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MODELING AND SIMULATION OF A JET DIFFUSION FLAME OF HYDROGEN SOLVED BY APPLYING THE ROSENBRACK METHOD

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ABSTRACT

Problems involving chemical reactions have an important characteristic called stiffness, indicating that the solutions of the involved ODE systems vary in different orders of magnitude. So, it is needed to choose suitable numerical methods for obtaining numerical solutions that are stable and convergent at a low computational cost. The most used methods for dealing with this type of problem are the implicit methods, since they have a region of unlimited stability in the complex plane that allows large variations in step size. In this work we employ an L-stable method: the fourth-order Rosenbrock method of four stages. The reduced mechanism for the combustion of hydrogen is simulated and the results have good agreement with data found in the literature.

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INTRODUCTION

Energy is an indispensable resource in everyone lives and combustion is the most used technology for conversion of it. For this reason, researchers have explored computational methods to develop practical combustion systems, specially as regards the reduction of the emission of pollutants into the atmosphere [1, 2]. The chemical kinetic modelling has become an important tool for interpreting and understanding the phenomena of combustion [3], leading to the development of several detailed and reduced reaction mechanisms to the combustion of different chemical compounds. Even today, fuels are predominantly derived from unsustainable mineral resources, petroleum and coal, whose combustion leads to environmental pollution, greenhouse gas emissions and problems with energy security [4]. But the high global demand of energy and the economic and environmental restrictions have leads to the pursuit for renewable sources of energy. Computer simulations with detailed kinetic mechanisms are complicated and, therefore, there is the need to develop, from these detailed mechanisms, the corresponding reduced mechanisms with fewer variables, maintaining a good level of accuracy and comprehensiveness for the desired applications [5].

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In this direction, based on the detailed mechanism given by Fisher *et al.* [6], available on the website of the Lawrence Livermore National Laboratory, the present paper develops a reduction strategy to obtain a two-step reduced kinetic mechanism for hydrogen. Reduced mechanisms for hydrogen combustion have been developed by many researches [7, 8, 9]. According to Peters and Rogg [7] the two-step mechanism is appropriate for hydrogen-air premixed and (non) diluted diffusion flames. There is an increasing interest in the study of hydrogen diffusion flames because of its key role in understanding hydrocarbon and biofuels combustion. Hydrogen can be obtained from fossil fuels or conveniently from renewable resources as a biofuel. The hydrogen is an important intermediate species in the oxidation of hydrocarbons and oxygenated fuels. The species H_2 , H , O , OH , HO_2 and H_2O_2 determine the composition of the radical pool in the majority of fuel reaction systems [10, 11]. Due to the existence of highly reactive radicals and fast reactions in the detailed mechanisms, the associate system of governing equations is stiff. One solution for this problem is the decrease of variables with the use of the assumptions of quasi-steady-state for species and partial equilibrium for reactions, whose purpose is to replace the differential equations by algebraic relations. This work is devoted to the study of a numerical method applied to H_2-O_2 chemical model, which is important

to evaluate the species concentration involved during the entire combustion process. The problems related to this process result in systems of ordinary differential equations (ODEs) with a special characteristic called stiffness, which occurs because the concentrations of the chemical species vary in different orders of magnitude. These are not the only problems with this type of characteristic, other examples appear in vibrations, electrical circuits and control theory. A system of equations is considered stiff when one or more variables change very quickly, while others change very slowly. This disparity over time is common in chemical systems in which reactions with radicals are very fast compared to reactions involving stable species. To solve stiff initial value problems, suitable numerical methods must be applied so that the numerical solution is stable and convergent at an acceptable computational cost. Although the treatment of stiff problems is quite frequent, there is not a mathematically precise definition that describes this characteristic well.

