

Analytical-numerical solution for turbulent jet diffusion flames of hydrogen

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Received: 30 August 2012 / Accepted: 27 September 2012 / Published online: 13 October 2012
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Abstract The hydrogen fuel seems to be a good candidate to replace the energy obtained from some fossil fuels. Therefore this work explains the process of obtaining a two-step reduced chemical kinetic mechanism for the hydrogen combustion. The development of a reduced mechanism consists in eliminating reactions that produce negligible influence on the combustion process. Moreover, for this mechanism, we obtain an analytical-numerical solution for a turbulent jet diffusion flame. To quantify the intermediate species, the mixture fraction is decomposed into three parts, each part directly related to the mass fraction of a species. The governing equations are discretized using the second order finite-difference approach and are integrated in time using the second order simplified three-step Runge-Kutta scheme. Obtained results compare favorably with data in the literature for a 50/50 % volume $H_2 - N_2$ jet diffusion flame. The main advantage of this strategy is the decrease of the work needed to solve the system of governing equations, by one order of magnitude for the hydrogen.

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Keywords Analytical-numerical solution · Diffusion flames · Hydrogen · Reduced kinetic mechanism

1 Introduction

Hydrogen can be obtained from fossil fuels or conveniently from renewable resources as a biofuel. Biofuels refer to liquid or gaseous fuels predominantly produced from biomass. In the context of reducing CO_2 emissions from power production, the hydrogen has recently drawn increased attention as a clean fuel [1]. Although it does not produce harmful emissions such as CO_2 , CO , soot and unburnt hydrocarbons, the high adiabatic temperatures of H_2 /air mixture originate large amounts of thermal NO_x in the flame. The hydrogen is an important intermediate species in the oxidation of hydrocarbons as well as of oxygenated fuels. The elementary kinetics of H , O , OH , HO_2 , H_2 and H_2O_2 determine the composition of the radical pool in hydrocarbon and oxygenated fuels reaction systems [2].

The ignition process of hydrogen with oxygen changes dramatically depending on the initial gas temperature and on the mixture fraction. Hydrogen combustion is strongly affected by molecular diffusion processes and has short ignition times, high laminar flame speed, and a wide flammability range. In a nonhomogeneous system, there are different reduced mechanisms appropriate for different zones, depending on the temperature and on the species concentrations [3].

There is an increasing interest in the study of hydrogen diffusion flames, since its kinetics is very well understood and because of its key role in hydrocarbon combustion. Reduced kinetics mechanisms for hydrogen combustion have been developed by several researchers, e. g., Peters and Rogg [4], Kreutz and Law [5], Saxena and Williams [6], Ströhle and Myhrvold [1], Lorenzetti et al. [7], among others. The basics of a reduced mechanism is the elimination of reactions that produce negligible influence on the overall combustion process [1]. According to Peters and Rogg [4], the two-step mechanisms are appropriate for hydrogen-air premixed and diluted and non-diluted diffusion flames.

The mixture fraction is a variable frequently used to describe nonpremixed flames. The mixture fraction measures the mixture of reagents and is mainly related to the large scale motions of the flow. However, with a single value of the mixture fraction it is not possible to account for products of incomplete combustion, or even the mixing of unburned fuel and oxygen. Instead, we need to decompose the mixture fraction into constitutive parts that represent the products of the different reactions [8]. The number of components depends on the complexity of the phenomenon.

In this work, we show the steps to develop a two-step reduced kinetic mechanism for hydrogen, and an analytical-numerical solution for a hydrogen jet diffusion flame, based on the decomposition of the mixture fraction. The set of governing equations is presented in the Favre averaging form. To validate the mechanism and the analytical procedure the numerical results for a H_2 - N_2 jet diffusion flame are compared with data from the literature.

