Finite Element Method Applied to the Solution of a Convective-Diffusive-Reactive Flow

Pedro H. Konzen, **Álvaro L. De Bortoli**, **Mark Thompson**,
Programa de Pós-Graduação em Matemática Aplicada, IM, UFRGS,
Av. Bento Gonçalves, 9500 - P.O. Box 15080 - Agronomia
91509-900 Porto Alegre - RS - BRASIL
E-mail: pedro.konzen@ufrgs.br

1. Introduction

The process of combustion appears in many practical situations in several industrial branches like in the automotive and the aeronautic industries. The need to decrease fuel consumption and pollutants due to this process have made the study of combustion models an increasingly active scientific research area.

The combustion phenomenon can be characterized by a high and irreversible heat release process with a non-linear reaction rate. The study of this phenomenon requires a description of the chemical reaction schemes (pollutants and combustion products yielding ignition, flame stability, etc.), chemical species mass transfer (by diffusion, convection and turbulent transport, etc.), heat transfer and the description of the flow field [11]; therefore, this process involves a multidisciplinary study.

Analytic solutions for combustion are known for only a few simple models. In order to overcome this difficulty several numerical methods have been proposed and considerable advances have been made [11]. However, the numerical simulation of more complex combustion models remains a great challenge. The numerical models have to deal with high gradients of temperature, species mass fraction and velocity fields. Moreover, the chemical scales of length and time as well as the species mass fractions can differ by many orders of magnitude.

The Finite Element Method (FEM) has been successfuly developed to solve transient flows and has gained significant popularity. This increasing popularity can be justified by the mathematical tools developed to analyze the FEM. This mathematical basis permits one to estimate local and global errors, convergence and stability of several problems [5, 6, 13].

In this work we present a numerical study of a set of reacting Navier-Stokes equations. The model describes the molecular mixture and the reaction-diffusion of two chemical species (fuel and oxidizer) yielding a product. The chemical scheme is supposed to be a single-step, irreversible, exothermic Arrhenius type reaction of a incompressible fluid [2]. The time integration follows the explicit Runge-Kutta three-stage scheme for second order time approximation. The FEM is used to the spacial discretization with triangular elements. A first order local error estimate is obtained for the aproximation of the exact solution of the problem by the FEM.

2. Governing Equations

The set of non-linear governing equations which describes a single-step, binary, irreversible, exothermic reaction between two species F and O to yield a product P as

$$v_f[F] + v_o[O] \Rightarrow v_p[P] + heat$$

can be expressed such as follows [2, 4, 11]. The governing equations for momentum and mass for an incompressible Newtonian fluid are expressed by the two-dimensional Navier-Stokes equations in the stream function-vorticity formulation as

$$\frac{\partial \omega}{\partial t} + \mathbf{u}\cdot\nabla\omega = \frac{1}{Re}\Delta\omega, \tag{1}$$

$$\Delta\psi = \omega, \tag{2}$$

where Re is the nondimensional Reynolds number, ψ and ω are the associated stream function and vorticity, respectively, related to the velocity $\mathbf{u}$ by

$$\mathbf{u} = \left(-\frac{\partial\psi}{\partial x_2}, \frac{\partial\psi}{\partial x_1}\right), \quad \omega = \frac{\partial u_2}{\partial x_1} - \frac{\partial u_1}{\partial x_2}.$$

The overall reaction rate is described by the Arrhenius kinetics law of the form

$$\dot{w} = K\ e^{-Ze/T},$$

where K is the frequency factor, Ze the non-dimensional Zel'dovich's number and T the absolute temperature. The diffusion-reaction equations for the mass fractions C_k of each of the species $k = \{F, O, P\}$, and the temperature T are given by

$$\frac{\partial C_k}{\partial t} + \mathbf{u}\cdot\nabla C_k - \frac{1}{ReSc_k}\Delta C_k = \mp v_k Da C_F C_O\ e^{-Ze/T} \quad (3)$$

$$\frac{\partial T}{\partial t} + \mathbf{u}\cdot\nabla T - \frac{1}{RePr}\Delta T = v_P HeDa C_F C_O\ e^{-Ze/T} \quad (4)$$

where v_k and Sc_k are the molar stoichiometric coefficients and the Schmidt number, respectively, for $k = \{F, O, P\}$. Da and Pr are the Damköhler and the Prandtl non-dimensional numbers, respectively, and He is the heat release parameter. The minus sign in equation (3) is used to $k \in \{F, O\}$ and the plus sign to $k \in \{P\}$.