Curtiss and Hirschfelder [12], were the first to conclude that stiff problems need implicit methods because they have the region of adequate stability. More precisely, these methods have a region of unlimited stability that covers the entire complex half-plane with a negative real part or at least an unlimited part thereof. Later, Shampine and Gear [13] gave us a definition: the initial value problem for EDOs is stiff if the Jacobian matrix of the system has at least one eigenvalue, for which the real part is negative with high modulus, while the solution within most of the integration interval slowly changes. This definition is the one that best characterizes stiffness, explaining that these problems present solutions in which some components decay much faster than others. In this work, the fourth-order four-stage Rosenbrock method is employed. It is a simple step method, with development based on diagonally implicit Runge-Kutta (DIRK) methods. The method allows size variation of the integration step due to the unlimited stability region, so that it uses a small step size where the solution changes more quickly, and allows to increase step size in regions where the solution is softer, obtaining a reduction in computational costs. The method will be used in the solution for hydrogen combustion. The reaction mechanism of hydrogen oxidation is widely used in rocket propulsion and also becomes important as a subsystem in the oxidation of hydrocarbons, as seen in Turns [14]. Chamousis [15] shows some advantages and disadvantages of the use of hydrogen as a transportation fuel. As advantages, it can be mentioned: high energy yield (122kJ/g), produced from many primary energy sources, high diffusivity, water vapor as the major oxidation product, is the most abundant element and the most versatile fuel. As disadvantages, there are: low density, large storage areas, not found free in nature, low ignition energy (similar to gasoline) and is currently expensive. In this way, the study of this fuel and its behavior is fundamental for advances in the field of combustion of hydrocarbons and biofuels.

Flow equations and their discretization procedure: Favred filtering becomes convenient when writing the governing equations for turbulent flows. The set of equations for the combustion process includes the momentum (Navier-Stokes), enthalpy, species mass fraction and pressure. They are written as follow:

$$\frac{\partial \bar{\rho} \bar{v}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_i \bar{v}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\frac{1}{Re} \sigma_{ij} \right), \quad \dots \dots \dots (1)$$

$$\frac{\partial \bar{\rho} \bar{Y}_i}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_j \bar{Y}_i}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\rho} \bar{\mu}_T}{\bar{\rho} \bar{\mu}_T} \frac{\partial \bar{Y}_i}{\partial x_j} \right), \quad \dots \dots \dots (2)$$

$$\frac{\partial \bar{\rho} \bar{h}}{\partial t} + \frac{\partial \bar{\rho} \bar{v}_j \bar{h}}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\rho} \bar{\mu}_T}{\bar{\rho} \bar{\mu}_T} \frac{\partial \bar{h}}{\partial x_j} \right), \quad \dots \dots \dots (3)$$

where $\bar{\rho}$ is the average density, \bar{v}_j the Favred averaged velocity, \bar{Y}_i the Favred averaged mass fraction of species i , $\bar{\mu}_T$ the reaction rate of the species i , $\bar{\mu}_T$ the eddy viscosity, the Favred averaged enthalpy.

The gradient of pressure can be obtained after solving a Poisson's equation of the form [16]

$$\nabla^2 \bar{p} = \Delta t \left(\frac{\partial (\bar{\rho} \bar{v}_i)}{\partial x_j} + \frac{\partial (\bar{\rho} \bar{v}_i)}{\partial t} \right) \quad \dots \dots \dots (4)$$

The reaction rate of each species is given by

$$\bar{w}_i = D_a Y_f Y_0 e^{-Z_e/R_e T_i} \quad \dots \dots \dots (5)$$

In these equations, R_e is the Reynolds, P_r the Prandtl, S_c the Schmidt, D_a the Damköhler and Z_e the Zel'dovich numbers. Temperature \bar{T} is obtained from enthalpy using a simple Newton iteration

$$\bar{h} = \sum_{i=1}^n \bar{Y}_i h_i(\bar{T}) \quad \dots \dots \dots (6)$$

and density can be relaxed by

$$\bar{\rho} = \frac{\bar{p}}{\frac{\eta}{1-\eta} \bar{T} + 1} \quad \dots \dots \dots (7)$$

with $0.1 < \eta < 0.8$ to avoid numerical instabilities, since variations in density affect all other equations.

The set of equations was solved numerically. A central finite difference scheme was adopted for spatial derivatives of first and second orders. A nonuniform structured mesh was used in order to concentrate enough points at the exit of the injector and along the burner centerline.

