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ASYMPTOTIC ANALYSIS OF STOICHIOMETRIC HYDROGEN-AIR FLAMES

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ARTICLE INFO	ABSTRACT
	This paper shows a mechanism for hydrogen combustion, an important submechanism in hydrocarbon oxidation and biofuels. Once exposed the equations derived from the chemical kinetics and concentration rates of each species involved, the complete mechanism of hydrogen oxidation is displayed. The strategy for obtaining a reduced mechanism with two reactions consists of four steps. This method involves the use of assumptions of steady-state for species and partial equilibrium for reactions. Jacobian matrices have extremely high stiffness ratio, which complicates the implementation of explicit methods. Thus, the fourth-order Rosenbrock method is applied with four stages, adaptive step control and specific parameters. The code is verified and shows good results for both the Robertson model and the reduced mechanism presented.

INTRODUCTION

The reaction mechanism of hydrogen oxidation is widely used in rocket propulsion calculations and also becomes important as a subsystem in the oxidation of hydrocarbons, as seen in Turns (2000). Chamousis (2000) 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. In the search for substitutes for fossil fuels, hydrogen appears as a good candidate, since it can be obtained from renewable raw materials and almost does not emit pollutants into the atmosphere. Chemical kinetic modelling has become a tool for the understanding of the combustion, leading to the development of different kinetic mechanisms. Anyway, computer simulations with detailed mechanisms are delicate because of the existence of highly reactive radicals, which brings stiffness to the system of equations. Therefore, it is necessary to develop reduced mechanisms with fewer variables and moderate stiffness, maintaining good precision and the behaviour of the mechanism. In next section will be presented the concepts of chemical kinetics, production and destruction rates, reaction rates, steady-state approximation and partial equilibrium. Following, complete mechanisms and asymptotic analysis for reducing the mechanism for the combustion of hydrogen are presented. Next, there is the Rosenbrock method presentation, its conditions of order and stability, and the implementation of a fourth-order four-stage method.

Chemical Kinetics

For the modeling of combustion it is necessary to know some important concepts in chemical kinetics, such as: elementary reaction rates, steady-state approximation and partial equilibrium. Most elementary reactions of greater interest in combustion are bimolecular and, considering an arbitrary bimolecular reaction, are of the form

$$A + B \rightarrow C + D, \tag{1}$$

that is, two molecules collide and react, forming two different molecules. The rate at which each reaction takes place is directly proportional to the concentration in $kmol/m^3$ of each of the reactant species, i.e.

$$\frac{d[A]}{dt} = -k[A][B]. \tag{2}$$

Equation (2) can be rewritten in order to suggest the dependence of the coefficient k in relation to temperature. If the temperature range of interest is not very wide, the bimolecular rate coefficient can be expressed by the empirical Arrhenius form,

$$k(T) = A \cdot e^{[-E_A/R_uT]}, \tag{3}$$

where A is a constant called pre-exponential or frequency factor. Comparing equations (6) and (7), we see that A is not constant but depends, based on collision theory, on $T^{1/2}$. Arrhenius plots of $\log k$ and $1/T$ for experimental data are used to obtain activation energy values, since the slope of such plots is $-E_A/R_u$. Even if the tabulation of experimental values for rate coefficients in Arrhenius form is common, the most frequent practice is to use the form with three parameters:

$$k(T) = AT^\beta \cdot e^{[-E_A/R_uT]}, \tag{4}$$

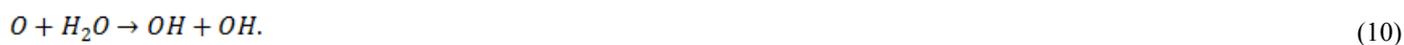where A, β and E_A are empirical values.

To simplify the chemical kinetics involved and favor the resolution of the problem, a reduction of the mechanism is made using some approximations, such as steady-state approximation 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 (Turns 2000). 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 (Peters 1988).