2 Reduced kinetic mechanism for the hydrogen

The main difficulty of the use of detailed kinetic mechanisms to analyze flames is that a conservation equation must be solved for each species. Therefore, it is desirable to use simplified kinetic mechanisms that describe the reaction system in terms of few species, obtained using the assumptions of steady-state and partial equilibrium, for example. Then, such mechanisms are valid for certain conditions, i. e., they produce good results for certain ranges of temperature and composition of the mixture [9].

For a homogeneous system, the steady-state assumption is valid for those intermediate species that are produced by slow reactions and consumed by fast reactions, so that their concentrations remain small. The partial equilibrium hypothesis is justified when the rate coefficients of forward and backward reactions are much larger than all the other rate coefficients of the reactions of the mechanism [10].

Consider the basic hydrogen mechanism shown in the Table 1 (with rate coefficients from Mehl et al. [11]). To obtain a reduced kinetic mechanism of two-step for the hydrogen, initially it is estimated the magnitude of the rate coefficients k using the modified equation of Arrhenius

$$k = AT^n \exp\left(-\frac{Ea}{RT}\right) \quad (1)$$

where A is the frequency factor, T the temperature, n the temperature exponent, Ea the activation energy, and R the gas constant. With this equation it is defined the main chain of the process: H_2-H_2O . For high temperatures ($T > 1, 800 K$) and $p = 1 bar$, the reaction rates of some forward and backward reactions are so high, that the partial

Table 1 Hydrogen mechanism rate coefficients (units are mol, cm^3, s, K and cal/mol)

Reaction	A	n	Ea
1f $H + O_2 = O + OH$	3.55E+15	-0.406	1.66E+04
1b $O + OH = H + O_2$	1.03E+13	-0.015	-1.33E+02
2f $O + H_2 = H + OH$	5.08E+04	2.670	6.29E+03
2b $H + OH = O + H_2$	2.64E+04	2.651	4.88E+03
3f $OH + H_2 = H + H_2O$	2.16E+08	1.510	3.43E+03
3b $H + H_2O = OH + H_2$	2.29E+09	1.404	1.83E+04
4f $OH + OH = O + H_2O$	1.45E+05	2.107	-2.90E+03
4b $O + H_2O = OH + OH$	2.97E+06	2.020	1.34E+04
5f $H + O_2 + M = HO_2 + M$	1.48E+12	0.600	0.00E+00
5b $HO_2 + M = H + O_2 + M$	3.09E+12	0.528	4.89E+04
6f $HO_2 + H = OH + OH$	7.08E+13	0.000	2.95E+02
6b $OH + OH = HO_2 + H$	2.03E+10	0.720	3.68E+04
7f $HO_2 + H = H_2 + O_2$	1.66E+13	0.000	8.23E+02
7b $H_2 + O_2 = HO_2 + H$	3.17E+12	0.348	5.55E+04
8f $HO_2 + OH = H_2O + O_2$	1.97E+10	0.962	-3.28E+02
8b $H_2O + O_2 = HO_2 + OH$	3.99E+10	1.204	6.93E+04

equilibrium can be considered for the reactions 1, 2 and 3 (see the Table 1). In this case, each reaction is in equilibrium and, therefore, the reaction rates of forward and backward reactions are similar, i. e.,

$$k_{1f}[H][O_2] \sim k_{1b}[O][OH] \tag{2}$$

$$k_{2f}[O][H_2] \sim k_{2b}[H][OH] \tag{3}$$

$$k_{3f}[OH][H_2] \sim k_{3b}[H][H_2O] \tag{4}$$

resulting in

$$[H] = \left(\frac{k_{1f}k_{2f}k_{3f}^2[O_2][H_2]^3}{k_{1b}k_{2b}k_{3b}^2[H_2O]^2} \right)^{\frac{1}{2}} \tag{5}$$

$$[O] = \frac{k_{1f}k_{3f}[O_2][H_2]}{k_{1b}k_{3b}[H_2O]} \tag{6}$$

$$[OH] = \left(\frac{k_{1f}k_{2f}[O_2][H_2]}{k_{1b}k_{2b}} \right)^{\frac{1}{2}} \tag{7}$$

