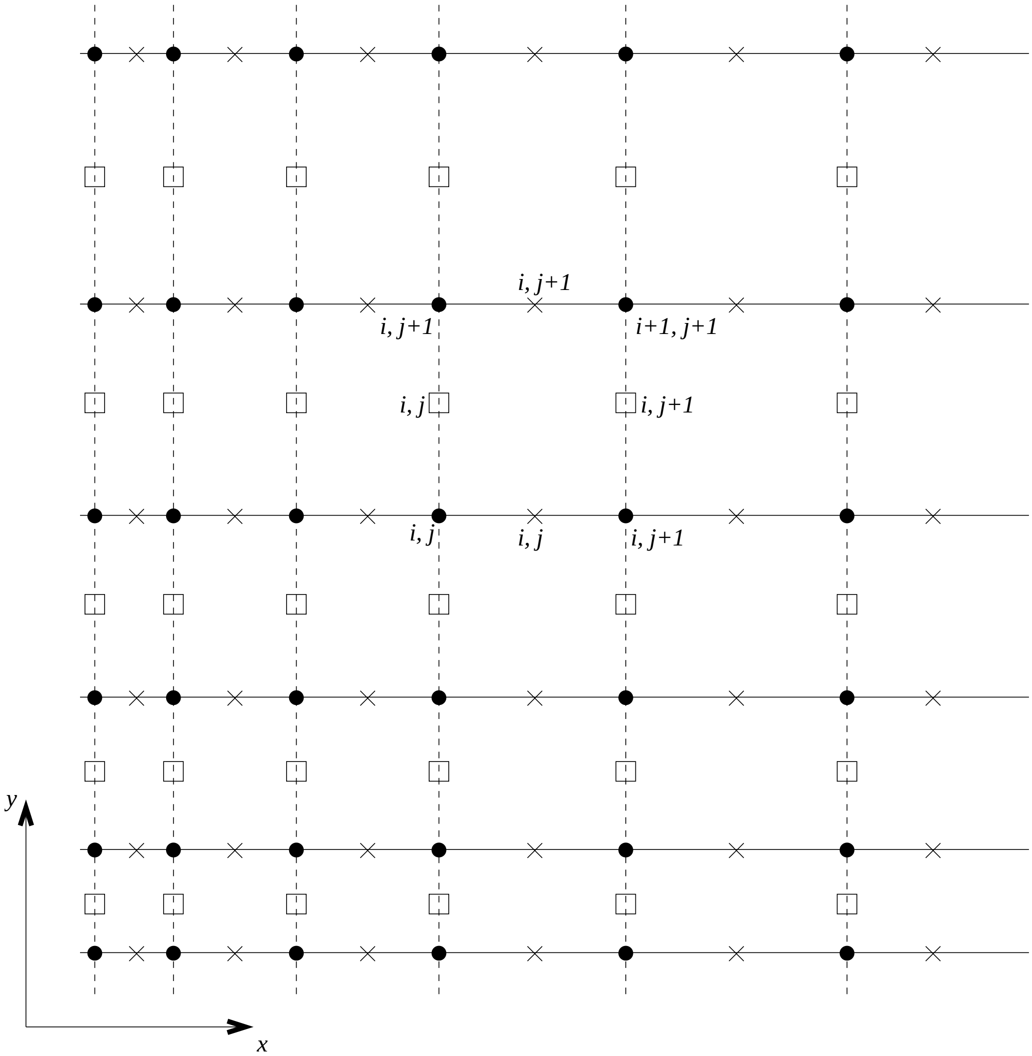

Figure 1: Finite difference discretization on staggered grid. Density ρ, temperature T and mass fraction of the k-th species Y_k are known at the grid points ($\bullet$); x-velocity components u and u_k are known at the "staggered" points in x ($\times$); y-velocity components v and v_k are known at the "staggered" points in y ($\square$).