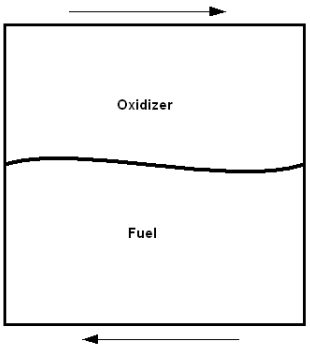

Figure 1: Initial condition: a two-sided lid-driven cavity flow.

2.1 Boundary Conditions

We formulated the problem as a driven cavity flow (see Figure 1). The non-slip boundary conditions associated to equations (1)-(4) are taken to be

$$\psi = 0, \qquad \frac{\partial \psi}{\partial \eta} = 0,$$

$$\frac{\partial C_k}{\partial \eta}, = 0 \quad k \in \{F, O, P\}, \qquad \frac{\partial T}{\partial \eta} = 0,$$

where η is the unit outer normal to the frontiers.

3. Local error estimate

In this section, we show a local error estimate for the approximation of the exact solution of (1)-(4) by FEM, which is a revised result from Zavaleta [14]. Local error estimates for the Navier-Stokes equation in polygon regions can be found in [7, 8]. We observe that the vorticity and the stream function are solved independently of the species concentrations and temperature in the problem. Thus, we assume that the vorticity and stream function are known.

More specific, we consider Ω a bounded open set in $\mathbb{R}^2$ with sufficient smooth boundary $\partial\Omega$ and external unit normal η. The problem is then reduced to a system formed just by equations (3) and (4) with $k \in \{F,\ O\}$. Here, $C_i = C_i(\mathbf{x}, t) : \Omega \times [0, \tau] \to \mathbb{R}$ for $i \in \{F, O\}$, $T = T(\mathbf{x}, t) : \Omega \times [0, \tau] \to \mathbb{R}$ and the known velocity $\mathbf{v} = \mathbf{v}(\mathbf{x}, t) : \Omega \times [0, \tau] \to \mathbb{R}^2$. We assume homogeneous Neumann boundary conditions and the initial conditions

$$C_F(\mathbf{x}, 0) = C_{F_0},\ C_O(\mathbf{x}, 0) = C_{O_0},\ T(\mathbf{x}, 0) = T_0,$$

$\forall\ \mathbf{x} \in \Omega$. Moreover, we set the non-negative constants α_F, α_O and α_T as $v_F Da$, $v_O Da$ and $v_P HeDa$, respectively; we take $\nu_F = \frac{1}{ReSc_F}$, $\nu_O = \frac{1}{ReSc_O}$ and $\nu_T = \frac{1}{RePr}$.

Here, the aim is to find a local error estimate for the approximate solution of the problem generated by the finite element method. In order to do this, we establish the variational formulation of the problem in an appropriate Hilbert space. In the sequel, we introduce the semi-discretized problem, which is defined in the finite element space. We want to estimate the difference between the solution of the variational problem (exact solution) and the solution of the semi-discretized problem (approximate solution).

The variational problem is to find $\mathbf{y} = (C_F,\ C_O,\ T) \in\ (H^1(\Omega))^3$ such that, for all $\phi \in\ (H^1(\Omega))^3$ we have

$$\left\langle \frac{\partial \mathbf{y}}{\partial t}, \phi \right\rangle + \langle \mathbf{u}\cdot\nabla\mathbf{y}, \phi\rangle - \langle D\Delta\mathbf{y}, \phi\rangle = \langle \mathbf{f}(\mathbf{y}), \phi\rangle \quad (5)$$

$$\mathbf{y}(0) = \mathbf{y}_0 \quad (6)$$

where $D = diag(\nu_F,\ \nu_O,\ \nu_T)$ is a diagonal matrix, $\langle\cdot,\ \cdot\rangle$ is the usual inner product in $(L^2(\Omega))^3$ and $f_k(\mathbf{y}) = \mp\alpha_k C_F C_O e^{-Ze/T(t)}$ with $k \in \{F, O, T\}$ and the "+" sign is used just when $k = T$.