After applying the steady-state hypothesis for the species HO_2 , OH and O , it is obtained the following two-step mechanism for the hydrogen



This mechanism can be justified by an asymptotic analysis, which is a method of describing limiting behavior. It employs the concept of a limit to identify reactions, critical conditions and other important parameters in nonlinear natural phenomena. Here it consists in assuming the steady-state hypothesis for certain species, obtaining algebraic equations among the reaction rates. Then, the global mechanism is defined by the stoichiometry of the balance equations.

For the set of elementary reactions shown in the Table 1, the balance equations for the hydrogen are written as

$$w_{H_2} = -w_2 - w_3 + w_7 \tag{10}$$

$$w_{O_2} = -w_1 - w_5 + w_7 + w_8 \tag{11}$$

$$w_{H_2O} = w_3 + w_4 + w_8 \tag{12}$$

$$w_H = -w_1 + w_2 + w_3 - w_5 - w_6 - w_7 \tag{13}$$

$$w_O = w_1 - w_2 + w_4 \tag{14}$$

$$w_{OH} = w_1 + w_2 - w_3 - 2w_4 + 2w_6 - w_8 \tag{15}$$

$$w_{HO_2} = w_5 - w_6 - w_7 - w_8 \tag{16}$$

The plus sign refers to species that appear on the right side of an elementary reaction, while the minus sign refers to species on the left. For example, in the reaction 1f:

$H + O_2 = O + OH$, $w_H = -w_{1f}$ and $w_{OH} = +w_{1f}$, repeating this procedure for all other species and reactions of the mechanism.

Note that

$$w_1 = w_{1f} - w_{1b} \quad (17)$$

$$w_2 = w_{2f} - w_{2b} \quad (18)$$

$$w_3 = w_{3f} - w_{3b} \quad (19)$$

$$w_4 = w_{4f} - w_{4b} \quad (20)$$

$$w_5 = w_{5f} - w_{5b} \quad (21)$$

$$w_6 = w_{6f} - w_{6b} \quad (22)$$

$$w_7 = w_{7f} - w_{7b} \quad (23)$$

$$w_8 = w_{8f} - w_{8b} \quad (24)$$

It is assumed that the species HO_2 , OH and O are in steady-state and, therefore, w_i is zero for these species, leading to three algebraic equations among the reaction rates w_k . Eliminating the fastest consumption rates, i. e., w_2 in the equation for the O , w_7 for HO_2 and w_8 for OH , it results in

$$w_2 = w_1 + w_4 \quad (25)$$

$$w_7 = -2w_1 + w_3 + w_4 + w_5 - 3w_6 \quad (26)$$

$$w_8 = 2w_1 - w_3 - w_4 + 2w_6 \quad (27)$$

Making the rates w_I and w_{II} equal to

$$w_I = w_1 + w_6 \quad (28)$$

$$w_{II} = w_5 \quad (29)$$

one obtains the following linear combinations

$$w_{H_2} = -3w_1 + w_5 - 3w_6 \quad (30)$$

$$w_{O_2} = -w_1 - w_6 \quad (31)$$

$$w_{H_2O} = 2w_1 + 2w_6 \quad (32)$$

$$w_H = 2w_1 - 2w_5 + 2w_6 \quad (33)$$

Therefore, the stoichiometry of these reactions corresponds to the mechanism given by Eqs. (8) and (9), with the corresponding reaction rates

$$\begin{aligned} w_I &= w_1 + w_6 \\ &= k_{1f}[H][O_2] - k_{1b}[O][OH] + k_{6f}[HO_2][H] - k_{6b}[OH]^2 \end{aligned} \quad (34)$$

$$\begin{aligned} w_{II} &= w_5 \\ &= k_{5f}[H][O_2][M] - k_{5b}[HO_2][M] \end{aligned} \quad (35)$$

The assumptions of steady-state and partial equilibrium help to simplify the system of kinetic equations, and to minimize the computational time required for their solution, but these hypotheses are not applied in regimes of low temperatures. These hypotheses can be used since the error between the simplified and complete solution is reduced to an acceptable level [12].

