



*Dedicated to Professor Ion Grosu
on the occasion of his 65th anniversary*

NUMERICAL STUDY OF PRESSURE AND COMPOSITION INFLUENCE ON LAMINAR FLAME PROPAGATION IN NITROGEN-DILUTED H₂-O₂ MIXTURES

Domnina RAZUS,^{a,*} Maria MITU,^a Venera GIURCAN,^a Codina MOVILEANU^a and Dumitru OANCEA^b

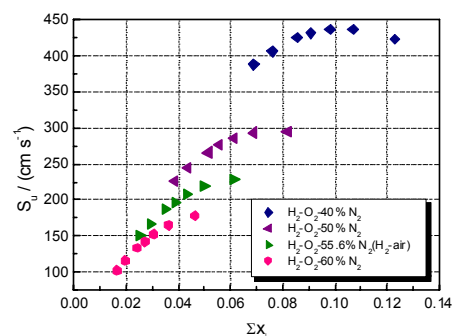
^a„Ilie Murgulescu” Institute of Physical Chemistry, 202 Spl. Independentei, 060021 Bucharest, Roumania

^bUniversity of Bucharest, Department of Physical Chemistry, 4-12 Elisabeta Blvd., 030018 Bucharest, Roumania

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The flame propagation in nitrogen-diluted stoichiometric H₂-O₂ mixtures ([N₂] = 10 – 60 vol%) was examined by the detailed chemical modelling of the isobaric deflagrations, at various initial pressures (1–10 bar). The modelling delivered the laminar burning velocity S_u and the temperature, volumetric heat release rate and species concentration profiles across the flame front, discussed in correlation with the initial composition and pressure of gaseous mixtures. For each mixture composition an empirical power law was used to examine the dependence of the laminar burning velocity on pressure, for a restricted range of pressure variation. The correlations found between the burning velocity and the mass fractions of reactive species in the flame front were discussed in connection with the non-monotonous S_u vs p dependence.

The overall activation parameters (reaction order and activation energy) of H₂-O₂ reaction in flames were determined from burning velocities dependencies on pressure and on average flame temperature.



INTRODUCTION

The laminar burning velocity is one of the most important characteristic properties of flammable fuel-oxidizer gaseous mixtures, directly correlated to the overall rate of fuel oxidation in flames. Knowledge of the laminar burning velocity is important for examining the stability of flames (connected to flashback process), for the design of various combustors and of active protection devices against damages of explosions. The laminar burning velocity is of fundamental importance for developing and testing theoretical and numerical models of laminar and

turbulent flame propagation. Together with the measured profiles of temperature, species concentrations and rate of heat delivery across the flame, the laminar burning velocity is used to validate the detailed mechanisms developed for modeling the flame propagation in various conditions of initial mixture: pressure, temperature and fuel/oxidizer ratio.^{1,2} At the same time, the laminar burning velocity is useful as input parameter for CFD (Computational Fluid Dynamics) simulations of deflagrations propagating in confined spaces or of vented explosions.^{3,4}

* Corresponding author: drazus@icf.ro; drazus@yahoo.com.

An important component of combustion research is the study of pressure influence on laminar burning velocity, meant to describe the flame propagation in real conditions and to offer information on the mechanism of fuel oxidation under flame conditions. For a constant initial composition of flammable mixtures, a frequently used relationship (especially for engineering applications) is the empirical power law which correlates S_u , the laminar burning velocity at pressure p , with reference values of the burning velocity and pressure:^{5,6}

$$S_u = S_{u,ref} \left(\frac{p}{p_{ref}} \right)^\nu \quad (1)$$

where ν is the baric coefficient and $S_{u,ref}$ is the laminar burning velocity at reference pressure p_{ref} (usually, the ambient pressure). The baric coefficient ν has negative values for most flammable gaseous mixtures, between -0.4 and -0.1.⁵⁻¹⁰ It is constant for limited ranges of initial temperature and pressure of flammable mixtures, but varies significantly by changing the fuel/oxidizer ratio and by adding inert gases to the flammable mixture.