The semi-discretized problem is constructed in the finite element space $(S_h)^3$ which is a finite dimensional space parameterized by the small parameter h. We illustrate the basic ideas used to construct S_h [3, 12]. For each $h > 0$ let $\mathcal{T}_h$ be a partition of $\overline{\Omega}$ (the closure

of Ω) into disjunct closed triangles κ such that the diameter of κ is bounded by h. In the $\mathcal{T}_h$, two triangles are either disjoint or share exactly either one side or one vertex.

We consider $\mathcal{T}_h$ an uniformly regular family of triangles. For each $h > 0$, the finite dimensional space S_h is defined by

$$S_h = \{u_h \in C(\Omega) : \ u_h|_\kappa \in \mathbb{P} \ \forall \ \kappa \in \mathcal{T}_h\}, \tag{7}$$

where $\mathbb{P}$ is the space of the polynomials in two variables of degree less or equal to one.

Then, the semi-discretized problem is to find $\tilde{\mathbf{y}}_h = (\tilde{C}_{Fh}, \ \tilde{C}_{Oh}, \ \tilde{T}_h)$, $\tilde{\mathbf{y}}_h : \ [0, \tau^*] \to (S_h)^3$ such that

$$\left\langle \frac{\partial \tilde{\mathbf{y}}_h}{\partial t}, \ \phi_h \right\rangle + \langle \mathbf{u} \cdot \nabla \tilde{\mathbf{y}}_h, \ \phi_h \rangle - \langle D\Delta_h \tilde{\mathbf{y}}_h, \ \phi_h \rangle = \langle f(\tilde{\mathbf{y}}_h), \ \phi_h \rangle \tag{8}$$

$$\tilde{\mathbf{y}}_h(0) = \tilde{\mathbf{y}}_{h0} \tag{9}$$

for all $\phi_h \in (S_h)^3$ and $t \in]0, \ \tau]$. Here, $\tilde{\mathbf{y}}_{h0}$ is the approximation of $\mathbf{y}_0$ in the finite element space and the discrete Laplace operator $\Delta_h : (S_h)^3 \to (S_h)^3$ is defined by

$$\langle -\Delta_h \psi, \ \phi \rangle = \langle \nabla \psi, \ \nabla \phi \rangle, \ \ \forall \ \phi \in (S_h)^3. \tag{10}$$

We introduce the orthogonal projection operators $P_h : L^2(\Omega) \to S_h$ and $R_h : H^1(\Omega) \to S_h$. These operators satisfy the following estimates for all $u \in H^{l+1}(\Omega)$, $0 \le l \le 1$ [12]:

$$\begin{aligned} &\|u - P_h u\|_{L^2(\Omega)} + \|u - R_h u\|_{L^2(\Omega)} \\ &+h \left(\|u - P_h u\|_{H^1(\Omega)} + \|u - R_h u\|_{H^1(\Omega)} \right) \\ &\le C h^{l+1} \|u\|_{H^{l+1}(\Omega)} \end{aligned} \tag{11}$$

To prove the local error estimate we will need the two following Lemma's. We will use $\|\cdot\|$ and $\langle \cdot, \cdot \rangle$ to the norm and inner product in $(L^2(\Omega))^3$, respectively. Moreover, $\|\cdot\|_m$ denote the norm on $(H^1(\Omega))^3$.

Lemma 1. *Let $P_h : \ (L^2(\Omega))^3 \to (S_h)^3$ be the orthogonal projection operator. The orthogonal projection $\mathbf{y}_h$ of the solution of (5)-(6) satisfies*

$$\begin{aligned} &\left\langle \frac{\partial \mathbf{y}_h}{\partial t}, \phi_h \right\rangle + \langle P_h \mathbf{u} \cdot \nabla \mathbf{y}_h, \phi_h \rangle + \left\langle P_h \mathbf{u} \cdot \nabla \mathbf{y}_h^\perp, \phi_h \right\rangle \\ &- \langle D\Delta_h \mathbf{y}_h, \phi_h \rangle - \left\langle D\Delta \mathbf{y}_h^\perp, \phi_h \right\rangle = \langle P_h f(\mathbf{y}), \phi_h \rangle \end{aligned} \tag{12}$$

$$\mathbf{y}_h(0) = P_h \mathbf{y}(0) \tag{13}$$

$\forall \ \phi_h \in (S_h)^3$ *with* $\mathbf{y} = \mathbf{y}_h + \mathbf{y}_h^\perp \doteq P_h \mathbf{y} + (I - P_h)\mathbf{y}$.