$$\left(\frac{\partial f}{\partial x} \right)_{(i,j,k)} = \frac{f_{(i+1,j,k)} - f_{(i-1,j,k)}}{2\Delta x} \quad \dots \dots \dots (8)$$

$$\left(\frac{\partial f}{\partial y} \right)_{(i,j,k)} = \frac{f_{(i,j+1,k)} - f_{(i,j-1,k)}}{2\Delta y} \quad \dots \dots \dots (9)$$

$$\left(\frac{\partial^2 f}{\partial x^2} \right)_{(i,j,k)} = \frac{f_{(i+1,j,k)} - 2f_{(i,j,k)} + f_{(i-1,j,k)}}{\Delta x^2} \quad \dots \dots \dots (10)$$

and in similar manner in other directions. This set of equations can be summarized as:

$$\begin{cases} \frac{\partial y}{\partial t} = f(y) \\ y(t_0) = y_0 \end{cases} \quad y = (\bar{\rho}, \bar{v}_i, \bar{Y}_k, \bar{h})^T.$$

Detailed kinetic systems for biodiesel surrogates generally have significant stiffness due to the difference between the time scales of the reactive species. The stiffness of the reduced mechanism strongly depends on the skeleton mechanism used [17]. This causes difficulties in the convergence of purely explicit numerical methods, because rigidity imposes severe limitations

on the time-step size [18]. The eigenvalues of the Jacobian matrix for f characterize the stability of the system. Generally, a system is considered stiff when its eigenvalues are very different in magnitude [19].

Rosenbrock method

For the solution of the differential equations a L-stable method (to be defined soon) is implemented based on a class of Runge-Kutta methods known as Rosenbrock method. The conditions for L-stability require that the method be implicit. Implicit or semi-implicit Runge-Kutta methods are known to satisfy conditions for good stability [20]. In order to propose an alternative for the resolution of systems of implicit equations, usually solved by iterative processes, Rosenbrock [21] presented a new method. He developed a new class of single-step methods, which is based on linearizations of implicit Runge-Kutta methods. This avoids the resolution of non-linear systems to solve a sequence of linear systems, which facilitates the implementation of the method. This method is also named in the literature as a linearly implicit Runge-Kutta method or as diagonally implicit Runge-Kutta.

Consider a system of ordinary differential equations,

$$y' = f(y), y(t_0) = y_0, \dots \dots \dots (12)$$

Where in $y = y(t) \in R^m, t \in R \text{ e } f: Rm \rightarrow Rm$.

The coefficients used in the Rosenbrock method determine new stability properties and order conditions, different from the conditions of the Runge-Kutta methods. According to Lambert [22], to obtain a p -order Runge-Kutta method, we must expand the equation of Runge-Kutta s -stages in Taylor's series to the desired order term and compare with the Taylor's series of the corresponding exact solution. More details on the development of high-order Runge-Kutta methods are contained in Butcher [20] or Wanner *et al.* [23]. The concept of L-stability is very important, since A-stable methods that are not damped maximally when $\lambda h \rightarrow -\infty$ do not generate satisfactory results [24]. This undesirable asymptotic behavior usually results in oscillatory solutions for very rigid systems. Thus, for extremely stiff systems it is desirable to develop L-stable rather than A-stable methods.

The four-stage fourth-order Rosenbrock method is given by:

$$y_{n+1} = y_n + h \sum_{i=1}^4 \gamma_i \kappa_i \tag{13}$$

$$\kappa_1 = f(y_n) / A(y_n) \tag{14a}$$

$$\kappa_2 = f(y_n + h a_{21} \kappa_1) / A(y_n) \tag{14b}$$

$$\kappa_3 = f(y_n + h(a_{31} \kappa_1 + a_{32} \kappa_2)) / A(y_n) \tag{14c}$$

$$\kappa_4 = f(y_n + h(a_{41} \kappa_1 + a_{42} \kappa_2 + a_{43} \kappa_3)) / A(y_n) \tag{14d}$$

where $A(y_n) = [I - h d \frac{\partial f(y_n)}{\partial y}]$.

The stability region of the method given by (13) with parameters from Table 1 and another four-stage A-stable fourth-order method developed by Bui [25], is shown in Figure 1.

The local error estimate, is:

$$E_{n+1} = \frac{\|y_{n+1}^* - y_{n+1}\|}{2^{\rho-1}} \tag{16}$$

with ρ the order of the method and the norm $\| \cdot \|$ is given by

$$\|y\| = \left[\frac{1}{\phi} \sum_{i=1}^{\phi} \left(\frac{y_{n+1}^i}{y_{max}^i} \right)^2 \right]^{1/2}, \tag{17}$$

where ϕ is the number of system variables.