4 Linearization

System (8) is clearly nonlinear in the unknowns $[\rho_l, T_l, u_l, v_l, u_{kl}, v_{kl}, Y_{kl}]$. Different choices are available to linearize and eventually solve it numerically. Here we prefer to employ Newton's method, i.e.

$$\mathbf{h}(\mathbf{u}) = \mathbf{h}(\bar{\mathbf{u}}) + \boldsymbol{J}(\bar{\mathbf{u}})(\mathbf{u} - \bar{\mathbf{u}}) = \bar{\mathbf{h}} + \overline{\boldsymbol{J}}(\mathbf{u} - \bar{\mathbf{u}}) = 0$$

or

$$\mathbf{u} = \bar{\mathbf{u}} - [\overline{\boldsymbol{J}}]^{-1}\bar{\mathbf{h}}, \tag{10}$$

where $\overline{\boldsymbol{J}} = \boldsymbol{J}(\bar{\mathbf{u}})$ denotes the Jacobian $\boldsymbol{J}$, computed in $\bar{\mathbf{u}}$.

The Jacobian is evaluated analytically, but alternatively it could have been computed numerically using the definition of derivative.

5 Steady solution of a time-dependent problem

The main drawback of Newton's method (10) is the strong dependence of its success on the initial guess. The differential problem is governed by partial differential equations supplemented by boundary conditions. Therefore, the initial guess is arbitrary and the algorithm might never converge if the initial guess is very far from the solution.

This weakness can be overcome by replacing the steady system (8) with a fake time-dependent, initial-value problem in the form

$$\begin{cases} \epsilon \dfrac{\partial \mathbf{u}}{\partial t} + \mathbf{h}(\mathbf{u}) = 0 \\ \\ \mathbf{u}(0) = \mathbf{u}_0 \end{cases} \tag{11}$$

where ϵ is a parameter that controls the "steadiness" of the problem. The solution of (8) is then

$$\mathbf{u} = \lim_{t\to\infty} \mathbf{u}(t).$$

If $\epsilon = 0$ the original system is retrieved, while $\epsilon > 0$ allows the solution to be rather independent of the initial condition $\mathbf{u}_0$. It goes without saying that problem (11) might require a long time t to reach the steady solution that satisfies the steady problem (8) ($t \to \infty$). However, convergence can be accelerated by increasing ϵ at the expense of a possible failure of Newton's method.

For the solution of problem (11) implicit second-order finite differences (backward differentiation formulas – BDF methods [2]) are used.

6 Linear-system solver

The linear system to be solved in the Newton iterative algorithm has some band structure but is clearly very *sparse* (that is, the number of nonzero elements of the matrix of dimension n is $\mathcal{O}(n)$ instead of $\mathcal{O}(n^2)$) due to the use of finite differences in two dimensions. Therefore, we used the matrix CSR (Compressed Storage Row) format, which requires one double array and one integer array of length equal to the number of non-zero elements and one integer array of length equal to the dimension of the system.

Being the LU decomposition not affordable in such conditions, we preferred to used a semi-iterative solver for (nonsymmetric) sparse matrices, namely the BiCGStab (BiConiugate Gradient Stabilized [9]) method preconditioned by ILU(0) (Incomplete LU factorization with no fill-in), already tailored to CSR format.

6.1 CSR format

We show with an example the CSR format and the matrix-vector product (required in the BiCGStab solver) in such a format. Given the matrix

$$A = \begin{pmatrix} 1.0 & -2.0 & 0 \\ 1.0 & -2.0 & 1.0 \\ 0 & 1.0 & -2.0 \end{pmatrix}$$

the CSR format is

$$\begin{aligned} \texttt{sysmat} &= \begin{bmatrix} 1.0 & -2.0 & 1.0 & -2.0 & 1.0 & 1.0 & -2.0 \end{bmatrix} \\ \texttt{ja} &= \begin{bmatrix} 1 & 2 & 1 & 2 & 3 & 2 & 3 \end{bmatrix} \\ \texttt{ia} &= \begin{bmatrix} 1 & 3 & 6 & 8 \end{bmatrix} \end{aligned}$$

Given the matrix A and a vector x, the matrix-vector product $y = Ax$ is performed by the algorithm reported in Table 1.

```
do i=1,n
   i1=ia(i)
   i2=ia(i+1)-1
   y(i)=0.0
   do j=i1,i2
      y(i)=y(i)+sysmat(j)*x(ja(j))
   end do
end do
```

Table 1: Matrix-vector product in CSR format.