Lemma 2. *If $w_F = C_{Fh} - \tilde{C}_{Fh}$, $w_O = C_{Oh} - \tilde{C}_{Oh}$ and $w_T = T_h - \tilde{T}_h$, then*

$$\begin{aligned} \mathbf{f}_i(\mathbf{y}) - \mathbf{f}_i(\tilde{\mathbf{y}}_h) = \pm\alpha_i \Big(&w_F w_O + w_F \tilde{C}_{Oh} + w_F \tilde{C}_{Oh}^\perp \\ &+ w_O \tilde{C}_{Fh} + \tilde{C}_{Fh} C_{Oh}^\perp + w_O C_{Fh}^\perp \\ &+ C_{Fh}^\perp \tilde{C}_{Oh} + C_{Fh}^\perp C_{Oh}^\perp \Big) e^{-Ze/|\tilde{T}_h|} \\ \pm\alpha_i C_F C_O \left(e^{-Ze/|w_T + \tilde{T}_h + T_h^\perp|} e^{-Ze/|\tilde{T}_h|} \right), \end{aligned} \tag{14}$$

where the sign "+" corresponds to $i = T$.

In the following theorem, we use C_i with i a positive integer to denote various constants which occurs in the arguments.

Theorem 1. *Let $\mathbf{y}$ the solution of (5)-(6), $\tilde{\mathbf{y}}_h$ the solution of (8)-(9) and we assume $\mathbf{y} \in (H^2(\Omega))^3$. Then, there exists an interval $[0, \ \tau]$ and a $C_\tau = C(\tau)$ such that*

$$\|\mathbf{y} - \tilde{\mathbf{y}}_h\| \le C_\tau h, \ \ 0 \le t \le \tau. \tag{15}$$

Proof. Take $\mathbf{y} - \tilde{\mathbf{y}}_h = \mathbf{y} - P_h \mathbf{y} + P_h \mathbf{y} - \tilde{\mathbf{y}}_h$ and from (11) we have

$$\|\mathbf{y} - P_h \mathbf{y}\| \le Ch \|\mathbf{y}\|_1, \qquad \|\mathbf{y} - P_h \mathbf{y}\| \le Ch^2 \|\mathbf{y}\|_2. \tag{16}$$

Thus, to establish the Theorem we have to show that exists a constant C_τ such that $\|P_h \mathbf{y} - \tilde{\mathbf{y}}_h\| \le Ch$. To do this, we define $\mathbf{w} = \mathbf{y}_h - \tilde{\mathbf{y}}_h = (w_F, \ w_O, \ w_T)$. Subtracting (8) of (12), taking $\phi_h = w_i$ and using the Lemma 2, we can obtain the inequality

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\|\mathbf{w}\|^2 + \sum_i \nu_i \|\nabla w_i\|^2 \le &\sum_i |\langle P_h v \cdot \nabla w_i, w_i \rangle| \\ &+ \sum_i \left| \left\langle P_h v \cdot \nabla C_{ih}^\perp, w_i \right\rangle \right| + \sum_i |\nu_i| \left| \left\langle \nabla C_{ih}^\perp, \nabla w_i \right\rangle \right| \\ &+ \sum_i |\alpha_i| \left| \left\langle P_h w_F C_O e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle \right. \\ &+ \left\langle P_h C_F w_O e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle - \left\langle P_h w_F w_O e^{-Ze/|\tilde{T}_h|}, \ w_i \right\rangle \\ &+ \left\langle P_h C_F C_{Oh}^\perp e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle - \left\langle P_h C_{Fh}^\perp C_{Oh}^\perp e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle \\ &- \left\langle P_h w_F C_{Oh}^\perp e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle + \left\langle P_h C_{Fh}^\perp C_O e^{-Ze/|\tilde{T}_h|}, w_i \right\rangle \\ &- \left\langle P_h C_{Fh}^\perp w_O e^{-Ze/|\tilde{T}_h|}, \ w_i \right\rangle + \\ &\left\langle P_h C_F C_O \left(e^{-Ze/|w_T + \tilde{T}_h + T_h^\perp|} - e^{-Ze/|\tilde{T}_h|} \right), \ w_i \right\rangle \Big| \end{aligned}$$