Recent measurements and computations for $\text{CH}_4\text{-N}_2\text{-O-N}_2$ mixtures revealed a weak pressure influence on laminar burning velocities: baric coefficients between $-0.1 < \nu < -0.06$ were determined for lean and stoichiometric $\text{CH}_4\text{-N}_2\text{-O-N}_2$ mixtures diluted by 40% N_2 whereas expected baric coefficients ($-0.2 < \nu < -0.1$) were determined for lean and stoichiometric $\text{CH}_4\text{-N}_2\text{-O-N}_2$ mixtures diluted with higher nitrogen amounts (50 and 60 vol %).¹¹ Such a behavior was already found for $\text{H}_2\text{-O}_2\text{-N}_2$ mixtures:^{12,13} for the stoichiometric $\text{H}_2\text{-O}_2$ mixture diluted with N_2 (concentrations within 0-30 vol%), characterized by faster flames when compared to $\text{H}_2\text{-air}$, a weak (poor) influence of pressure on laminar burning velocities was observed, shown by absolute baric coefficients between 0.1 and 0.05. In nitrogen-diluted $\text{H}_2\text{-O}_2$ mixtures with N_2 concentrations higher than 30 vol% (including $\text{H}_2\text{-air}$) slower flames propagate and a stronger pressure influence on S_u is measured (absolute baric coefficients between 0.1 and 0.3). From extended measurements of laminar burning velocity in $\text{H}_2\text{-O}_2\text{-N}_2$ mixtures¹⁴⁻¹⁸ the pressure exponent was found dependent on temperature and dilution degree by nitrogen as well. The data confirm earlier suggestions of Günther¹⁹ and Lewis and von Elbe²⁰

who postulated the baric coefficient as being a function only of flame velocity, not of the system considered and/or the state of the flammable mixture. Other studies on flame propagation in $\text{H}_2\text{-air}$ and $\text{H}_2\text{-O}_2$ mixtures diluted by He, Ar, N_2 or steam^{18, 21-23} examined the flame structure and outlined the influence of pressure on consumption and production rates of HO, H and HO_2 radicals in the reaction zone of these flames, in order to explain the variation of their baric coefficients.

In the present paper the laminar burning velocity of the stoichiometric $\text{H}_2\text{-O}_2$ mixture diluted with various nitrogen concentrations between 10 and 60 vol% are examined, at various initial pressures between 1 and 10 bar. The $\text{H}_2\text{-O}_2$ mixtures are widely used for engine propulsion and for fuel cells.^{3,4,6} Their burning velocities, obtained by the detailed kinetic modeling of their flames, are examined in connection with variations of peak mass fractions for important radical species H, HO and O, and with the peak rate of volumetric heat release in the flame. Sensitivity analyses in respect to laminar burning velocity are used to outline the reactions most influenced by pressure variation, with impact on reactive species concentrations.

COMPUTING PROGRAM

The kinetic modelling of $\text{H}_2\text{-O}_2\text{-N}_2$ flames was performed with 1D COSILAB package developed by Rogg and Peters.²⁴ Premixed adiabatic laminar free flames were examined. As solvers, the package uses a steady Newton solver (usually 25 iterations, relative tolerance 10^{-5} ; absolute tolerance 10^{-8}), an unsteady Newton solver (usually 15 iterations, relative tolerance 10^{-4} ; absolute tolerance 10^{-6}) and an unsteady Euler solver. For the adaptive grid parameters, we used $\text{GRAD} = 0.1$, $\text{CURV} = 0.2$ and a maximum ratio of adjacent cell size between 1.3 and 1.1. The runs, performed for isobaric combustion of $\text{H}_2\text{-O}_2\text{-N}_2$ at various pressures within 1 and 10 bar and various mole fractions of N_2 , delivered the laminar burning velocities of gaseous mixtures, along with the temperature, volumetric rate of heat release and species profiles across the flame front. The modeling used an improved version of Warnatz mechanism^{12,13,25-27} based on 9 chemical species which participate to 19 elementary reactions, shown in the Appendix. The input data were taken from thermodynamic and molecular databases of Sandia National Laboratories, USA, according to the international standard (format for CHEMKIN).

In the examined mixtures the nitrogen concentration was expressed as % from the total mixture volume ($H_2 + O_2 + N_2$).

RESULTS AND DISCUSSION

1. The laminar burning velocities of H_2 - O_2 - N_2 flames

The laminar burning velocities of N_2 -diluted H_2 - O_2 flames containing various nitrogen concentrations, calculated for a constant initial temperature of 300 K, were plotted in Fig. 1(a) and 1(b) as functions of the initial pressure. At ambient initial conditions the calculated burning velocity of the stoichiometric H_2 -air mixture was $S_{u,ref} = 228$ cm/s. The reference experimental data from literature vary between 260 cm/s, data measured on flames anchored on a burner²⁸ and 210 cm/s, data measured on outwardly spherical flames propagating in a bomb and corrected for stretch effects in the early stage of flame propagation.^{16,17,29,30} At pressures higher than ambient the computed laminar burning velocities of H_2 - O_2 - N_2 flames are also close to literature values.^{16-18,21-23}