7 Discrete equations

By employing the discretization introduced in §3, one gets
Continuity:

$$
\begin{aligned}
&\frac{2}{x_{i+1,j}-x_{i-1,j}}\left[\frac{\rho_{i+1,j}+\rho_{i,j}}{2}u_{i,j}-\frac{\rho_{i,j}+\rho_{i-1,j}}{2}u_{i-1,j}\right]+\\
&\frac{2}{y_{i,j+1}-y_{i,j-1}}\left[\frac{\rho_{i,j+1}+\rho_{i,j}}{2}v_{i,j}-\frac{\rho_{i,j}+\rho_{i,j-1}}{2}v_{i,j-1}\right]=0
\end{aligned}
\tag{12}
$$

x-momentum:

$$
\begin{aligned}
&\frac{1}{x_{i+1,j}-x_{i,j}}\left[\rho_{i+1,j}\left(\frac{u_{i+1,j}+u_{i,j}}{2}\right)^2-\rho_{i,j}\left(\frac{u_{i,j}+u_{i-1,j}}{2}\right)^2\right]+\\
&\frac{2}{y_{i,j+1}-y_{i,j-1}}\left[\left(\frac{\rho_{i,j}+\rho_{i+1,j}+\rho_{i+1,j+1}+\rho_{i,j+1}}{4}\right)\left(\frac{u_{i,j}+u_{i,j+1}}{2}\right)\left(\frac{v_{i,j}+v_{i+1,j}}{2}\right)-\right.\\
&\qquad\left.\left(\frac{\rho_{i,j-1}+\rho_{i+1,j-1}+\rho_{i+1,j}+\rho_{i,j}}{4}\right)\left(\frac{u_{i,j-1}+u_{i,j}}{2}\right)\left(\frac{v_{i,j-1}+v_{i+1,j-1}}{2}\right)\right]=\\
&\qquad-\overline{R}\frac{\rho_{i+1,j}T_{i+1,j}-\rho_{i,j}T_{i,j}}{x_{i+1,j}-x_{i,j}}
\end{aligned}
\tag{13}
$$

y-momentum:

$$
\begin{aligned}
&\frac{2}{x_{i+1,j}-x_{i-1,j}}\left[\left(\frac{\rho_{i,j}+\rho_{i+1,j}+\rho_{i+1,j+1}+\rho_{i,j+1}}{4}\right)\left(\frac{u_{i,j}+u_{i,j+1}}{2}\right)\left(\frac{v_{i,j}+v_{i+1,j}}{2}\right)-\right.\\
&\qquad\left.\left(\frac{\rho_{i-1,j}+\rho_{i,j}+\rho_{i,j+1}+\rho_{i-1,j+1}}{4}\right)\left(\frac{u_{i-1,j}+u_{i-1,j+1}}{2}\right)\left(\frac{v_{i-1,j}+v_{i,j}}{2}\right)\right]+\\
&\frac{1}{y_{i,j+1}-y_{i,j}}\left[\rho_{i,j+1}\left(\frac{v_{i,j+1}+v_{i,j}}{2}\right)^2-\rho_{i,j}\left(\frac{v_{i,j}+v_{i,j-1}}{2}\right)^2\right]=\\
&-\overline{R}\frac{\rho_{i,j+1}T_{i,j+1}-\rho_{i,j}T_{i,j}}{y_{i,j+1}-y_{i,j}}
\end{aligned}
\tag{14}
$$

production of k-th species:

$$\frac{2}{x_{i+1,j}-x_{i-1,j}}\left[\frac{\rho_{i+1,j}Y^k_{i+1,j}+\rho_{i,j}Y^k_{i,j}}{2}(u_{i,j}+u^k_{i,j})-\frac{\rho_{i,j}Y^k_{i,j}+\rho_{i-1,j}Y^k_{i-1,j}}{2}(u_{i-1,j}+u^k_{i-1,j})\right]+$$

$$\frac{2}{y_{i,j+1}-y_{i,j-1}}\left[\frac{\rho_{i,j+1}Y^k_{i,j+1}+\rho_{i,j}Y^k_{i,j}}{2}(v_{i,j}+v^k_{i,j})-\frac{\rho_{i,j}Y^k_{i,j}+\rho_{i,j-1}Y^k_{i,j-1}}{2}(v_{i,j-1}+v^k_{i,j-1})\right]=$$