Now, taking estimates in the Sobolev norms the last inequality yields

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\|\mathbf{w}\|^2 + \nu' \|\nabla \mathbf{w}\|^2 \le C_1 \|\mathbf{w}\|^2 + C_2 \|\mathbf{w}\| \|\nabla \mathbf{w}\|^2 \\ &+ C_3 \|\mathbf{w}\|^3 + C_4 h^4 + \epsilon \left(\frac{3}{2} h^2 + 1 \right) \|\nabla \mathbf{w}\|^2 + C_5 h^2 \end{aligned} \tag{17}$$

where $C_1, C_2, C_3, C_4, C_5, \nu'$ and ϵ are positive constants. For ϵ and h sufficiently small we have $C_4 h^4$ is small compared to $C_5 h^2$ and, $\nu' > \epsilon \left(\frac{3}{2} h^2 + 1 \right)$. Then, we have $\nu'' = \nu' - \epsilon \left(\frac{3}{2} h^2 + 1 \right) > 0$ and

$$\begin{aligned} &\frac{d}{dt}\|\mathbf{w}\|^2 + 2\nu'' \|\nabla \mathbf{w}\|^2 \le 2C_1 \|\mathbf{w}\|^2 + \\ &2C_2 \|\mathbf{w}\| \|\nabla \mathbf{w}\|^2 + 2C_3 \|\mathbf{w}\|^3 + 2C_4 h^2 \end{aligned} \tag{18}$$

From the theory of differential inequalities, for all (h, τ), there exists an interval $[0, \ s]$ such that $\forall \ t \in [0, \ s]$ we have

$$\|\mathbf{w}\| \le \frac{\nu''}{2C_2}. \tag{19}$$

Hence, we see that

$$\frac{d}{dt}\|\mathbf{w}\|^2 \leq C_1\|\mathbf{w}\|^2 + C_6 h^2. \tag{20}$$

We use the Gronwall's Lemma to find

$$\|\mathbf{w}\| \leq \sqrt{\frac{C_6}{C_1}} h e^{C_1\tau/2} \leq \frac{\nu''}{2C_2} \tag{21}$$

provided $h \leq \sqrt{\frac{C_1}{C_6}}\frac{\nu''}{2C_2}e^{-C_1\tau/2}$ Now, by contradiction, we can conclude that $\|\mathbf{w}\| \leq C_\tau h$ is valid for all $t \in [0,\ \tau]$. □

4. Numerical results

In this section, numerical results are presented for mixing flows including chemical reaction. We show the evolution of the concentration of the reactants and product and the temperature and reaction rate due to a set of parameters.

In the numerical simulation we consider a square box $[0,1] \times [0,1]$. Initially, the two reactants F (fuel) and O (oxidizer) are placed in contact as shown in (Fig. 1). We assume that the diffusivities D_i of the initial mixed quantities are equal to the viscosity of the fluid. Therefore, we have taken $Sc_i = 1$ for $i \in \{F, O, P\}$. We take $Pr = 1$, $He = 10$, $Ze = 7$ and the molar stoichiometric coefficients to be $v_F = v_O = v_P = 1$.

4.1 Spatial Discretization

For the spatial discretization with the FEM, we apply the Galerkin's method [15, 16]. The two-dimensional computational domain Ω is discretized using triangular linear elements. A non-uniform 65×65 grid points has been used such that there is a cell concentration near the cavity walls. Hence, inside each element the variables are approximated as

$$\omega \approx \omega^e = N_J(\xi,\eta)\omega^J(t), \qquad \psi \approx \psi^e = N_J(\xi,\eta)\psi^J(t),$$
$$C_k \approx C_k^e = N_J(\xi,\eta)C_k^J(t), \quad T \approx T^e = N_J(\xi,\eta)T^J(t),$$

where ω^J, ψ^J, C_k^J, T^J are, respectively, the variables ω, ψ, C_k and T taken in the node J; as before, $k \in \{F, O, P\}$. Moreover, we have assumed the following approximation in each element