Table 1. Parameters for the fourth-order Rosenbrock method with four stages

$\gamma_1 = 0,9451564786$	$\gamma_2 = 0,341323172$	$\gamma_3 = 0,5655139575$
$\gamma_4 = -0,8519936081$	$a_{31} = -0,1012236115$	$a_{32} = 0,9762236115$
$a_{21} = -0,5000000000$	$a_{42} = 0,7151140251$	$a_{43} = 0,1430371625$
$a_{41} = -0,3922096763$		

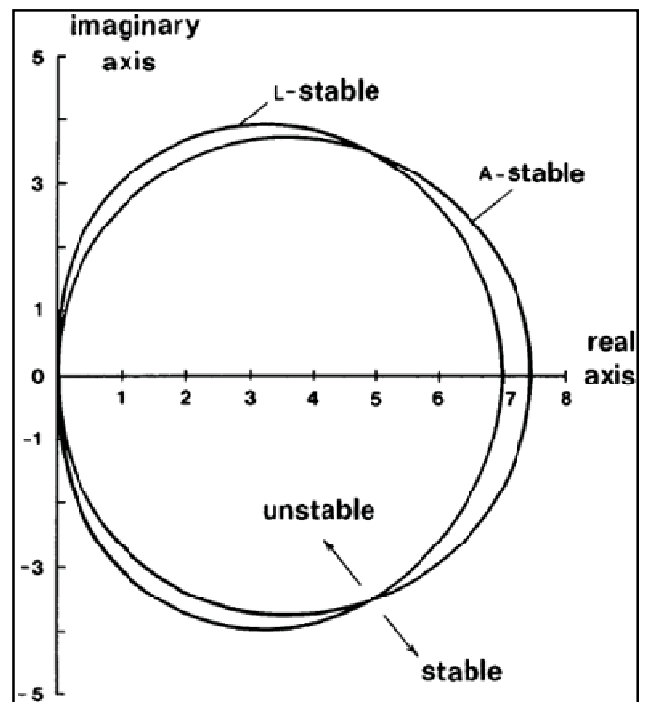


Figure 1. Stability region of an A-stable and a L-stable four-stage fourth-order method, adapted from [25].

For a tolerance ϵ , the following procedure can be used to determine the time increase:

- If $E_{n+1} > \epsilon$, the step is rejected and h should be reduced.
- If, the step is accepted, but h should be reduced.
- If, the step is accepted and h is accepted.
- If, the step is accepted and h can be increased.

In this way, instead of using a small time-step across the whole integration interval to control regions with greater stiffness, we use an adaptive step control. Thus, in regions where the step should be reduced, it is done, whereas in regions with lower stiffness the step is increased in order to decrease the whole computational time to solve the system of equations. The variables y_{n+1} and y_{n+1}^* are calculated using time-steps h and $h/2$, respectively. To avoid divergence during the iterative process the increment for the step needs to be limited, which can be done by the following relation:

$$h_{n+1} = h_n \min \left(10, \max \left(0,1 ; \frac{0,9}{\Delta y} \right)^2 \right) \dots \dots \dots (18)$$

It is also necessary that the step values are limited by a maximum and minimum values, the initial time increase

should be sufficiently small and, in the case of rejection of h_{n+1} the growth factor in the next iteration is made equal to 1, instead of 10, as in equation (18).

Table 2. Hydrogen mechanism rate coefficients (units are mol, cm³, s, K and cal= mol).

Reaction	A	β	E_A
1. $OH + H_2 = H + H_2O$	2.14E+08	1.52	3449
1b. $H + H_2O = OH + H_2$	5.09E+09	1.30	18588
2. $O + OH = O_2 + H$	2.02E+14	-0.40	0
3. $O + H_2 = OH + H$	5.06E+04	2.67	6290
4. $H + O_2 + M = HO_2 + M$	4.52E+13	0.00	0
5. $OH + HO_2 = H_2O + O_2$	2.13E+28	-4.83	3500
6. $H + HO_2 = OH + OH$	1.50E+14	0.00	1000
7. $H + HO_2 = H_2 + O_2$	6.63E+13	0.00	2126
8. $H + HO_2 = O + H_2O$	3.01E+13	0.00	1721
9. $O + HO_2 = O_2 + OH$	3.25E+13	0.00	0
10. $2OH = O + H_2O$	3.57E+04	2.40	-2112
11. $H + H + M = H_2 + M$	1.00E+18	-1.00	0
12. $H + OH + M = H_2O + M$	2.21E+22	-2.00	0
13. $H + O + M = OH + M$	4.71E+18	-1.00	0
14. $O + O + M = O_2 + M$	1.89E+13	0.00	-1788
15. $HO_2 + HO_2 = H_2O_2 + O_2$	4.20E+14	0.00	11982
16. $OH + OH + M = H_2O_2 + M$	1.24E+14	-0.37	0
17. $H_2O_2 + H = HO_2 + H_2$	1.98E+06	2.00	2435
18. $H_2O_2 + H = OH + H_2O$	3.07E+13	0.00	4217
19. $H_2O_2 + O = OH + HO_2$	9.55E+06	2.00	3970
20. $H_2O_2 + OH = H_2O + HO_2$	2.40E+00	4.04	-2162