3 Mathematical formulation and solution procedure for jet diffusion flame

Consider a hydrogen jet diffusion flame in which the fuel, delivered from a round nozzle, with diameter d and exit velocity u_0 , mixes with the surrounding air by convection and diffusion, as shown in the Fig. 1. The jet flame is chosen because it represents the

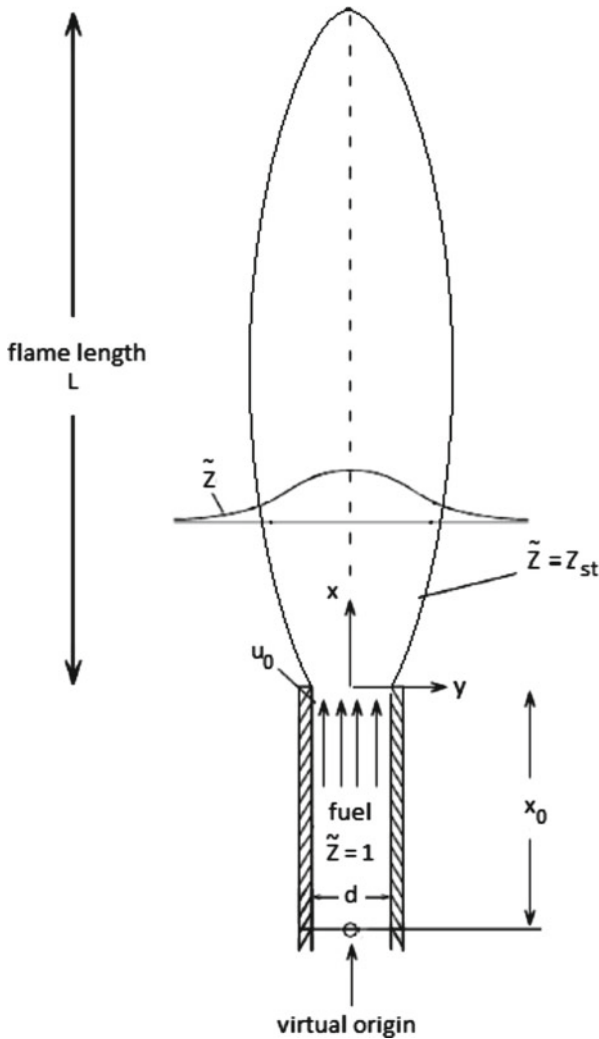


Fig. 1 Jet diffusion flame sketch

class of nonpremixed flames. Here, the effects of buoyancy and pressure gradients in the flame were neglected.

This problem is governed by the equations of continuity, momentum, mass fraction of the species i , mixture fraction and temperature. Favre filtering is used to write them conveniently.

In a homogeneous system, where a fuel stream is mixed with an oxidizer stream, the mixture fraction can be defined as the ratio between the mass fraction of the fuel, in the unburnt mixture, and the mass fraction of fuel, in the original fuel stream, $Z = Y_{F,u}/Y_{F,1}$, and is related with the fuel and the oxidizer mass fractions through the relation

$$Z = \frac{\nu Y_F - Y_{O_2} + Y_{O_{2,2}}}{\nu Y_{F,1} + Y_{O_{2,2}}} \quad (36)$$

where $\nu = (\nu_{O_2} W_{O_2})/(\nu_F W_F)$, $Y_{O_{2,2}}$ is the mass fraction of O_2 in the oxidizer stream, and W_i the molecular weight of the species i .

When solving the analytical problem for the two-step mechanism, corresponding to the Eqs. (8) and (9), the mixture fraction needs to be decomposed into parts that represent the intermediate species.