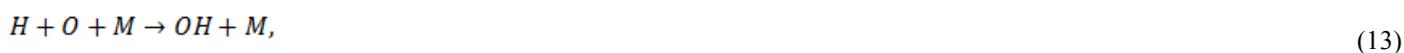## MECHANISMS OF HYDROGEN COMBUSTION

According to Turns (2000), the initiation reactions are

$$H_2 + M \rightarrow H + H + M, \tag{5}$$

$$H_2 + O_2 \rightarrow HO_2 + H. \tag{6}$$

The steps of chain-reaction involving O, H and OH radicals are

$$H + O_2 \rightarrow O + OH, \tag{7}$$

$$O + H_2 \rightarrow H + OH, \tag{8}$$

$$H_2 + OH \rightarrow H_2O + H, \tag{9}$$

$$O + H_2O \rightarrow OH + OH. \tag{10}$$

Chain-terminating steps that involves O, H and OH radicals are the three-body recombination reactions:

$$H + H + M \rightarrow H_2 + M, \tag{11}$$

$$O + O + M \rightarrow O_2 + M, \tag{12}$$

$$H + O + M \rightarrow OH + M, \tag{13}$$

$$H + OH + M \rightarrow H_2O + M. \tag{14}$$

With the objective of completing the mechanism, reactions involving HO_2, the hydroperoxy radical, and H_2O_2, hydrogen peroxide, are included. When the reaction below becomes active,

$$H + O_2 + M \rightarrow HO_2 + M, \tag{15}$$

then the following reactions enter the system:

$$HO_2 + H \rightarrow OH + OH, \tag{16}$$

$$HO_2 + H \rightarrow H_2O + O, \tag{17}$$

$$HO_2 + O \rightarrow O_2 + OH, \tag{18}$$

and

$$HO_2 + HO_2 \rightarrow H_2O_2 + O_2, \tag{19}$$

$$HO_2 + H_2 \rightarrow H_2O_2 + H, \tag{20}$$

With

$$H_2O_2 + OH \rightarrow H_2O + HO_2, \tag{21}$$

$$H_2O_2 + H \rightarrow H_2O + OH, \tag{22}$$

$$O_2 + H \rightarrow HO_2 + H_2, \tag{23}$$

$$H_2O_2 + M \rightarrow OH + OH + M. \tag{24}$$

Depending on the temperature and pressure conditions, the reverse reactions may be relevant too. Therefore, in the modeling of the $H_2 - O_2$ system can be taken into account up to forty reactions involving the eight species: H_2, O_2, H_2O, OH, O, H, HO_2 and H_2O_2. For the set of elementary reactions (5-24), the balance equations for the hydrogen, using the operator $\omega_i = k_i[A][B]$ for the reaction i defined by $A + B = C + D$, can be written as (Peters 1992; De Bortoli 2012):

$$\frac{d[H_2]}{dt} = -\omega_1 + \omega_{1b} - \omega_3 + \omega_7 + \omega_{11} + \omega_{17},$$

$$\frac{d[H]}{dt} = +\omega_1 - \omega_{1b} + \omega_2 + \omega_3 - \omega_4 - \omega_6 - \omega_7 - \omega_8 - 2\omega_{11} - \omega_{13} - \omega_{17} - \omega_{18},$$

$$\frac{d[O_2]}{dt} = +\omega_2 - \omega_4 + \omega_5 + \omega_7 + \omega_9 + \omega_{14} + \omega_{15},$$

$$\frac{d[O]}{dt} = -\omega_2 - \omega_3 + \omega_8 - \omega_9 + \omega_{10} - \omega_{13} - 2\omega_{14} - \omega_{19},$$

$$\frac{d[H_2O]}{dt} = +\omega_1 - \omega_{1b} + \omega_5 + \omega_8 + \omega_{10} + \omega_{12} + \omega_{18} + \omega_{20},$$

$$\frac{d[OH]}{dt} = -\omega_1 + \omega_{1b} - \omega_2 + \omega_3 - \omega_5 + 2\omega_6 + \omega_9 - 2\omega_{10}$$
$$-\omega_{12} + \omega_{13} - 2\omega_{16} + \omega_{18} + \omega_{19} - \omega_{20},$$

$$\frac{d[HO_2]}{dt} = +\omega_4 - \omega_5 - \omega_6 - \omega_7 - \omega_8 - \omega_9 - 2\omega_{15} + \omega_{17} + \omega_{19} + \omega_{20},$$

$$\frac{d[H_2O_2]}{dt} = +\omega_{15} + \omega_{16} - \omega_{17} - \omega_{18} - \omega_{19} - \omega_{20}. \tag{25}$$