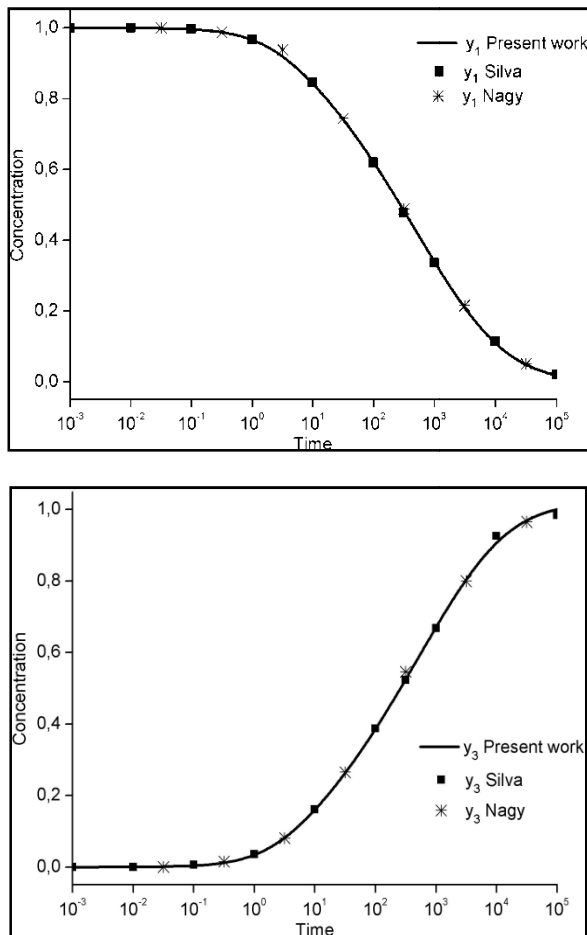


Figure 2. First (left side) and third (right side) variables of Robertson model

Code verification

To check the implementation of the method used, a system of ordinary differential equations usually applied in numerical tests for stiff equations, called the Robertson model, was selected. The kinetic model of Robertson [26] is one of the

most known problems for the analysis of stiff methods. The model describes the kinetics of an autocatalytic reaction and the structure of the reactions is given by



$y_2 + y_3 \rightarrow y_1 + y_3$ where k_1 , k_2 and k_3 are the specific velocities given by $k_1 = 0,04$, $k_2 = 3 \cdot 10^7$ and $k_3 = 10^4$ and y_1 , y_2 and y_3 are the chemical species involved. The model proposed by Robertson has no defined units. The model can be described as:

$$\begin{aligned} \frac{dy_1}{dt} &= -0,04y_1 + 10^4 y_2 y_3, \\ \frac{dy_2}{dt} &= 0,04y_1 - 10^4 y_2 y_3 - 3 \times 10^7 y_2, \\ \frac{dy_3}{dt} &= 3 \times 10^7 y_2 \end{aligned} \quad (20)$$

The integration interval used was $[10^{-3}, 10^5]$ with initial conditions

$$\begin{aligned} y_1(t_0) &= 1, \\ y_2(t_0) &= 0, \\ y_3(t_0) &= 0. \end{aligned} \quad (21)$$

The points obtained by the integration of the model with the Rosenbrock method are compared next with the work of Silva [27], which used the Modified Extended Backward Differentiation Method (MEBDF), and with the work of Nagy [28], in which a package for Mathematica software is developed (called Reaction Kinetics) and compared with a MATLAB internal command. The results shown in Figure 2 are in good agreement with those observed in the literature.