To obtain an expression for the mixture fraction, a linear combination of formation rates of the species H_2 , H and H_2O is made as

$$2w_{H_2} + 2w_{H_2O} + w_H = 0 \quad (37)$$

which can also be written as

$$2 \frac{dY_{H_2}}{W_{H_2}} + 2 \frac{dY_{H_2O}}{W_{H_2O}} + \frac{dY_H}{W_H} = 0 \quad (38)$$

Integrating this equation from time zero (unburned mixture) to a given time t , one obtains the expression

$$2 \frac{Y_{H_2} - Y_{H_2,u}}{W_{H_2}} + 2 \frac{Y_{H_2O} - Y_{H_2O,u}}{W_{H_2O}} + \frac{Y_H - Y_{H,u}}{W_H} = 0 \quad (39)$$

Using the equation $Z = Y_{F,u}/Y_{F,1}$, and considering that the concentrations of H and H_2O at the beginning of the combustion are zero, i. e., $Y_{H_2O,u} = Y_{H,u} = 0$, the mixture fraction turns

$$\tilde{Z} = \left(Y_{H_2} + \frac{W_{H_2}}{W_{H_2O}} Y_{H_2O} + Y_H \right) \frac{1}{Y_{H_2,1}} \quad (40)$$

Thus, the mixture fraction is composed by three parts

$$\tilde{Z}_1 = \frac{Y_{H_2}}{Y_{H_2,1}} \quad (41)$$

$$\tilde{Z}_2 = \frac{W_{H_2}}{W_{H_2O}} \frac{Y_{H_2O}}{Y_{H_2,1}} \tag{42}$$

$$\tilde{Z}_3 = \frac{Y_H}{Y_{H_2,1}} \tag{43}$$

Consider the equation for the mass fraction of the species i and for the temperature ($i, j = 1, 2, 3$)

$$\frac{\partial(\bar{\rho}\tilde{Y}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Y}_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Sc} \frac{\partial\tilde{Y}_i}{\partial x_j} \right) + \tilde{m}_i \tag{44}$$

$$\frac{\partial(\bar{\rho}\tilde{T})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{T})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Pr} \frac{\partial\tilde{T}}{\partial x_j} \right) + \tilde{m}_T \tag{45}$$

where ρ is the density, t the time, x_j the spacial coordinate, u_j the velocity vector, μ_t the turbulent viscosity (Smagorinsky model), T the temperature, Re the Reynolds number, Sc the Schmidt number, Pr the Prandlt number, \tilde{m}_i the production rate of the species i , and \tilde{m}_T the heat release due to chemical reactions. It results the following three equations for the mass fraction components

$$\frac{\partial(\bar{\rho}\tilde{Z}_1)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z}_1)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Sc} \frac{\partial\tilde{Z}_1}{\partial x_j} \right) + \frac{W_{H_2}}{Y_{H_2,1}} (\tilde{w}_{H_2,I} + \tilde{w}_{H_2,II}) \tag{46}$$

$$\frac{\partial(\bar{\rho}\tilde{Z}_2)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z}_2)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Sc} \frac{\partial\tilde{Z}_2}{\partial x_j} \right) - \frac{2}{3} \frac{W_{H_2}}{Y_{H_2,1}} \tilde{w}_{H_2,I} \tag{47}$$

$$\frac{\partial(\bar{\rho}\tilde{Z}_3)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Z}_3)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\frac{\bar{\mu}_t}{Re Sc} \frac{\partial\tilde{Z}_3}{\partial x_j} \right) - \frac{W_{H_2}}{Y_{H_2,1}} \left(\frac{1}{3} \tilde{w}_{H_2,I} + \tilde{w}_{H_2,II} \right) \tag{48}$$

where $\tilde{w}_{H_2,I}$ and $\tilde{w}_{H_2,II}$ correspond to the hydrogen production rate of reactions I and II of the two-step mechanism shown in (8) and (9), respectively. After adding the Eqs. (46)–(48), the source term must cancel, and it results an unique equation for the mixture fraction.