$$Ae^{-\frac{E}{RT_{i,j}}} \tag{15}$$

x-Fick-law for the k-th species:

$$u^k_{i,j}\frac{Y^k_{i,j}+Y^k_{i+1,j}}{2}=-D_k\frac{Y^k_{i+1,j}-Y^k_{i,j}}{x_{i+1,j}-x_{i,j}} \tag{16}$$

y-Fick-law for the k-th species:

$$v^k_{i,j}\frac{Y^k_{i,j}+Y^k_{i,j+1}}{2}=-D_k\frac{Y^k_{i,j+1}-Y^k_{i,j}}{y_{i,j+1}-y_{i,j}} \tag{17}$$

Energy equation:

$$\frac{2c_p}{x_{i+1,j}-x_{i-1,j}}\left[\frac{\rho_{i+1,j}T_{i+1,j}+\rho_{i,j}T_{i,j}}{2}u_{i,j}-\frac{\rho_{i,j}T_{i,j}+\rho_{i-1,j}T_{i-1,j}}{2}u_{i-1,j}\right]+$$

$$\frac{2c_p}{y_{i,j+1}-y_{i,j-1}}\left[\frac{\rho_{i,j+1}T_{i,j+1}+\rho_{i,j}T_{i,j}}{2}v_{i,j}-\frac{\rho_{i,j}T_{i,j}+\rho_{i,j-1}T_{i,j-1}}{2}v_{i,j-1}\right]+$$

$$-\lambda\left[\frac{2}{x_{i+1,j}-x_{i-1,j}}\left(\frac{T_{i+1,j}-T_{i,j}}{x_{i+1,j}-x_{i,j}}-\frac{T_{i,j}-T_{i-1,j}}{x_{i,j}-x_{i-1,j}}\right)\right]+$$

$$-\lambda\left[\frac{2}{y_{i,j+1}-y_{i,j-1}}\left(\frac{T_{i,j+1}-T_{i,j}}{x_{i,j+1}-x_{i,j}}-\frac{T_{i,j}-T_{i,j-1}}{x_{i,j}-x_{i,j-1}}\right)\right]+$$

$$\rho_{i,j}\sum_{k=1}^{K}Y^k_{i,j}c_{p_k}\left[\left(\frac{u^k_{i-1,j}+u^k_{i,j}}{2}\right)\left(\frac{T_{i+1,j}-T_{i-1,j}}{x_{i+1,j}-x_{i-1,j}}\right)+\left(\frac{v^k_{i,j-1}+v^k_{i,j}}{2}\right)\left(\frac{T_{i,j+1}-T_{i,j-1}}{y_{i,j+1}-y_{i,j-1}}\right)\right]=$$

$$-\sum_{k=1}^{K}h_kAe^{-\frac{E}{RT_{i,j}}} \tag{18}$$

By introducing the following quantities,

$$D^1_{x0}=\frac{1}{x_{i+1}-x_{i-1}};\qquad D^1_{x\mathrm{f}}=\frac{1}{x_{i+1}-x_i};\qquad D^1_{x\mathrm{b}}=\frac{1}{x_i-x_{i-1}};$$

$$D^1_{y0} = \frac{1}{y_{j+1} - y_{j-1}}; \qquad D^1_{y\mathrm{f}} = \frac{1}{y_{j+1} - y_j}; \qquad D^1_{y\mathrm{b}} = \frac{1}{y_j - y_{j-1}};$$
$$D^2_{x0} = -2D^1_{x0}\left(D^1_{x\mathrm{f}} + D^1_{x\mathrm{b}}\right); \qquad D^2_{x\mathrm{f}} = 2D^1_{x0}D^1_{x\mathrm{f}}; \qquad D^2_{x\mathrm{b}} = 2D^1_{x0}D^1_{x\mathrm{b}};$$

the Jacobian can be written as

$$\begin{aligned} &D^1_{x0}\left[(\rho_{i+1,j} + \rho_{i,j})u_{i,j} - (\rho_{i,j} + \rho_{i-1,j})u_{i-1,j}\right] + \\ &D^1_{y0}\left[(\rho_{i,j+1} + \rho_{i,j})v_{i,j} - (\rho_{i,j} + \rho_{i,j-1})v_{i,j-1}\right] = 0 \end{aligned} \tag{19}$$