Assuming the steady-state hypothesis for the species O, OH, HO_2 and H_2O_2, their differential operators are equal to zero, which leads to four equations among the reaction rates ω_i:

$$\omega_6 = +\omega_4 - \omega_5 - \omega_7 - \omega_8 - \omega_9 - \omega_{15} + \omega_{16} - \omega_{18},$$
$$\omega_{12} = -\omega_1 + \omega_{1b} - 2\omega_2 + 2\omega_4 - 3\omega_5 - 2\omega_7 - \omega_8 - 2\omega_9$$
$$-\omega_{10} - 2\omega_{14} - 3\omega_{15} - \omega_{16} + \omega_{17} + \omega_{19},$$
$$\omega_{13} = -\omega_2 - \omega_3 + \omega_8 - \omega_9 + \omega_{10} - 2\omega_{14} - \omega_{19},$$
$$\omega_{20} = +\omega_{15} + \omega_{16} - \omega_{17} - \omega_{18} - \omega_{19}. \tag{26}$$

Making the rates ω_I e ω_{II} equal to $\omega_I = -\omega_2 + \omega_4 - \omega_5 - \omega_7 - \omega_9 - \omega_{14} - \omega_{15}$ and $\omega_{II} = -\omega_1 + \omega_{1b} - 3\omega_2 - \omega_3 + 3\omega_4 - 3\omega_5 - 2\omega_7 - 3\omega_9 + \omega_{11} - 3\omega_{14} - 3\omega_{15} + \omega_{17},$ results the following linear combinations:

$$\frac{d[H_2]}{dt} = -3\omega_I + \omega_{II}$$

$$\frac{d[H]}{dt} = +2\omega_I - 2\omega_{II}$$

$$\frac{d[O_2]}{dt} = -\omega_I$$

$$\frac{d[H_2O]}{dt} = +2\omega_I \tag{27}$$

The stoichiometry of these balance equations corresponds to the global mechanism of two-step for the hydrogen, where M is an inert needed to remove the bond energy that is liberated during recombination (Peters 1992):

$$
\begin{aligned}
I \quad & 3H_2 + O_2 = 2H + 2H_2O \\
II \quad & H + H + M = H_2 + M
\end{aligned}
\tag{28}
$$

The main advantage of this mechanism is the reduction of the system stiffness, reducing the time required for the solution of reactive flows. This method can be used for obtaining reduced mechanisms for more complex fuels, such as methanol, ethanol and biodiesel.

ROSENBROCK METHODS

It is desirable that the method to be implemented for numerical integration of stiff systems of ordinary differential equations be stable in a large region of the real negative part of the complex λh-plane, as well as accurate in some neighbourhood of the origin. Most explicit methods have a bounded region of stability, which requires small step sizes of integration even for moderately stiff systems (Bui 1979b). For extremely stiff systems, it is desirable to develop a L-stable method rather than A-stable or stiffly stable methods, since in general these last methods, which are not damped maximally as $\lambda h \to -\infty$, are not satisfactory (Bui 1979c). This undesirable asymptotic behaviour often results in oscillatory solutions for stiff problems. In this work, an L-stable method is implemented based on a class of Runge-Kutta methods known as the 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 of good stability (Butcher 1964). In order to propose an alternative for the solution of implicit equations, Rosenbrock (1963) presented a new method. He developed a new class of single-step methods, which is based on linearizations of the implicit Runge-Kutta methods. Thus, it is avoided the resolution of non-linear systems to solve a sequence of linear systems, which facilitates the implementation of the method. This method is also found in the literature as a linearly implicit Runge-Kutta method or as diagonally implicit Runge-Kutta method.

Table 1. Parameters of fourth-order L-stable Rosenbrock method [Bui 1977]

w_1	0.9451564786	a_{31}	0.1012236115
w_2	0.341323172	a_{32}	0.9762236115
w_3	0.5655139575	a_{41}	0.3922096763
w_4	0.8519936081	a_{42}	0.7151140251
a_{21}	0.5	a_{43}	0.1430371625
b_{ij}	$0, for\ i = 2,3,4\ and\ j = 1,2,\dots,i$	1	

Table 2. Comparison between present work, Lorenzetti et al [2010] and experimental values

X/D	Present work	Lorenzetti et al [2010]	Experimental value [Sandia 2010]
5	0,00733082	0,00073848	0,00156
10	0,02198189	0,0080656	0,0251
15	0,04515112	0,02755	0,0583
20	0,07386720	0,068598	0,0924
25	0,10484718	0,11501	0,127
30	0,13507058	0,15291	0,15
35	0,16220864	0,16148	0,154
40	0,13610308	0,14699	0,132
45	0,10345754	0,12357	0,105
50	0,07984447	0,099465	0,0909
55	0,06405627	0,082871	0,0673
60	0,05448827	0,066507	0,0619
65	0,04950991	0,054543	0,0514