The set of governing Eqs. (46–48) with their corresponding boundary conditions is solved numerically. A forward finite difference scheme for the time derivative is employed,

$$\left(\frac{\partial f}{\partial t} \right)_{(i,j,k,t+1)} \sim \frac{f(i,j,k,t+1) - f(i,j,k,t)}{\Delta t} \tag{49}$$

and a central finite difference scheme for spatial derivatives of first-order is adopted

$$\left(\frac{\partial f}{\partial x} \right)_{(i,j,k,t)} \sim \frac{f(i+1,j,k,t) - f(i-1,j,k,t)}{2\Delta x} \tag{50}$$

$$\left(\frac{\partial f}{\partial y} \right)_{(i,j,k,t)} \sim \frac{f(i,j+1,k,t) - f(i,j-1,k,t)}{2\Delta y} \tag{51}$$

$$\left(\frac{\partial f}{\partial z}\right)_{(i,j,k,t)} \sim \frac{f(i,j,k+1,t) - f(i,j,k-1,t)}{2\Delta z} \quad (52)$$

The second-order spatial derivatives are approximated using the central finite difference scheme

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_{(i,j,k,t)} \sim \frac{f(i+1,j,k,t) - 2f(i,j,k,t) + f(i-1,j,k,t)}{(\Delta x)^2} \quad (53)$$

$$\left(\frac{\partial^2 f}{\partial y^2}\right)_{(i,j,k,t)} \sim \frac{f(i,j+1,k,t) - 2f(i,j,k,t) + f(i,j-1,k,t)}{(\Delta y)^2} \quad (54)$$

$$\left(\frac{\partial^2 f}{\partial z^2}\right)_{(i,j,k,t)} \sim \frac{f(i,j,k+1,t) - 2f(i,j,k,t) + f(i,j,k-1,t)}{(\Delta z)^2} \quad (55)$$

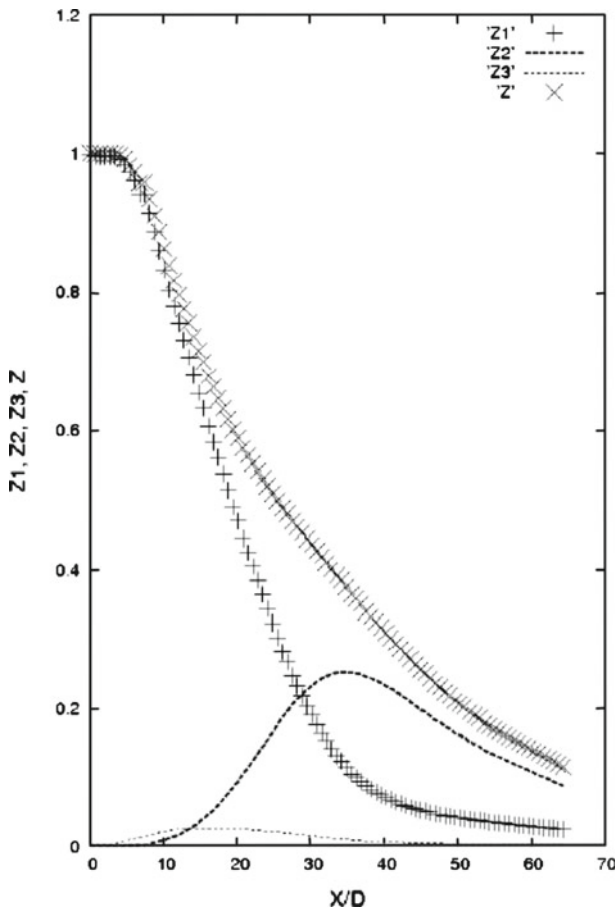


Fig. 2 Mixture fraction Z and its components Z_1 , Z_2 and Z_3 along the burner centerline