The data in Fig. 1 show different patterns of S_u variation when pressure increases from 1 to 10 bar: a steady increase of S_u for H_2 - O_2 - N_2 mixtures with $[N_2] = 0$ -20 vol% and a steady decrease of S_u for H_2 - O_2 - N_2 mixtures with $[N_2] = 55.6$ vol% (*i.e.* H_2 -air mixture) and 60 vol%. Between them, the H_2 - O_2 - N_2 mixtures with $[N_2] = 30, 40$ and 50 vol%

have a non-monotonous of S_u versus p_0 , with maxima around 2-3 bar. Similar results were reported by Sun *et al.*³¹ for H_2 -air mixtures of variable equivalence ratios. In a rich mixture ($\varphi = 1.8$) S_u increased with pressure from 0.6 atm until it reached a maximum at about 2 atm, and then decreased with pressure. Dayma *et al.*,¹⁷ Lu *et al.*¹⁸ and Kuznetsov *et al.*²² confirmed the non-monotonic behavior of the laminar burning velocity at pressure variation in their research on H_2 -air mixtures with various equivalence ratios. This behavior was assigned by Sun *et al.*³¹ and Law³² to the decrease of overall reaction orders at pressure increase.

The present data on H_2 - O_2 - N_2 mixtures delivered positive baric coefficients (in mixtures with $[N_2] = 0$ - 20 vol%) and negative baric coefficients (mixtures with $[N_2] = 40$ - 60 vol%), determined by means of the power law equation (1) applied to the increasing part of data from Fig. 1(a) and to the decreasing part of data from Fig. 1(b). Between them, the stoichiometric H_2 - O_2 mixture containing 30% N_2 seems to have positive baric coefficients at pressures within 1 and 4 bar, then negative baric coefficients at pressures within 4 and 10 bar. The results are given in Table 1. Similar to this, Szabo *et al.*²³ found that the baric coefficients of laminar burning velocities for the stoichiometric H_2 -air mixture diluted with steam are dependent on pressure and on added inert concentration.

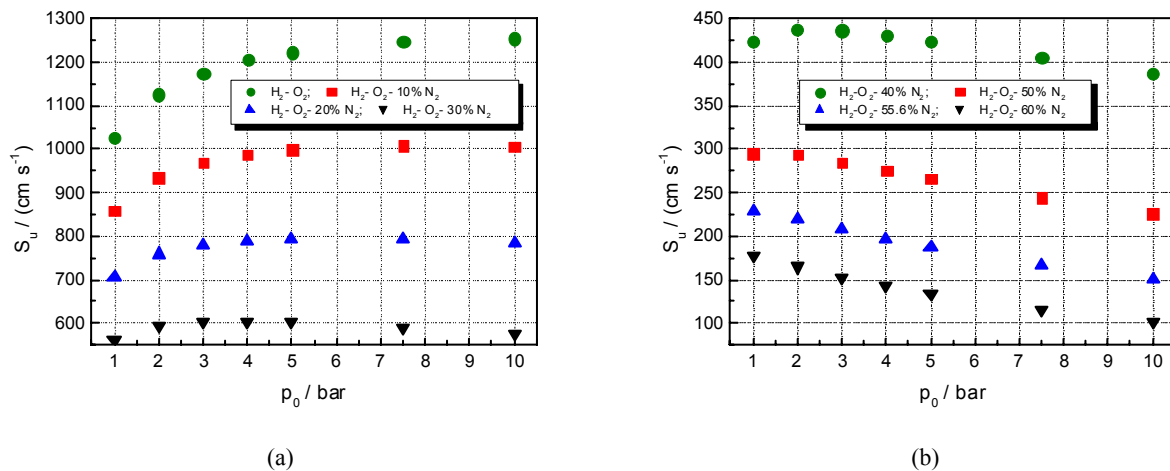


Fig. 1 – Computed laminar burning velocities of stoichiometric H_2 - O_2 - N_2 flames at various initial pressures.

Table 1

Baric coefficients, v , of laminar burning velocities for stoichiometric H_2 - O_2 - N_2 mixtures with various nitrogen concentrations, at 300 K

$[N_2]$ /vol%	0	10	20	40	50	55.6*	60
v	0.080	0.062	0.038	-0.044	-0.118	-0.177	-0.236