According to Bui (1979a), the s-stage Rosenbrock procedure for solving the following system

$$
\begin{aligned}
\frac{dy}{dx} &= f(y) \qquad x > x_0 \\
y(x_0) &= y_0
\end{aligned}
\tag{29}
$$

where $x \in \mathbb{R}$, $y(x) \in \mathbb{R}^n$, $y_0 \in \mathbb{R}^n$ and $f: \mathbb{R}^n \to \mathbb{R}^n$ is assumed to be analytic in the neighbourhood of y_0. The Rosenbrock method is given by:

$$y_{m+1} = y_m + h \sum_{i=1}^{s} w_i \kappa_i ,$$

$$\kappa_i = f\left(y_m + h \sum_{j=1}^{i-1} a_{ij}\kappa_j\right) + d_i h \frac{\delta f}{\delta y}\left(y_m + h \sum_{j=1}^{i-1} b_{ij}\kappa_j\right)\kappa_i.$$

(30)

The conditions of L-stability are:

- $|y_{m+1}/y_m| \leq 1$ on Real(λh) = 0.
- y_{m+1}/y_m has lower numerator degree than denominator degree in $q = \lambda h$.

Consider that

$$\frac{y_{m+1}}{y_m} = \frac{\sum_{i=0}^{r} \alpha_i q^i}{\prod_{i=1}^{s}(1 - d_i q)} = R_{r,s}(q) \ where \ r \leq s \ and \ \alpha_0 = 1,$$

(31)

where $d_i = d$ (for all i) is the inverse of one of the roots of the Laguerre polynomial of degree s.

Four-Stage Method of Order Four

The roots of the Laguerre polynomial of degree 4 are 0.3225476896, 1.7457611012, 4.5366202969 and 9.3950709123, so the parameter d should have one of the following values: $d_1 = 3.100316735$, $d_2 = 0.5728160625$, $d_3 = 0.2204284103$ or $d_4 = 0.1064387921$. Using d_2 for the parameter d, Bui (1977) developed a fourth-order L-stable method which also minimizes the error constant. This method is defined by the set of parameters contained in Table 1.

Order conditions

The coefficients used in the Rosenbrock method determine new properties of stability and order conditions, different from the conditions of the Runge-Kutta methods. According to Lambert (1991), to obtain a Runge-Kutta method of highest order, we must expand the equation in Taylor series to the desired order and compare the results with the Taylor's correct answer. Further details on the development for high-order Runge-Kutta methods are contained in Butcher (1964) or Hairer; Norsett; Wanner (1987). Similarly, the order conditions for the fourth-order Rosenbrock method are:
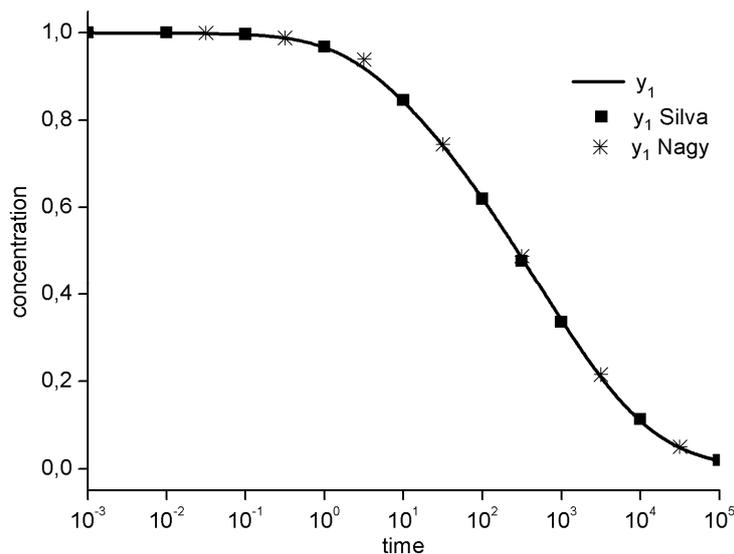

Figure 1: First variable of Robertson's model.

$$\sum_{i=1}^{4} w_i = 1$$

(32a)