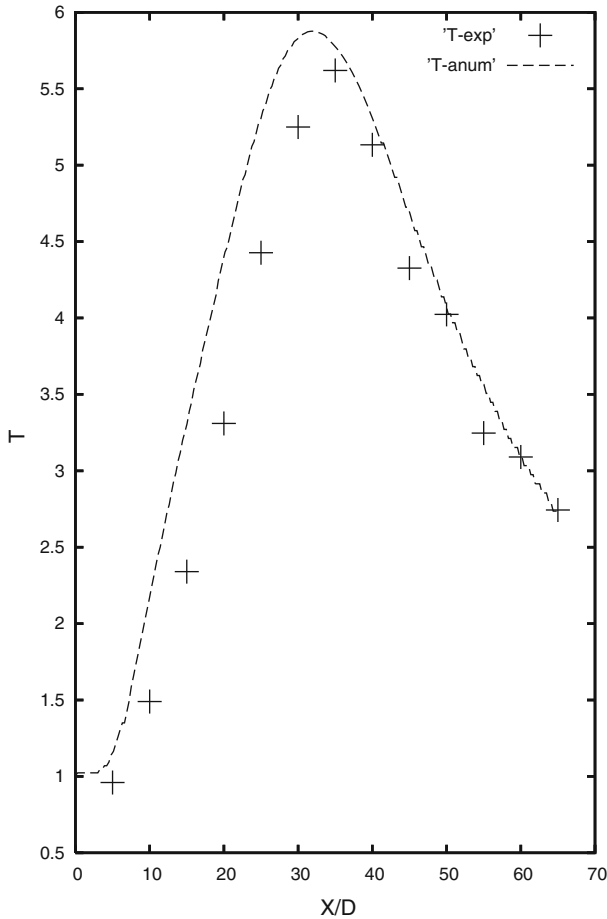


Fig. 3 Comparison of the experimental values (T-exp) [13] with the analytical-numerical values (T-anum) for the temperature mean value along the flame axis

The numerical simulations were realized using the simplified Runge-Kutta multi-step scheme. This scheme is given by

$$\vec{W}_{i,j,k}^{(0)} = \vec{W}_{i,j,k}^{(n)} \tag{56}$$

$$\vec{W}_{i,j,k}^{(r)} = \vec{W}_{i,j,k}^{(0)} - \alpha_r \Delta t \vec{R}_{i,j,k}^{(r-1)} \tag{57}$$

$$\vec{W}_{i,j,k}^{(n+1)} = \vec{W}_{i,j,k}^{(3)} \tag{58}$$

where $\vec{W}_{i,j,k} = \{\tilde{Z}_1, \tilde{Z}_2, \tilde{Z}_3, \tilde{Y}_i, \tilde{T}\}^T$, $r = 1, 2, 3$ the number of stages, and the coefficients α_r are given by $\alpha_1 = 1/2, \alpha_2 = 1/2$ and $\alpha_3 = 1$. For low Mach-numbers the Courant Friedrich-Lewy (CFL) is the convergence condition, resulting in $\Delta t = CFL \frac{V_{i,j,k}}{\lambda^i + \lambda^j + \lambda^k}$, where λ^i is the spectral ratio of the Jacobian matrix related to