Solution of a Hydrogen Turbulent jet Diffusion Flame: To simplify the chemical kinetics involved and favor the resolution of the problem, a reduced mechanism is made using some hypotheses, such as steady-state and partial equilibrium. The steady-state hypothesis is valid for intermediate species that are produced by slow reactions and consumed by fast reactions, so their concentrations remain small [14]. The hypothesis of partial equilibrium is justified when the velocities of the forward and backward reactions are much greater than the other specific velocities of the mechanism [29].

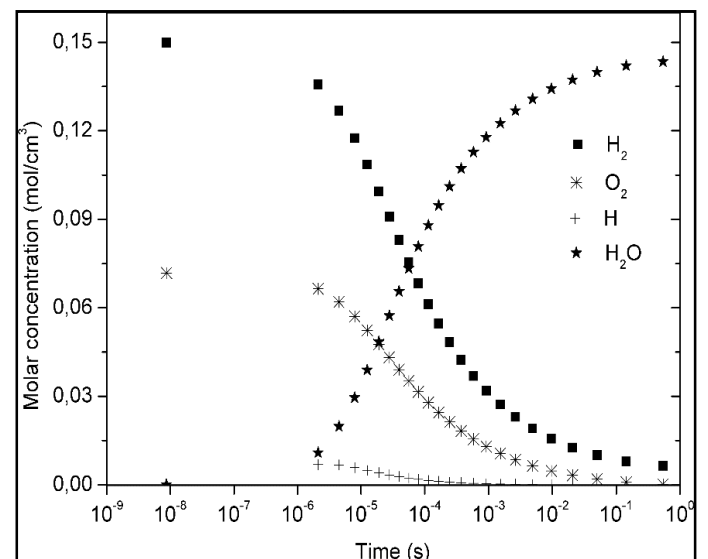
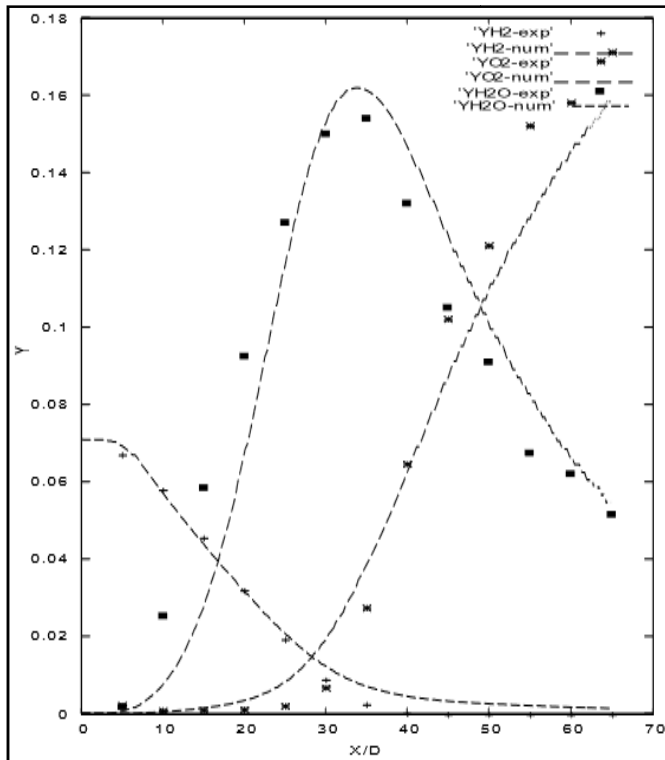


Figure 3. Molar concentrations obtained by integration of the reduced mechanism for H_2 combustion

Table 3. Comparison between the equilibrium mole fractions

Species	Present work	Gaseq
H_2	0.0149	0.015
O_2	$2.11E-9$	0.006
H	$3.74E-9$	no info
H_2O	0.3470	0.324
N_2	0.638	0.646

**Figure 4. Sketch of a jet flame**

Mechanisms of hydrogen combustion: Consider the reactions 1-20 presented by Marinov [30], according to Table 2. After applying the hypothesis of partial equilibrium for those reactions with high specific forward and backward velocities, it remains the reactions 1, 3, 11, 12, 13 and 14. Considering the steady-state assumption for the species OH , it results the following two-step mechanism among four species for hydrogen



where M is an inert needed to remove the bond energy that is liberated during recombination [29].