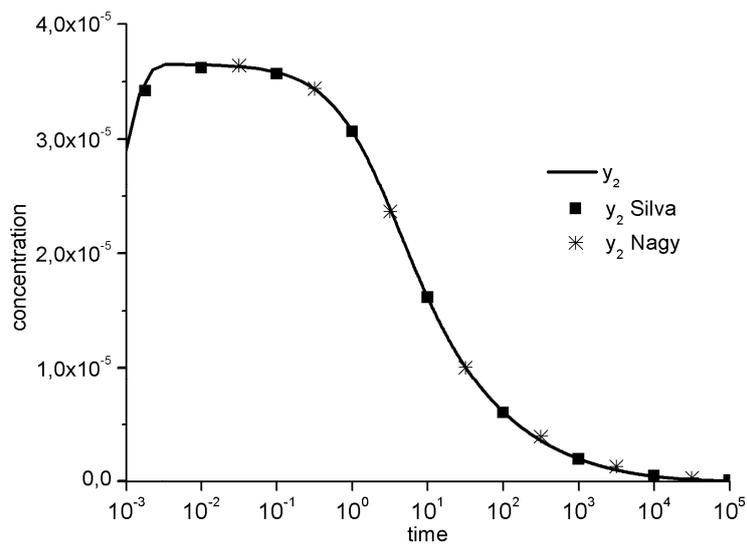$$\sum_{i=1}^{4} w_i \alpha_i = \frac{1}{2} - d$$

(32b)

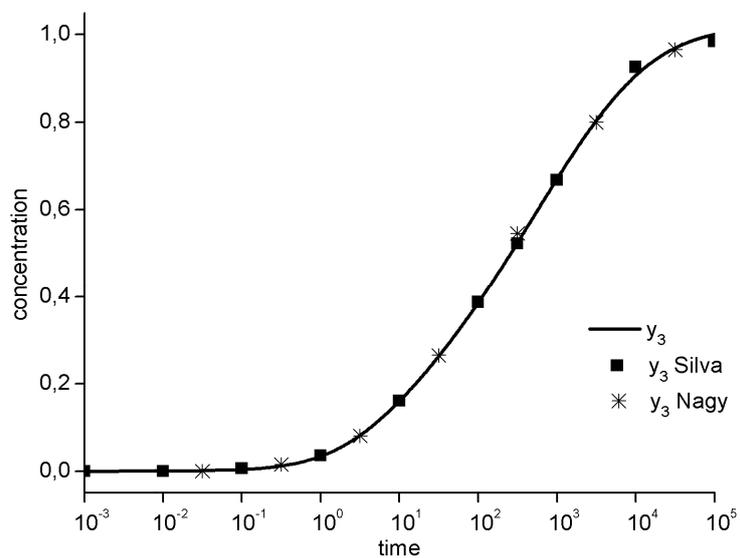**Figure 2: Second variable of Robertson's model**

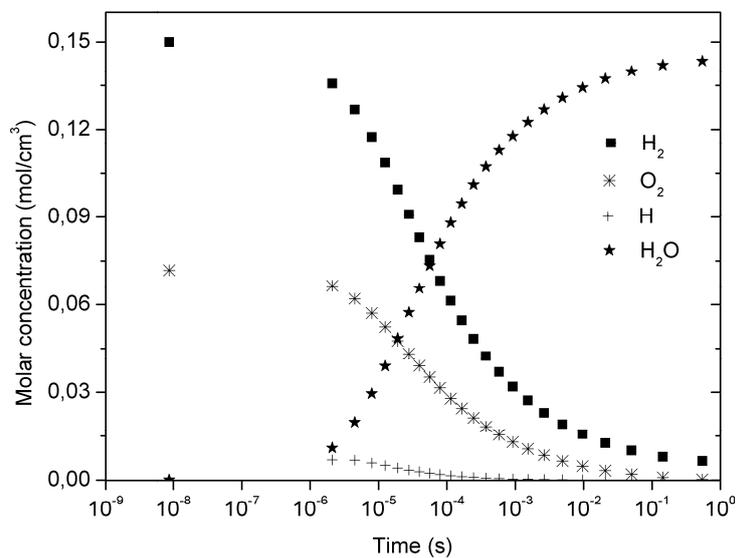**Figure 3: Third variable of Robertson's model.**
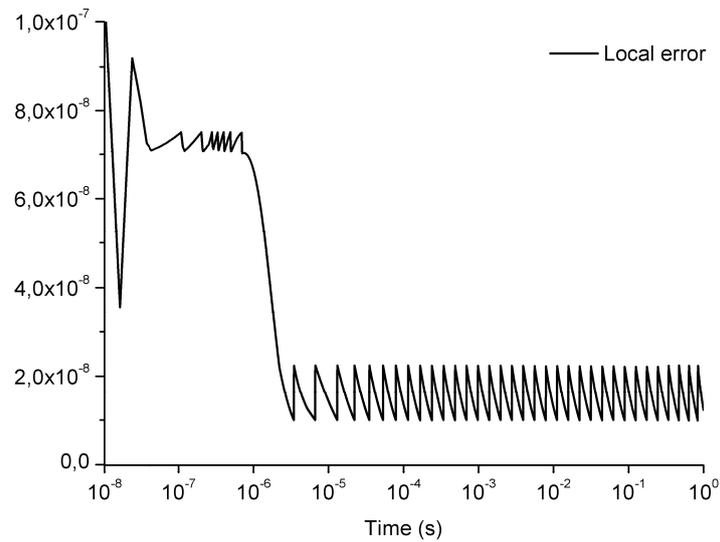

