An analysis of flame instabilities based on Sivashinky equation

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1 Introduction

Since its first derivation in 1977 [1] the integro-differential equation of Sivashinsky has been a fascinating topic for the combustion researchers. This equation allow the analysis of the flame instability via a single evolution equation that describes the dynamics of the flame interface. Since the time of its initial integration [2], the enormous potential for the reproduction and modeling of the different flames instabilities has been recognized. Because of the clarity of its application and interpretation for the Darrieus-Landau, Thermo-Diffusive and Rayleigh-Taylor instabilities, we may use in our subsequent analysis the presentation of the equation that can be found in the excellent review [3]. In this variant the equation reads,

$$F_t + 4\nabla^4 F + [\frac{1}{2}\beta(1 - Le) - 1]\nabla^2 F + \frac{1}{2}(\nabla F)^2 = \phi_{DR} + \phi_{RT} \tag{1}$$

where ϕ_{DR} and ϕ_{RT} are therms that take into account the Darrieus-Landau and Rayleigh-Taylor instabilities, Le is the Lewis number and β the Zeldovich number. With $\phi_{DR} = \phi_{RT} = 0$ only the thermo-diffusive instability is considered. The term

$$\phi_{DR} = \frac{1 - \sigma}{8\pi^2} \int_{-\infty}^{\infty} |k| e^{ik(x-z)} F(z, t) dk dz \tag{2}$$

were σ is the expansion ratio and will take into account the hydrodynamic instability and

$$\phi_{RT} = -G(F - \langle F \rangle), \tag{3}$$

where G is the dimensionless acceleration, allow accounting for the Rayleigh-Taylor instability [4].

The initial investigation, [1] and [2], that was focused in the two dimensional pattern of the thermo-diffusive and Darrieus-Landau instability was rapidly and naturally extended to three dimensional configurations still in the early times of the investigation of the formulation, [5]. The formulation, that originally considered exclusively a free boundary problem, was also ameliorated to study two dimensional circular flames [6]. In a subsequent continuation of the analysis, three dimensional spherical flames were examined in the monograph studies [7] and [8]. The formulation was also significantly extended to take into account the effect of buoyancy, upward or downward propagating flames, including thus the Rayleigh-Taylor instability [4].

In the last years, a very significant development have been undertaken by Matalon and his co-workers [9]. In their studies, the evolution of weakly curved flames is studied by the analysis of the Michelson-Sivashinsky equation, which is analogous to the equation (1) but without the $\nabla^4 F$ term. Most notably, the results that these researchers have achieved include the analytic solution of the Michelson-Sivashinsky equation [10]. The solution allows to analyze the combined effect of the Darrieus-Landau instability and the intensity of the turbulence and other turbulence related parameters in the wrinkling of the flame and its propagation [11] and [12].

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Surprisingly, the modeling of the flame instabilities have been introduced only in the last years [13] for large scale calculations. In such a methodology the effective burning velocity was modeled as a product of the laminar burning velocity and a flame surface wrinkling factor Ξ. The surface wrinkling factor is analyzed taking into account [14] a transport equation

$$\Xi_t + \vec{u} \cdot \nabla \Xi = G(\Xi - 1) - R(\Xi - 1)^{\frac{3}{2}} \tag{4}$$

in which G and R are sub-grid wrinkling generation and removal rates. Although such a formulation allow for the most desirable modeling of the instabilities it has serious restrictions.

The objective of our work is to integrate the Sivashinsky equation to evaluate the wrinkling factor for different H_2-air mixtures in order to compare with experimental data on 2D-flame-instability and to find out the flame velocity enhancement due to the corrugation of the flame in 2D-geometry.