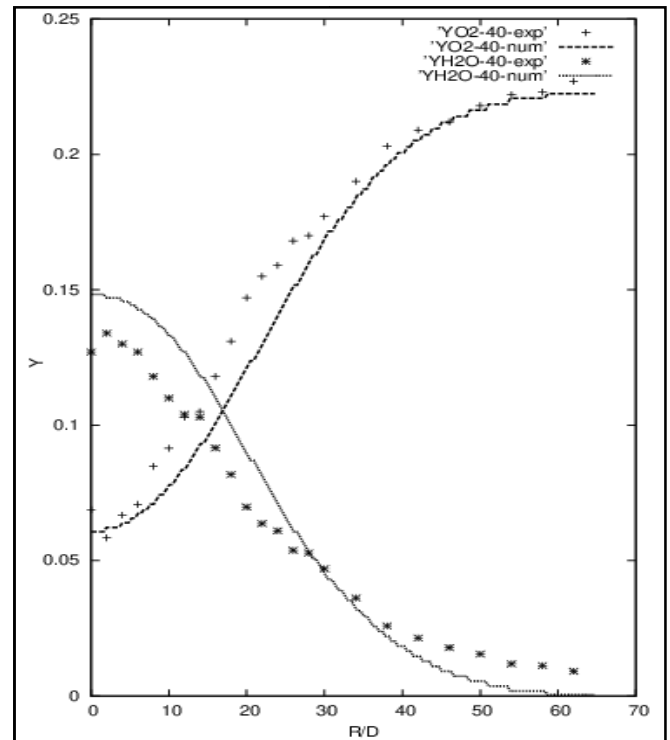
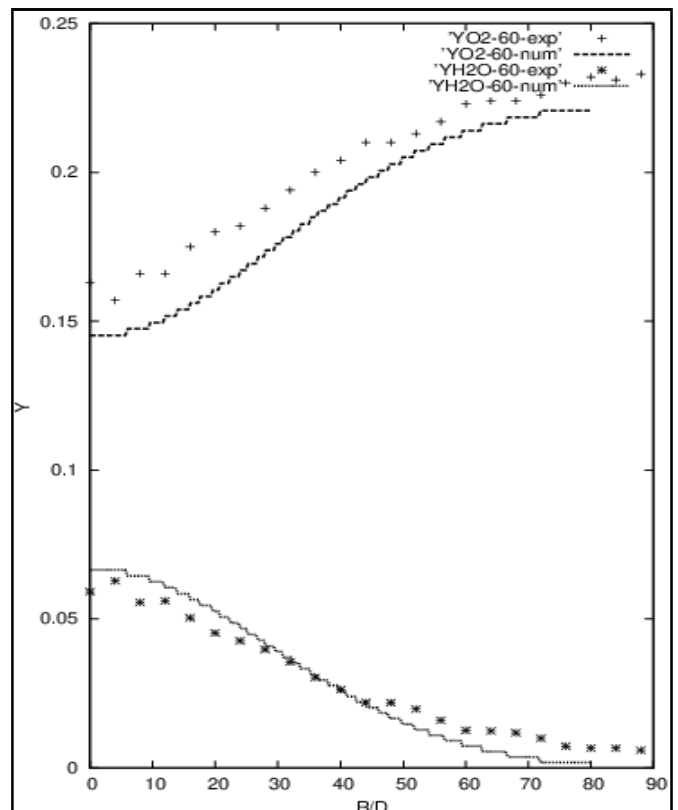
The system of ordinary differential equations resulting from these reactions is

$$\begin{aligned} d[H_2]/dt &= -3\omega_I' + \omega_{11}' \\ d[H]/dt &= 2\omega_I' - 2\omega_{11}' \\ d[O_2]/dt &= -\omega_I' \\ d[H_2O]/dt &= 2\omega_I' \end{aligned} \quad (23)$$

NUMERICAL RESULTS

To obtain the behavior of the species concentration in relation to time, the system of reactive equations was solved by the fourth order Rosenbrock method with four stages defined by

the equation 13 and using the parameters of Bui [31] shown in the table 1. The tolerance for the error used was $\epsilon = 10^{-7}$. The simulations were done assuming a temperature of 800K. In Figure 3 the species molar concentrations in relation to time are shown. In the Table 3 a comparison is made with the data generated through the Gaseq program (<http://www.gaseq.co.uk/>), which provides the molar fraction of the species when the equilibrium is obtained. Gaseq uses a method based on the minimisation of free energy (NASA method).