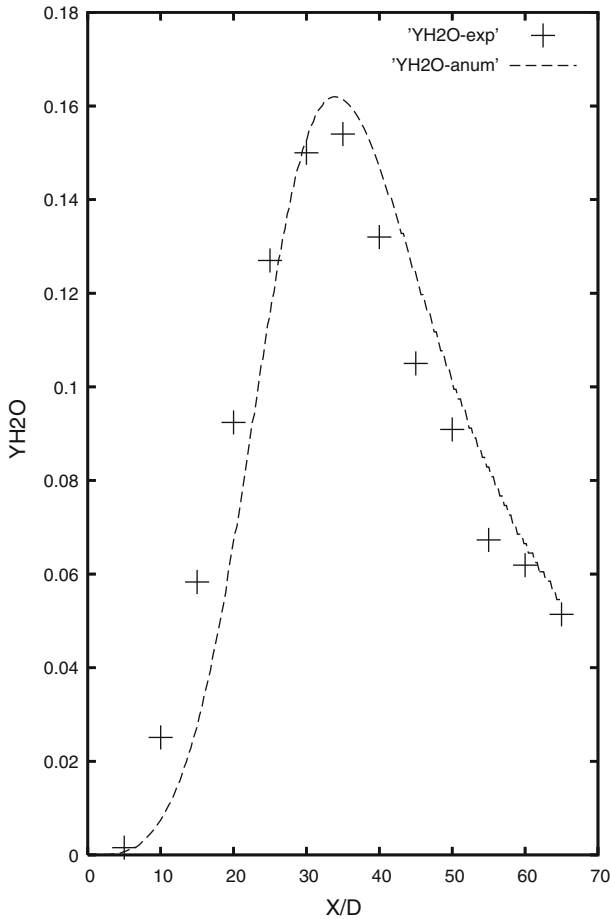


Fig. 4 Comparison of the experimental values (YH2O-exp) [13] with the analytical-numerical values (YH2O-anum) for the water vapor mean value along the flame axis

the direction \vec{i} , and similarly for λ in other directions; the CFL number is of order 2 for the Runge-Kutta of three stages.

4 Analytical/numerical results

The 50–50% volume H_2/N_2 flame [13] is chosen to obtain the results for the mixture fraction, as shown in the Fig. 2. The $\tilde{Z}_1 = Y_{H_2}/Y_{H_2,1}$ decreases with the increase of the ratio X/D , while the $\tilde{Z}_2 = (W_{H_2}Y_{H_2O})/(W_{H_2O}Y_{H_2,1})$ starts as zero and increases in the reaction zone. The same behavior is observed for $\tilde{Z}_3 = Y_H/Y_{H_2,1}$, but the magnitude of H is smaller. Due to the advection and diffusion the water vapor value remains important as X/D increases, but its magnitude is not so high far downstream from the reaction zone, due to the increase of the flame jet diameter.

Figures 3 and 4 show the nondimensional temperature and the water vapor profiles, respectively. The temperature profile is in reasonable agreement with the experiment. It rises downstream the jet entrance in the rich part of the flame and decreases by expansion in the lean flame region. It is overpredicted in the rich part of the flame due to the radiation, which is not considered in the present model. The H_2O mass fraction compares reasonably with the experiment too; the jet flame spreading is adequately captured.

In these figures, “exp” means the values of the experiment and “anum” the analytical-numerical values. The relations for T and Y_{H_2O} as a function of the mixture fraction can also be easily found in the literature (see Peters [14] and Warnatz [15]).

5 Conclusions

In this work we show the development of a reduced kinetic mechanism for hydrogen diffusion flames, considering steady-state and partial equilibrium assumptions. The main advantage of the strategy is the decrease of the work needed to solve the resultant system of chemical equations, by one order of magnitude for the hydrogen.

The main contribution of the present work is the split of the mixture fraction into three parts to obtain the intermediate species for a hydrogen jet diffusion flame, resulting in a system of three differential equations. These equations were solved for a 50–50% $H_2 - N_2$ diffusion flame, giving consistent results in comparison with the experiment.

Acknowledgments This research is being developed at the Federal University of Rio Grande do Sul - UFRGS. Andreis thanks the financial support from the *Coordenação de Aperfeiçoamento de Pessoal de Nível Superior* - CAPES - Brazil, and Prof. De Bortoli gratefully acknowledges the financial support from the *Conselho Nacional de Desenvolvimento Científico e Tecnológico* - CNPq - Brazil, under process 303007/2009-5.

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