*stoichiometric H_2 -air

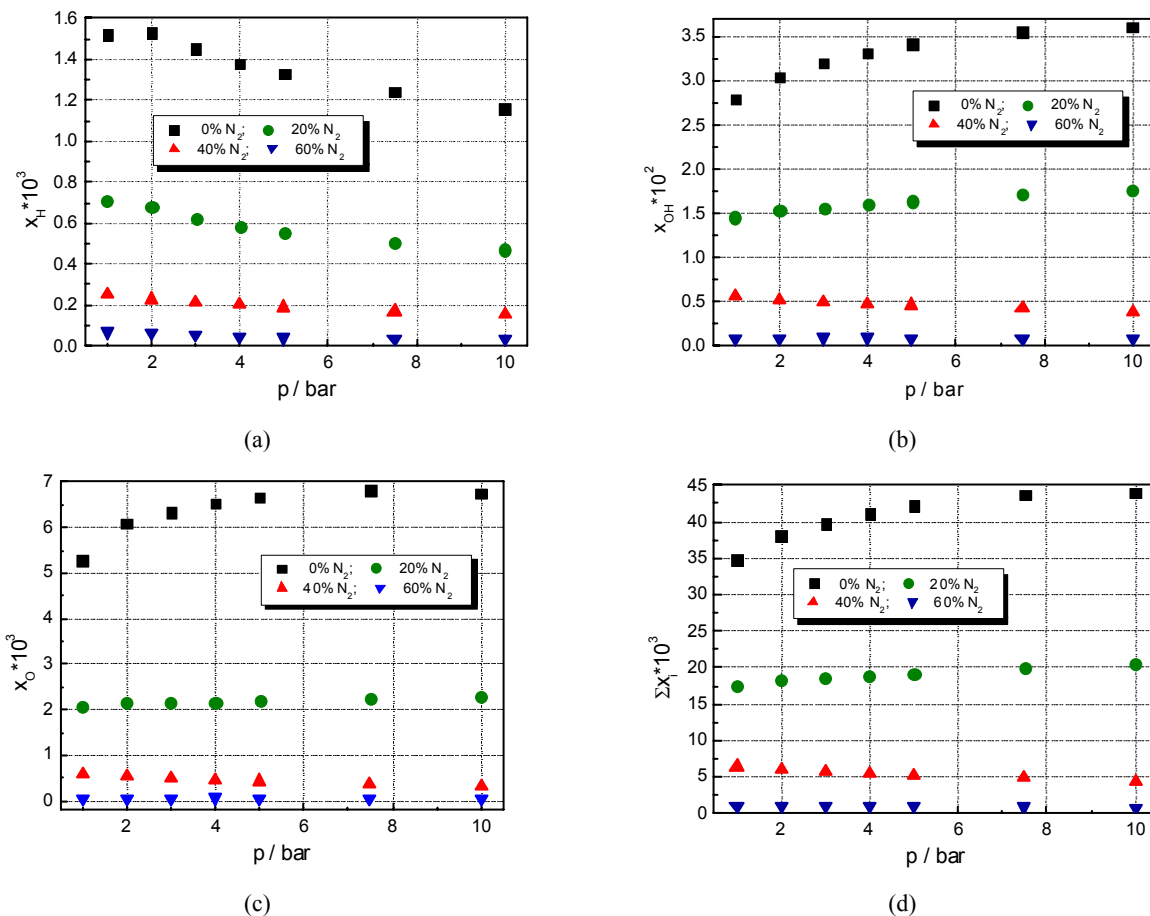


Fig. 2 – Peak mass fractions of H, OH and O ((a)-(c)) and the sum of their peak mass fractions (d) in stoichiometric H₂-O₂-N₂ flames with various N₂ concentrations as functions of the total initial pressure.

Warnatz examined the dependence of S_u on pressure for H₂-O₂-N₂ mixtures within a much wider pressure range (0.01-100 bar).^{12,13} His diagrams of $\log S_u$ vs $\log p$ for H₂-O₂ were linear at very low and at very high pressures corresponding to a power law with the baric coefficient $\nu = +0.20$. According to Warnatz¹² for each of these pressure ranges a different set of competing elementary reactions account for the observed pressure dependence of S_u . Sensitivity analyses performed at the kinetic modeling of H₂-air flames confirmed this (Dayma *et al.*,¹⁷ Lu *et al.*,¹⁸ Aung *et al.*,³⁰ Konnov³³). Hu *et al.*¹⁶ assumed that the suppression (or enhancement) of overall chemical reaction with the increase of initial pressure is due to the decrease (or increase) of H and OH mole fractions in flames. Indeed, for laminar premixed hydrogen-oxygen flames Qiao *et al.*²¹ found a linear correlation between the laminar burning velocities and (H + OH) peak mole fractions, obtained at the condition where the mole fraction of H was a maximum.

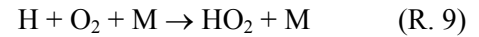
In accord to these opinions, it is important to examine first the pressure influence on H, OH and O peak mass fractions of H₂-O₂-N₂ flames (x_H , x_{OH} and x_O) with various nitrogen concentrations, shown in plots from Figures 2(a)-(c). In Figure 2(d) the sum of H, OH and O peak mass fractions is plotted against pressure; the common aspect of plots from Figures 2(a), (c) and (d) is the monotonous decrease of radical concentration with pressure. The exception is found in Figure 2(b) showing that pressure has little influence on peak mass fractions of OH, at all nitrogen dilutions.

