Development of an analytical–numerical solution for a steady and axisymmetric turbulent jet diffusion flame for the hydrogen based on a reduced kinetic mechanism

F.N. Pereira [a], G.S.L. Andreis [a,b], A.L. De Bortoli [a,c,*], N.R. Marcílio [a]

[a] Graduate Program in Chemical Engineering, Federal Univ. of Rio Grande do Sul, Brazil
[b] Federal Institute of Education, Science and Technology of Rio Grande do Sul, Brazil
[c] Graduate Program in Applied Mathematics, Federal Univ. of Rio Grande do Sul, Brazil

ARTICLE INFO

ABSTRACT

The hydrogen fuel is considered to be an ideal source of energy, because its complete combustion generates no pollutants, only water vapor. Therefore, the hydrogen has been suggested as a clean fuel. A detailed kinetic mechanism for the combustion of hydrogen that comprises eight species ($H_2, O_2, O, OH, H_2O, H, HO_2$ and H_2O_2) and 20 elementary reactions, was reduced to two-step mechanism for nonpremixed flames involving four reactive species (H_2, O_2, H, H_2O). We performed, for this mechanism, a numerical analysis of the equations, including the velocity, mixture fraction, mass fractions and temperature. To quantify the components of intermediary reactions, the mixture fraction is decomposed into three parts, each part directly related to the mass fraction of each species. The results compare favorably with data in the literature for a jet diffusion flame of 50/50% in volume of $H_2 - N_2$. The main advantage of the strategy employed here is to decrease the work needed to solve the system of equations of the reactive flow.

© 2013 Elsevier Inc. All rights reserved.

1. Introduction

Biohydrogen is a replacement for fossil fuel and renewable liquid fuels, and is produced from biorenewable feedstocks by chemical, thermochemical, biological, biochemical, and biophotolytical methods [1]. Hydrogen is used in many industries as a chemical raw material, especially in the production of fertilizer, and also for producing dyes, drugs, and plastics. This fuel is used in the processing of oils and fats, as a fuel for welding, to make gasoline from coal, and to produce methanol. The supercold liquid hydrogen, in combination with liquid oxygen, is a powerful fuel for the Space Shuttle and other rockets [2]. Hydrogen gas has properties that make it suitable as a fuel for internal combustion engines in automobiles [1].

Flames of Hydrogen/air are special because no more than about 20 elementary reactions are relevant to their primary chemical kinetics, and the rate parameters for these are known better than those for other flames [3]. Usually, the computations with detailed mechanisms are complicated by the existence of highly reactive radicals, which induces significant stiffness to the governing equations due to the differences in the time scales of the species. Consequently, there exists the need to develop, from these detailed mechanisms, the corresponding reduced mechanisms of fewer variables and moderated stiffness, while maintaining the accuracy and comprehensiveness of the detailed mechanisms [4].

---

* Corresponding author. Address: Graduate Program in Applied Mathematics (PPGMAp), Federal University of Rio Grande do Sul (UFRGS), Av. Bento Gonçalves 9500, Zip Code 91509-900, PO Box 15080, Porto Alegre, RS, Brazil. Tel.: +55 51 3308 6189; fax: +55 51 3308 7301.
E-mail addresses: felipe.norte.p@gmail.com (F.N. Pereira), greice.andreis@caxias.ifrs.edu.br (G.S.L. Andreis), dbortoli@mat.ufrgs.br (A.L. De Bortoli), nilson@enq.ufrgs.br (N.R. Marcílio).

In the works from Peters [5], Peters and Rogg [6], Griffiths [7], Leung and Lindstedt [8], Marinov [9], Jazbec et al. [10], Liakos et al. [11], Lindstedt and Meyer [12], Fernández-Tarrazo et al. [13], Seiser et al. [14], and Lorenzzetti et al. [15], among many others, it is treated the reduction of chemical kinetic mechanisms. In the book from Peters and Rogg [6], it is proposed more than one reduced mechanism to the same fuel. According to them, the mechanisms of two-step are appropriate for premixed flames and diffusion flames of hydrogen-air.