$$C_F^e C_O^e e^{-Ze/T^e} \approx \sum_J N_J C_F^J(t) C_O^J(t) e^{-Ze/T^J(t)}.$$

A Galerkin approximation solution to the set of equations (1)-(4) is given using a variational formulation of the problem. Then, if we use the natural coordinate system we can write the element equations as

$$[M_L]\{\dot{W}\} + ([B(\psi)] - [C(\psi)])\{W\} = -\frac{1}{Re}[K]\{W\},$$
$$[K]\{\Psi\} = [M]\{W\},$$
$$[M_L]\{\dot{\mathcal{C}}_k\} + ([B(\psi)] - [C(\psi)])\{\mathcal{C}_k\} + \frac{1}{ReSc_k}[K]\{\mathcal{C}_k\} = \mp v_k Da[M]\{\mathcal{H}\},$$
$$[M_L]\{\dot{\mathcal{T}}_k\} + ([B(\psi)] - [C(\psi)])\{\mathcal{T}_k\} + \frac{1}{RePr}[K]\{\mathcal{T}_k\} = v_P HeDa[M]\{\mathcal{H}\},$$

where the point indicates temporal derivative, $\{W\}$, $\{\Psi\}$, $\{\mathcal{C}_k\}$ and $\{\mathcal{T}\}$ are column vectors whose components are the nodal variable ω_J, ψ_J, C_k^J and T_J, respectively. The other matrices have the following components

$$M_{i,j} = \frac{\Delta x \Delta y}{4}\int_{-1}^{1}\int_{-1}^{1} N_i N_j \, d\xi d\eta$$
$$B_{i,j} = \int_{-1}^{1}\int_{-1}^{1} N_i \frac{\partial \psi^e}{\partial \eta}\frac{\partial N_j}{\partial \xi} \, d\xi d\eta$$
$$C_{i,j} = \int_{-1}^{1}\int_{-1}^{1} N_i \frac{\partial \psi^e}{\partial \xi}\frac{\partial N_j}{\partial \eta} \, d\xi d\eta$$
$$K_{i,j} = \int_{-1}^{1}\int_{-1}^{1} \left(\frac{\partial N_i}{\partial \xi}\frac{\partial N_j}{\partial \xi} + \frac{\partial N_i}{\partial \eta}\frac{\partial N_j}{\partial \eta}\right) d\xi d\eta$$

The matrix $[M_L]$ is the known lumped mass matrix associated to the consistent mass matrix $[M]$. This approximation makes the computational process much simpler and less expensive because it allows the application of explicit methods [10, 15, 16].

4.2. Time-stepping scheme

We have seen that FEM, when applied to the problem under study, yields EDO's systems which have to be solved. In order to solve these EDO's with high accuracy and low storage requirements the Runge-Kutta method was chosen. To extend the stability region and to obtain second order time approximation three stages are employed [9].

4.3. Simulations

Here, we present some results of simulations (see Figure 2). Initially, the two reactants F (fuel) and O (oxidizer) are placed in contact as shown in Figure 1. We assume that the diffusivities D_i of the initial mixed quantities are equal to the viscosity of the fluid. Therefore, we have taken $Sc_i = 1$ for $i \in \{F, O, P\}$. We have set $Re = 400$, Pr $= 1$, He $= 10$ and the molar stoichiometric coefficients to be $v_F = v_O = v_P = 1$.