Figure 4. Reduced mechanism integrated by Rosenbrock
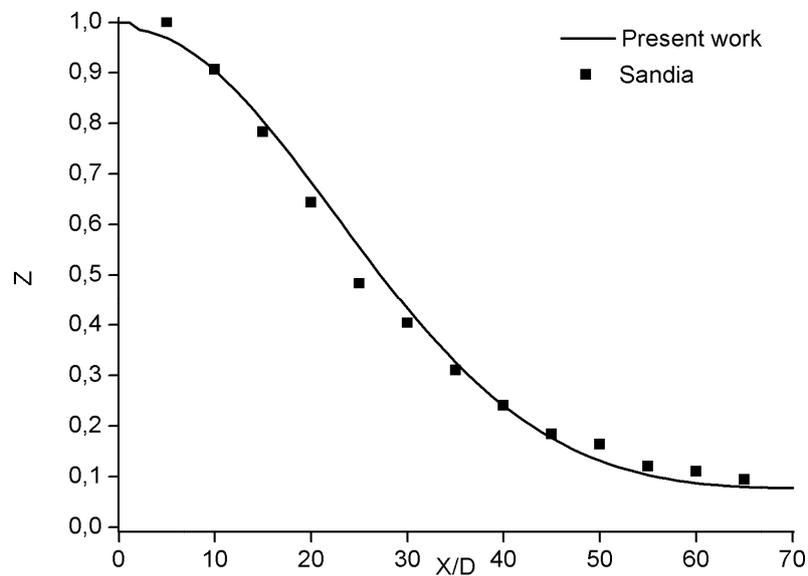
Figure 5: Local error over time interval.

Figure 6. Comparison of the mixture fraction for H_2/N_2 jet with experiment.

$$\sum_{i=1}^{4} w_i \alpha_i^2 = \frac{1}{3}$$

(32c)

$$\sum_{i=1}^{4} w_i \alpha_i^3 = \frac{1}{4}$$

(32d)

$$\alpha_2 a_{32} w_3 + (\alpha_2 a_{42} + \alpha_3 a_{43}) w_4 = d^2 - d + \frac{1}{6}$$

(32e)

$$\alpha_2^2 a_{32} w_3 + (\alpha_2^2 a_{42} + \alpha_3^2 a_{43}) w_4 = \frac{1}{12} - \frac{d}{3}$$

(32f)

$$\alpha_2 \alpha_3 a_{32} w_3 + (\alpha_2 a_{42} + \alpha_3 a_{43}) \alpha_4 w_4 = \frac{1}{24} - \frac{d}{3}$$

(32g)