The influence of the mass fractions of H, and of Σx_i (the sum of peak mass fractions of H, OH and O) on the laminar burning velocities of nitrogen-diluted stoichiometric H₂-O₂ flames is shown in Figures 3 and 4. A steady decrease of the laminar burning velocity with Σx_i is observed for H₂-O₂ and H₂-O₂-10 vol % N₂ flames. In contrast to them, the H₂-O₂ flames diluted with 40...60 vol% N₂ are characterized by a steady increase of the laminar

burning velocity with Σx_i . Both trends are valid for the examined pressure range, between 1 and 10 bar. A special situation is observed for H₂-O₂ flames diluted with 20 or 30 vol% N₂ where S_u reaches a maximum when examined against Σx_i .

The sensitivity analysis, revealing the influence of various elementary reactions on the laminar burning velocity, was performed for runs on stoichiometric H₂-O₂ flames diluted by N₂ at various pressures between 1 and 10 bar. The sensitivity coefficients of these reactions with respect to the laminar burning velocity of H₂-O₂ flames diluted by 30 vol% N₂ are plotted in Fig 5(a), near the plot of burning velocity against pressure shown in Fig 5(b). Data referring to reaction (R. 2) (O + H₂ → OH + H) were not plotted in Fig 5(a); the sensitivity coefficients for

this reaction in respect to the laminar burning velocity ($SC_{r,2}$) were almost constant for the pressure range between 1 and 10 bar ($SC_{r,2} = 0.156 - 0.157$). Different trends of variation are observed for the examined sensitivity coefficients at increasing pressure. Among analyzed reactions, the termolecular reaction:



is influenced in a greater extent by pressure when compared to other reactions. The sensitivity coefficients for this reaction in respect to S_u reach a peak at 2 bar, a trend of variation which is followed by the laminar burning velocity when examined against pressure (Fig. 5(b)).

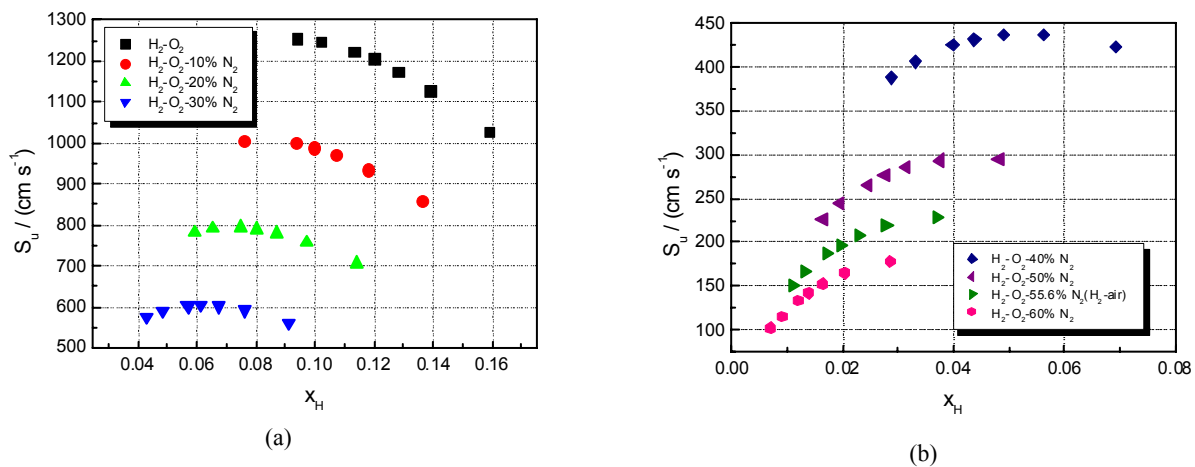


Fig. 3 – The laminar burning velocity of stoichiometric H₂-O₂-N₂ mixtures versus the peak mass fraction of H; each data set corresponds to computations at various initial pressures.