x-momentum:

$$\begin{aligned} &D^1_{x\mathrm{f}}\left[\rho_{i+1,j}\left(\frac{u_{i+1,j} + u_{i,j}}{2}\right)^2 - \rho_{i,j}\left(\frac{u_{i,j} + u_{i-1,j}}{2}\right)^2\right] + \\ &D^1_{y0}\left[\left(\frac{\rho_{i,j} + \rho_{i+1,j} + \rho_{i+1,j+1} + \rho_{i,j+1}}{2}\right)\left(\frac{u_{i,j} + u_{i,j+1}}{2}\right)\left(\frac{v_{i,j} + v_{i+1,j}}{2}\right) - \right. \\ &\quad \left.\left(\frac{\rho_{i,j-1} + \rho_{i+1,j-1} + \rho_{i+1,j} + \rho_{i,j}}{2}\right)\left(\frac{u_{i,j-1} + u_{i,j}}{2}\right)\left(\frac{v_{i,j-1} + v_{i+1,j-1}}{2}\right)\right] + \\ &\quad \overline{R}D^1_{x\mathrm{f}}(\rho_{i+1,j}T_{i+1,j} - \rho_{i,j}T_{i,j}) = 0 \end{aligned} \tag{20}$$

y-momentum:

$$\begin{aligned} &D^1_{x0}\left[\left(\frac{\rho_{i,j} + \rho_{i+1,j} + \rho_{i+1,j+1} + \rho_{i,j+1}}{2}\right)\left(\frac{u_{i,j} + u_{i,j+1}}{2}\right)\left(\frac{v_{i,j} + v_{i+1,j}}{2}\right) - \right. \\ &\quad \left.\left(\frac{\rho_{i-1,j} + \rho_{i,j} + \rho_{i,j+1} + \rho_{i-1,j+1}}{2}\right)\left(\frac{u_{i-1,j} + u_{i-1,j+1}}{2}\right)\left(\frac{v_{i-1,j} + v_{i,j}}{2}\right)\right] + \\ &D^1_{y\mathrm{f}}\left[\rho_{i,j+1}\left(\frac{v_{i,j+1} + v_{i,j}}{2}\right)^2 - \rho_{i,j}\left(\frac{v_{i,j} + v_{i,j-1}}{2}\right)^2\right] = \\ &-\overline{R}D^1_{y\mathrm{f}}(\rho_{i,j+1}T_{i,j+1} - \rho_{i,j}T_{i,j}) \end{aligned} \tag{21}$$

production of k-th species:

$$\begin{aligned} &D^1_{x0}\left[(\rho_{i+1,j}Y^k_{i+1,j} + \rho_{i,j}Y^k_{i,j})(u_{i,j} + u^k_{i,j}) - (\rho_{i,j}Y^k_{i,j} + \rho_{i-1,j}Y^k_{i-1,j})(u_{i-1,j} + u^k_{i-1,j})\right] + \\ &D^1_{y0}\left[(\rho_{i,j+1}Y^k_{i,j+1} + \rho_{i,j}Y^k_{i,j})(v_{i,j} + v^k_{i,j}) - (\rho_{i,j}Y^k_{i,j} + \rho_{i,j-1}Y^k_{i,j-1})(v_{i,j-1} + v^k_{i,j-1})\right] = \\ &Ae^{-\frac{E}{RT_{i,j}}} \end{aligned} \tag{22}$$

x-Fick-law for the k-th species:

$$u^k_{i,j}(Y^k_{i,j} + Y^k_{i+1,j}) = -2D^1_{x\mathrm{f}} D_k (Y^k_{i+1,j} - Y^k_{i,j}) \tag{23}$$

y-Fick-law for the k-th species:

$$v^k_{i,j}(Y^k_{i,j} + Y^k_{i,j+1}) = -2D^1_{y\mathrm{f}} D_k (Y^k_{i,j+1} - Y^k_{i,j}) \tag{24}$$