$$\alpha_2 a_{32} a_{43} w_4 = -d^3 + \frac{3}{2} d^2 - \frac{1}{2} d + \frac{1}{24}$$
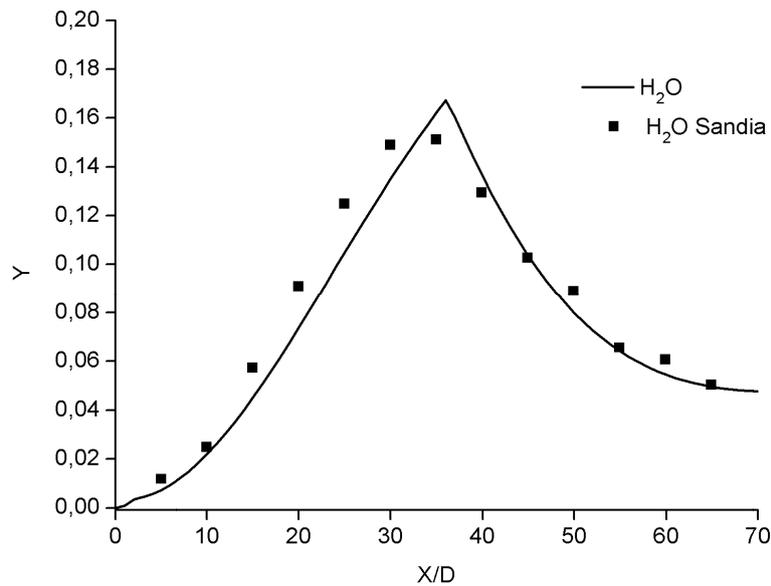
(32h)

Figure 7. Mass fraction of H_2O along the burner centerline.

and considering $\alpha_i = \sum_{j=1}^{i-1} a_{ij}$, for $i = 2, 3, 4$ and $\alpha_1 = 0$.

The local error estimation is given by

$$E_{n+1} = \frac{\|y_{n+1}^* - y_{n+1}\|}{(2^4 - 1)},$$

(33)

considering the norm $\| \cdot \|$ as

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

(34)

The variables y_{n+1}^* and y_{n+1} are calculated using step-size 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 equation, agreeing with De Bortoli (2015):

$$h_{n+1} = h_n \min \left[10, max \left(0.1; \frac{0.9}{\Delta y} \right)^2 \right].$$

(35)

It is also necessary that the values of the step-size be limited by maximum and minimum values. The initial time increment must be small enough and, in case of h_{n+1} rejection, the growth factor should be replaced by 1, instead of 10, in the next iteration.

Code verification

To evaluate the efficiency of the method used, some differential equation systems usually applied in numerical tests were selected. Robertson's (1966) model is one of the most well known problems for the analysis of stiff systems. The model describes the kinetics of an autocatalytic reaction whose reaction structure is given in.

$$y_1 \xrightarrow{k_1} y_2$$
$$y_2 + y_2 \xrightarrow{k_2} y_2 + y_3$$
$$y_2 + y_3 \xrightarrow{k_3} y_1 + y_3$$

(36)

where k_1, k_2 and k_3 are the specific rates 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 species involved.

The model equation can be written as

$$\frac{dy_1}{dt} = -0.04y_1 + 10^4 y_2 y_3,$$

(37a)

$$\frac{dy_2}{dt} = 0.04y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2,$$

(37b)

$$\frac{dy_3}{dt} = 3 \cdot 10^7 y_2^2.$$

(37c)

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

$$y_1(t_0) = 1,$$
$$y_2(t_0) = 0,$$
$$y_3(t_0) = 0.$$

(38)

The points obtained from the integration developed by Silva (2013), using the Modified Extended Backward Differentiation Formulae (MEBDF), are shown in figures 1, 2 and 3 by squares. The stars corresponds to results obtained by Nagy *et al.* (2014) using MATLAB and the continuous line shows the results of fourth order Rosenbrock method.

RESULTS AND DISCUSSION

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 and an adaptive control for the time-step. The numerical method was implemented in Fortran language. A tolerance for error $\varepsilon = 10^{-7}$ was assumed. Figure 4 shows the results and Figure 5 shows the local error. As no experimental data for comparison of molar concentration of hydrogen was found in the literature, in the following the mixture fraction was compared to experimental values obtained from the researches of the Sandia National Laboratory (2010). The result for the mixture fraction (Z), shown in Figure 6, indicates the decay of the centerline velocity with downstream distance from the entrance. Based on the Burke-Schumann analytical solution (Warnatz *et al* 2006) and the equations presented by Lorenzetti *et al* (2010), the mass fraction of H_2O along the burner centerline is presented. The nitrogen acts as an inert, not affecting the jet diffusion flame. The result, shown in Figure 7, is satisfactory, despite the use of a simple model. The results obtained for the H_2O mixture fraction can now be compared with those of Lorenzetti *et al* (2010), and with the experimental data of Sandia National Laboratories (2010). The comparison is shown in Table 2. In some intervals, the values obtained are now closer to the experimental ones, as seen at X/D between 10 to 20 and 40 to 45, for example.

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