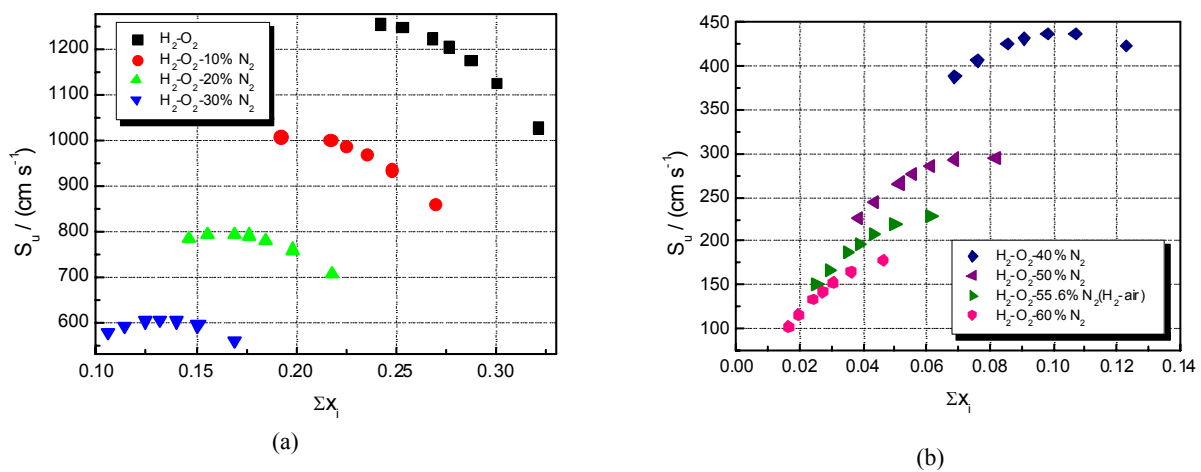
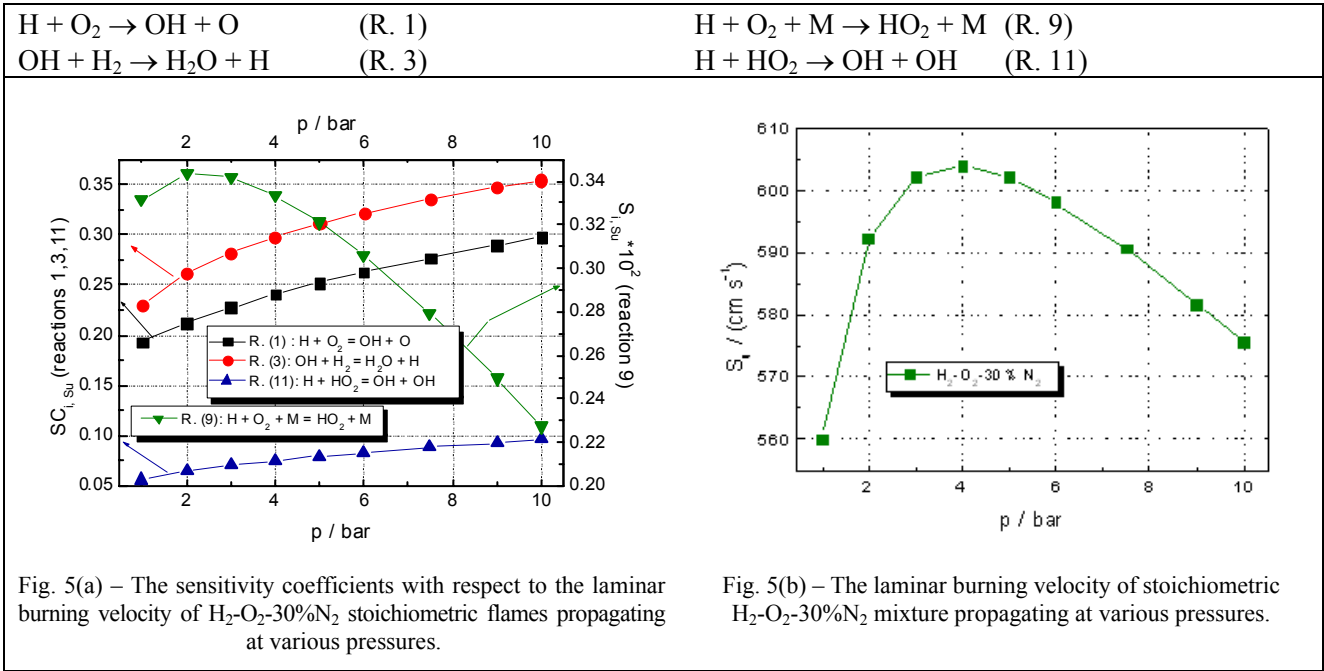


Fig. 4 – The laminar burning velocity of stoichiometric H₂-O₂-N₂ mixtures versus the sum of peak mass fractions of H, O and OH; each data set corresponds to computations at various initial pressures.