Energy equation:

$$\begin{aligned}
&c_p D^1_{x0}\left[(\rho_{i+1,j}T_{i+1,j} + \rho_{i,j}T_{i,j})u_{i,j} - (\rho_{i,j}T_{i,j} + \rho_{i-1,j}T_{i-1,j})u_{i-1,j}\right] + \\
&c_p D^1_{y0}\left[(\rho_{i,j+1}T_{i,j+1} + \rho_{i,j}T_{i,j})v_{i,j} - (\rho_{i,j}T_{i,j} + \rho_{i,j-1}T_{i,j-1})v_{i,j-1}\right] + \\
&-\lambda\left[D^2_{x\mathrm{f}}T_{i+1,j} + D^2_{x\mathrm{b}}T_{i-1,j} + D^2_{y\mathrm{f}}T_{i,j+1} + D^2_{y\mathrm{b}}T_{i,j-1} + (D^2_{x0} + D^2_{y0})T_{i,j}\right] + \\
&\rho_{i,j}\sum_{k=1}^{K} Y^k_{i,j} c_{p_k}\left[D^2_{x0}\left(\frac{u^k_{i-1,j} + u^k_{i,j}}{2}\right)(T_{i+1,j} - T_{i-1,j}) + \right. \\
&\left. D^2_{y0}\left(\frac{v^k_{i,j-1} + v^k_{i,j}}{2}\right)(T_{i,j+1} - T_{i,j-1})\right] = \\
&-\sum_{k=1}^{K} h_k A e^{-\frac{E}{RT_{i,j}}}
\end{aligned} \tag{25}$$

8 Implementation and attempts

We first concentrated on a one-reaction system based on

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

where the reacting mixture is made of CH_4 and air and the product H_2O of the reaction is first neglected.

After several attempts it was recognized that the discretized equations derived in §7 lead to a ill-conditioned matrix system. Other staggered grids were employed but it was not possible to improve the numerical convergence of the scheme.

In order to reduce the problems due to the nature of the Euler equations, the full compressible Navier-Stokes equations were solved using finite differences. This made the code much more complex and, unfortunately, did not solve completely the convergence problems.

Therefore, it was decided to follow a different approach by reconsidering the model and simplifying the governing equations. First of all, the number of equations was reduced by noting that equations (5) and (6) can easily be substituted into equations (4) and (7), where they are actually needed. The number of equations and unknowns thus dropped from $4 + K \times 3$ to $4 + K$, K being the total number of species. The next attempt was to neglect the pressure gradient in the x- and y-momentum equations, which is reasonable because it is mainly a recirculation flow. However, numerical difficulties were encountered also in this case.

It was then decided to further simplify the model to a 2-dimensional flow where the velocity field was assigned analytically. In fact, the similarity solution of a 2D jet is known [7]. This led to the solution of the numerical difficulties but to unreasonable temperature profiles (constant).

The model was further simplified to a one-dimensional system of equations. The continuity equation reduced to $(\rho u)_x = 0 \Rightarrow \rho u = \rho_0 u_0$, where the subscript $_0$ denotes the values at the burner. The x-momentum equation was replaced by $u(x)$ where x is the distance from the jet exit so that u decades as $x^{-1/3}$. The energy equation was simplified too and the following form was employed: $c_p \rho u T_x - \lambda T_{xx} + (E_1 A_1 + E_2 A_2) e^{-E/(R*T)} = 0$. It is clear that Y_k is not present in this equation and therefore the energy equation is completely decoupled from the others.

However, since $E/R = 2.4358E + 04$, the energy equation practically reduces to $AT_x + BT_{xx} = 0$. If the temperature at the burner (T_0) and far away from it (T_∞) are the same, the trivial solution $T = T_0 = T_\infty$ is found. On the other hand, if $T_0 \neq T_\infty$, the solution oscillates due to the fact that $A >> B$ (because of the constants employed) and thus the effect of T_x prevails on the effect of T_{xx}.

Another problem found with this simple 1D model was that, since $\rho u =$ const and $u_\infty \to 0$ then $\rho_\infty \to \infty$.

9 Suggestions for future work

Based on the problems experienced so far, possible future developments are as follows.

- To restart from scratch by reconsidering the model employed for the description of the phenomenon. The natural evolution should be from a one-dimensional model to its extension to a two-dimensional case.

- Improvement of the chemistry. Maybe not enought species are used and the combustion is not properly (physically and realistically) developed.

- To try to overcome the numerical difficultied of the general formulation by using forward or backward (non-centered) finite differences.

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