**Figure 5. Mass fraction of H_2 , O_2 and H_2O along the burner centerline****Figure 6. Mass fraction of H_2 and H_2O at positions $X/R=40$ and 60**

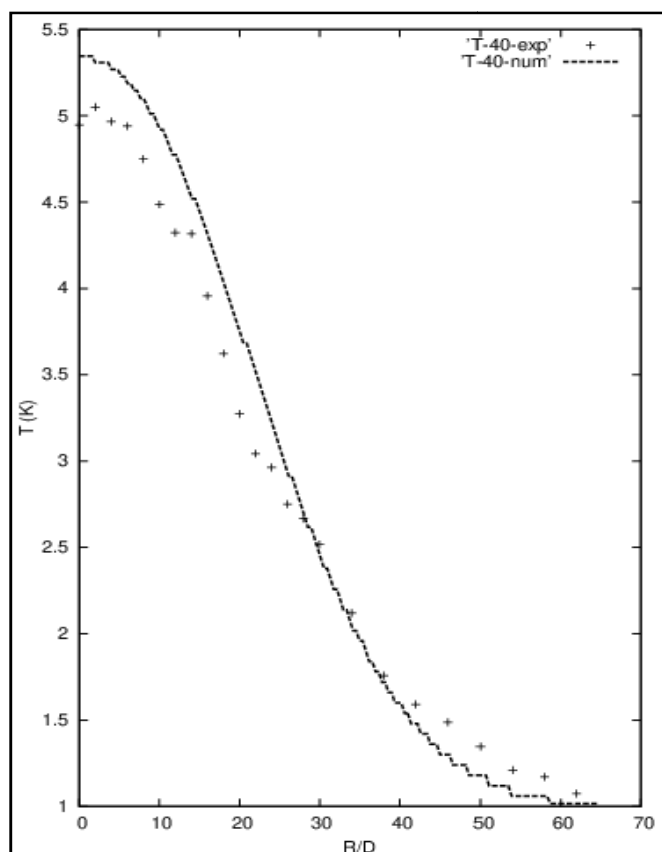


Figure 7. Temperature T profile at position $X/R=40$

We suppose air as a mixture composed of 23.7% of O_2 and 76.28% of N_2 . The results are consistent with those provided by Gaseq, but while Gaseq only report the concentration at equilibrium, our data provide information on the whole process. Following, we present the results for a turbulent jet diffusion flame as shown in Fig. 4. Numerical results of the jet flame are indicated as "num" in the figures. The jet flame was chosen because it represents the class of nonpremixed flames. One employs a duct of cylindrical cross section with diameter $D_e = 0.3$ and the fuel is injected from a tube of diameter $D = 0.07$. The duct length corresponds to $10 D_e$. The H_2 flame is used to compare the results (www.ca.sandia.gov/TNF). Since the flame is governed by hydrodynamics, occurs an axial decreasing of the mixture fraction along the burner centerline. The mass fraction of fuel H_2 , oxidizer O_2 and product H_2O are shown in Fig. 5. The radial mass fraction distribution, shown in Fig. 6, can be reasonably approximated by a Gaussian function. The temperature profile, presented in Fig. 7, shows a reasonable agreement with the experiment. It rises rapidly in the rich part of the flame and decreases by expansion in the lean flame region.

Conclusions

In this work the four-stage fourth-order Rosenbrock method is employed for solving a turbulent jet diffusion flame of hydrogen. It is applied in the EDOs system resulting from the modeling of chemical kinetics for hydrogen combustion. Also is presented a reduced mechanism for hydrogen with two reactions and four species, which represents well the behavior of the complete system containing 21 reactions and eight species. It is believed that the great impact of this work is on the qualitative and quantitative model for the development of research involving stiffness equations, especially in the field of combustion, since the numerical simulation of mechanisms

that represent this phenomenon, can become difficult since it involves highly reactive radicals, which brings stiffness to the system. In this way, the simplifications used in this paper contribute to the achievement of good results, with reduced stiffness of the system. Furthermore, the numerical method presented here contains features that allow reduction in computational cost and stability that allows a great variation in the temporal step, which may represent an advance in other researches. For future works, it is suggested to apply the same procedure for a larger biofuel molecules, such as methanol, ethanol and biodiesel.

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