The pathway analysis of H_2 in H_2 - O_2 flames diluted by He, performed by Lu et al.,¹⁸ confirmed the decrease of H fraction at pressure increase, in spite of increased OH fraction via $H / HO_2 / OH$. According to these authors, a poorer radical pool would restrain the overall reaction rate and lead to reduction of overall reaction order and to the non-monotonic behavior of laminar burning velocities.¹⁸

2. The overall activation parameters of H_2 - O_2 reaction

According to the thermal theory of flame propagation, the laminar burning velocity is related to the overall reaction rate in the flame front:³

$$S_u \approx \left(\frac{\lambda}{\rho C_p} \cdot C_0^{1-n} \cdot \exp(-E_a / RT_{f,av}) \right)^{1/2} \quad (2)$$

where λ is the thermal conductivity, ρ - the density and C_p - the specific heat of the unburned gas; C_0 - the initial fuel concentration, $T_{f,av}$ is

the average temperature of the flame front, n and E_a are the overall activation parameters (reaction order and activation energy, respectively) and R is the universal gas constant.

At constant temperature eq. (2) can be written as:

$$S_u \approx p_0^{(1-n)/2} \quad (3)$$

after assuming that the terms involving the pressure dependence of average flame temperature $T_{f,av}$ and of thermal diffusivity $\lambda/(\rho C_p)$ have very small values and can be neglected.³⁴ According to eq. (3) the overall reaction orders, n , can be obtained from ν , the baric coefficients of burning velocities:

$$n = 2(\nu + 1) \quad (4)$$

The overall reaction orders of H_2 oxidation with O_2 in their nitrogen-diluted flames, calculated from the baric coefficients of their burning velocities, are given in Table 2.

Table 2

Overall reaction orders, n , of H_2 - O_2 reaction in N_2 -diluted flames

N_2 /vol%	0	10	20	30	40	50	55.6*	60
ν	0.080	0.062	0.038	0	-0.044	-0.118	-0.177	-0.236
n	2.16	2.12	2.08	2.00	1.91	1.76	1.65	1.53

* stoichiometric H_2 -air

Table 3

Overall (apparent) activation energy of H₂ oxidation with O₂ in stoichiometric H₂-O₂-N₂ flames, E_a / (kJ mol⁻¹); mixtures at T₀ = 300 K

p ₀ / bar	1.0	2.0	3.0	5.0	7.5	10.0
E _a / (kJ mol ⁻¹)	121	141	154	174	193	208

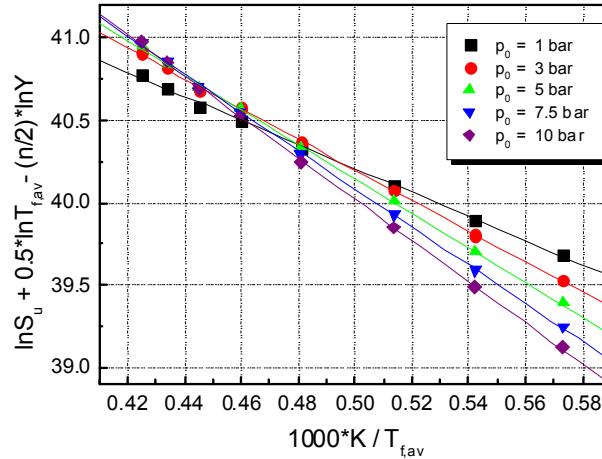


Fig. 6 – Variation of laminar burning velocity, included in the left term of eq.(5), against the reciprocal average flame temperature, for H₂-O₂-N₂ mixtures with various N₂ concentrations.

For H₂-O₂-N₂ mixtures a common trend is observed: the increase of the dilution degree results in a steady decrease of overall reaction orders, from 2.16 down to 1.65 in H₂-air mixtures and still lower (1.53) in a H₂-O₂ mixture diluted with 60% N₂. Literature data are quite scattered: for the stoichiometric H₂-air mixture, Iijima and Takeno³⁵ reported overall reaction orders between 2.3 and 2.5 whereas Sun *et al.*,³¹ and Law³² found $n = 2.0$ at 1 bar.

Using the present reaction orders, n , the overall activation energies were determined with equation (2) modified in order to account for the flame temperature variation determined by the dilution with an inert additive:

$$\ln S_u + \frac{1}{2} \ln T_{f,av} - \frac{n}{2} \ln Y = \text{const} - \frac{E_a}{2RT_{f,av}} \quad (5)$$

where Y is the mole fraction of reactive components (fuel + oxidant) in the examined mixture and $T_{f,av}$ is the average temperature in the flame front, calculated according to Burke *et al.*³⁶

$$T_{f,av} = T_0 + 0.74(T_f - T_0) \quad (6)$$

Plots of the left term of eq. (5) versus the reciprocal value of the average flame temperature are given in Fig. 6, for using the laminar burning velocities of H₂-O₂ mixtures diluted with various amounts of N₂, at ambient initial pressure and with

various N₂ concentrations. The overall activation energies were determined from the slopes of the linear correlations given by eq. (5). Similar graphs were drawn for higher initial pressures, within the examined range.