Diffusion flame structures can be conveniently represented employing the mixture fraction as the independent variable. The mixture fraction represents the fuel quantity and has the value $Z = 0$ in the oxidizer stream and $Z = 1$ in the fuel stream. Most of the chemistry typically occurs near the stoichiometric value [3].

In this work, it is obtained a reduced mechanism of two steps for the hydrogen, and it is developed an analytical–numerical solution for a hydrogen diffusion flame, using the mechanism found. The set of governing equations is presented in the Favre averaged form, and includes the conservation of the mass, the momentum, the mass fraction of species, the mixture fraction and the energy. To validate the mechanism and the analytical procedure, numerical results are presented and compared with experimental values for a flame of 50/50% in volume of $H_2 - N_2$.

2. Reduced kinetic mechanism

Consider the mechanism presented by Marinov [9] for the oxidation of the hydrogen, composed by 20 reactions among eight reactive species, listed in the Table 1.

The reduced kinetic mechanism is obtained by the introduction of appropriate hypotheses of steady-state and partial equilibrium to the detailed mechanism and after neglecting terms and reactions of lesser importance [3]. The strategy consists of 5 steps:

1. Estimate the order of magnitude of the rate of reactions and define the main chain;
2. Introduce steady-state and partial equilibrium assumptions;
3. Identify the global reactions and their principal rates;
4. Justify the assumptions through asymptotic analysis;
5. Identify the limitations of the strategy.

To estimate the order of magnitude of the reactions, consider the specific rate k of each elementary reaction κ, given by the relation

$$k_\kappa = AT^\beta \exp\left(-\frac{E}{RT}\right), \tag{1}$$

where A is the frequency factor, T temperature, β the exponent of temperature, E the activation energy, and R the gas constant. With this, it is defined the main chain of the process. For the reactions of the Table 1, considering $T = 900K$, it results the main chain for the hydrogen oxidation: H_2, H, H_2O.

For a homogeneous system, the steady-state assumption is valid for those intermediate species that are produced by slow reactions and are consumed by fast reactions, so that their concentrations remain small. The partial equilibrium hypothesis

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

	Reaction	A	β	E
1	$OH + H_2 = H + H_2O$	2.14E + 08	1.520	3449
2	$O + OH = O_2 + H$	2.02E + 14	−0.400	0
3	$O + H_2 = OH + H$	5.06E + 04	2.670	6290
4	$H + O_2 + M = HO_2 + M$	4.52E + 13	0.000	0
5	$OH + HO_2 = H_2O + O_2$	2.13E + 28	−4.827	3500
6	$H + HO_2 = OH + OH$	1.50E + 14	0.000	1000
7	$H + HO_2 = H_2 + O_2$	6.63E + 13	0.000	2126
8	$H + HO_2 = O + H_2O$	3.01E + 13	0.000	1721
9	$O + HO_2 = O_2 + OH$	3.25E + 13	0.000	0
10	$2OH = O + H_2O$	3.57E + 04	2.400	-2112
11	$H + H + M = H_2 + M$	1.00E + 18	−1.000	0
12	$H + OH + M = H_2O + M$	2.21E + 22	−2.000	0
13	$H + O + M = OH + M$	4.71E + 18	−1.000	0
14	$O + O + M = O_2 + M$	1.89E + 13	0.000	-1788
15	$HO_2 + HO_2 = H_2O_2 + O_2$	4.20E + 14	0.000	11982
16	$OH + OH + M = H_2O_2 + M$	1.24E + 14	−0.370	0
17	$H_2O_2 + H = HO_2 + H_2$	1.98E + 06	2.000	2435
18	$H_2O_2 + H = OH + H_2O$	3.07E + 13	0.000	4217
19	$H_2O_2 + O = OH + HO_2$	9.55E + 06	2.000	3970
20	$H_2O_2 + OH = H_2O + HO_2$	2.40E + 00	4.042	−2162