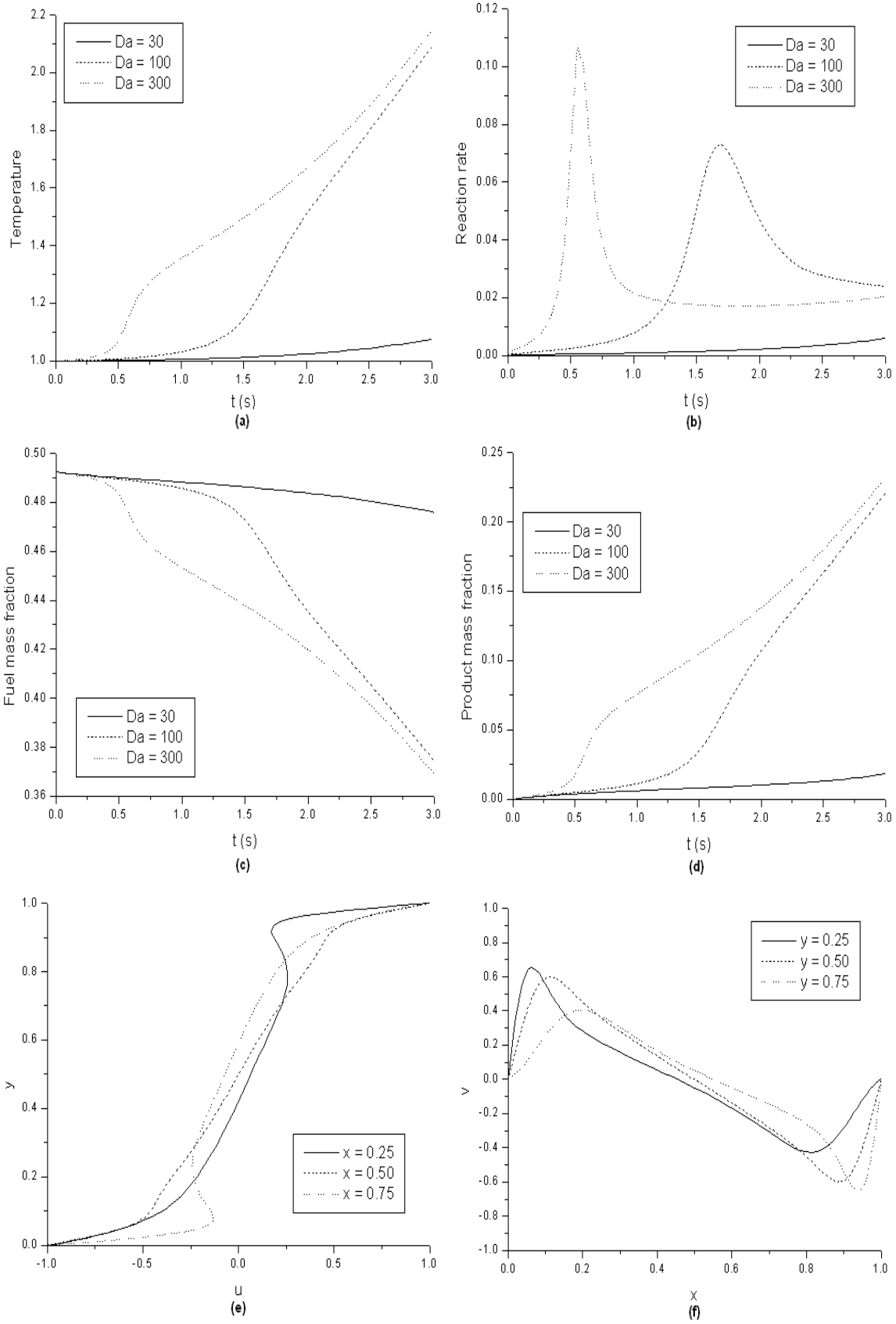

Figure 2: Simulation results for $Re = 400$, $Pr = 1$, $Sc = 1$, $Ze = 6$ and $He = 10$: (a) temperature evolution; (b) reaction rate evolution; (c) fuel mass fraction evolution; (d) product mass fraction evolution; (e) stationary horizontal velocity; (f) stationary vertical velocity.

We can observe that the Damköhler number changes significantly the reaction rate behavior, as shown in Figure 2(b). The reaction rate increases rapidly at the beginning of the process and then it decreases slowly until all fuel is consumed. As is expected, increasing Da increases the reaction rate. This implies increase of the temperature and product formation (see Figure 2(a) and Figure 2(d)).

5. Conclusions

In this work we have applied FEM to the numerical simulation of reacting flows in a two-sided lid-driven cavity. A non-uniform grid and the a Runge-Kutta three time-stepping scheme were choose to improve the stability and the simplicity of the code. The numerical results show how changes in the Damköhler affect the mixing and reaction process. Furthermore, the mathematical nature of FEM has been explored here. We have shown a local error estimate for the approximation of the solution of the problem with FEM. This estimate of order h is valid only for small t and h. In [7], it is observed that the constant in the estimate of the local error grows exponentially with time. In a future work we intend to establish global error estimates for the solutions based on FEM.

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