The overall activation energies of H₂ oxidation with O₂ in nitrogen-diluted flames are given in Table 3. These activation energies increase steadily with pressure, in contrast to the activation energies of methane oxidation with O₂ in N₂-diluted flames, which change by less than 5% in the pressure range from 1 to 10 bar.³⁷

The overall activation energy reported in literature was found dependent on pressure, as well. For the stoichiometric H₂-air flame Iijima and Takeno³⁵ reported $E_a = 234$ kJ mol⁻¹ at 1 atm and $E_a = 196$ kJ mol⁻¹ at 10 atm. In contrast to these results, Sun *et al.*³¹ found that pressure increase results in an increase of the activation energy and reported $E_a = 113$ kJ mol⁻¹ for the same flame at 1 bar, in agreement with our data. The activation energies reported later by Law for the stoichiometric H₂-air flame: $E_a = 142$ kJ mol⁻¹ at 1 bar and 209 kJ mol⁻¹ at 20 bar³² confirm well the present data.

CONCLUSIONS

The laminar burning velocities obtained by kinetic modeling of flame propagation in H₂-O₂-N₂ stoichiometric mixtures were examined in

correlation with the initial pressure and nitrogen content. At constant initial composition and temperature, the laminar burning velocities of H₂-O₂-N₂ mixtures are strongly influenced by their nitrogen content and follow a non-monotonous variation against pressure, determined by the complex nature of chemical reaction mechanism.

The computed flame structure revealed a nonlinear variation of active species concentrations and of laminar burning velocities in response to pressure variation, through the various pressure-dependent chain mechanisms. The suppression of overall chemical reaction with the increase of

initial pressure is thus explained by the decrease of H, OH and O mass fractions in flames.

The overall activation parameters (reaction order and activation energy) of H₂ oxidation with O₂ in flames, determined by assuming a simple one-step kinetics over the range of initial conditions, were found dependent on initial composition (nitrogen content) and on pressure, which influenced the flame temperature.

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Appendix – Elementary reactions and their rate constants for H₂ combustion with O₂

$$k = A (T/K)^b \exp(-E/RT);$$

Both k and A are given in units of (cm³ mol⁻¹)ⁿ⁻¹ s⁻¹ with n = the reaction order

Nr.	Reaction	A	b	E (cal/mol)	Reference
1	H + O ₂ ↔ O + OH	1.9150E+014	0.0000	16440.0000	25
2	O + H ₂ ↔ H + OH	5.0800E+004	2.6700	6292.0000	25
3	OH + H ₂ ↔ H + H ₂ O	2.1600E+008	1.5100	3430.0000	25
4	O + H ₂ O ↔ OH + OH	2.9700E+006	2.0200	13400.0000	25
5	H ₂ + M ↔ H + H + M	4.5770E+019	-1.4000	104440.0000	25
6	O ₂ + M ↔ O + O + M	4.5150E+017	-0.6400	118900.0000	25
7	OH + M ↔ O + H + M	9.8800E+017	-0.7400	102100.0000	26
8	H ₂ O + M ↔ H + OH + M	1.9120E+023	-1.8300	118500.0000	26
9	H + O ₂ (+M) ↔ HO ₂ (+M)	1.4750E+012	0.6000	0.0000	26
10	HO ₂ + H ↔ H ₂ + O ₂	1.6600E+013	0.0000	823.0000	26
11	HO ₂ + H ↔ OH + OH	7.0790E+013	0.0000	295.0000	26
12	HO ₂ + O ↔ OH + O ₂	3.2500E+013	0.0000	0.0000	26
13	HO ₂ + OH ↔ H ₂ O + O ₂	2.8900E+013	0.0000	-497.0000	26
14	H ₂ O ₂ + O ₂ ↔ HO ₂ + HO ₂	4.6340E+016	-0.3500	50670.0000	27
15	H ₂ O ₂ (+M) ↔ OH + OH (+M)	2.9510E+014	0.0000	4843.0000	12
16	H ₂ O ₂ + H ↔ H ₂ O + OH	2.4100E+013	0.0000	3970.0000	12
17	H ₂ O ₂ + H ↔ H ₂ + HO ₂	6.0250E+013	0.0000	7950.0000	12
18	H ₂ O ₂ + O ↔ OH + HO ₂	9.5500E+006	2.0000	3970.0000	12
19	H ₂ O ₂ + OH ↔ H ₂ O + HO ₂	1.0000E+012	0.0000	0.0000	12

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