2 Analysis

2.1 Integration of the Sivashinsky equation for H_2-air mixtures. Conditions of calculation

Certainly, the equation (1) may be transformed into a formulation similar to the equation (4). Considering the length $ds = \sqrt{1 + (F_x)^2} dx$ we may define $\Xi = \left(\int_{x-\frac{L}{2}}^{x+\frac{L}{2}} \sqrt{1 + F_x^2} dx \right) / L$. From this, a change of variables must be carried out to obtain a closed system in Ξ. Note that for sufficiently big L, Ξ will be statistically independent of x and thus, Ξ will be a function of time only. Nevertheless, such a change of variables is very complicated to be implemented. Not the staleness difficulty is the fact that, in order to be consistent with the physics, L should be big enough ($L \to \infty$) and thus series expansion of the variables pose mathematical difficulties.

For these reasons, it would be very valuable to clarify for which mixtures and for what timescales should the Darrieus-Landau and the Thermo-Diffusive instability be modeled. Also, before further analysis with Sivashinsky equation (1) will be undertaken, it would be convenient to find out if the weakly nonlinear character of the *standard* Sivashinsky equation is adequate and sufficient to try to derive a compelling model. Thus, we undertake the solution of the Sivashinsky equation particularized for different H_2-air mixtures at normal conditions.

The integration of the equation (1) has been carried out utilizing a second order finite differences method following the procedure described in detail by Michelson in [2]. For the time integration, the second order Predictor-Corrector methodology [15] has been utilized in a periodic domain.

As initial condition, a planar surface perturbed with a white noise has been selected. For the simulations, a ratio of 10^{-9} between the average amplitude of the perturbation and the total surface of the flame has been considered, corresponding to approximately 10^{-7} m rms.

2.2 Analysis of results

After an initial period in which the propagation does not appear in a coherent manner the cusps are formed and the typical surface of a cellular flame is established. The surface obtained as a result of numerical integration of eq. (1) shows qualitative agreement with the results already exhibited in [2], [16] and [3]. The cells that form in the profile are in a status of continuous irregular motion, see Figure 1, which is one of the characteristics of the solutions of this equation. In the Figure 1 the flame has been represented as *heatmap* in which the local position of the flame relative to its average position is represented. The cusps are shown in white and form the typical bifurcation annihilation pattern. The surface wrinkling factors obtained from the calculations have been represented in the Figure 2. Two very clear qualitative differentiate patterns can be observed. For very lean mixtures, up to 12 % vol in H_2 (Figures 2a and 2b), an initial plateau exists, representing a regime in which the Thermo-Diffusive instability accounts for the most of the excess of surface. This regime is followed by a more or less fast transition that culminates in a regime in which the surface wrinkling factor oscillates in a relatively thin channel (for the width of the channel see the standard deviation in Table 1). Clearly, the intermediate stage no longer exists for richer mixtures, 2b, 2c, 2d, 2e and 2f where the transition is fast and is followed immediately by the final stage. This transition can be studied utilizing the dimensionless time that appears to happen between

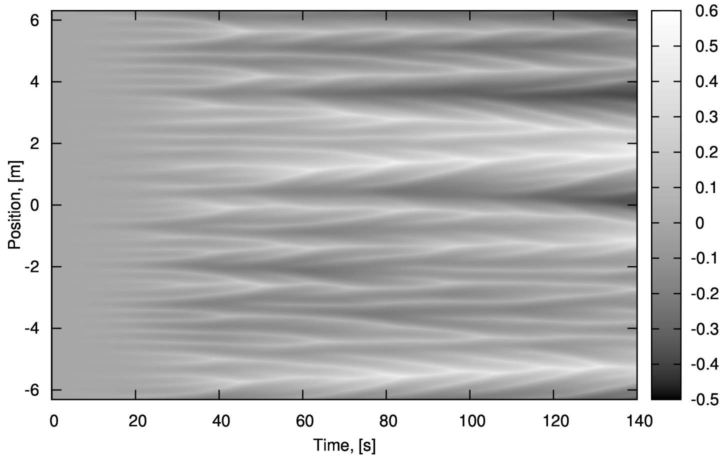


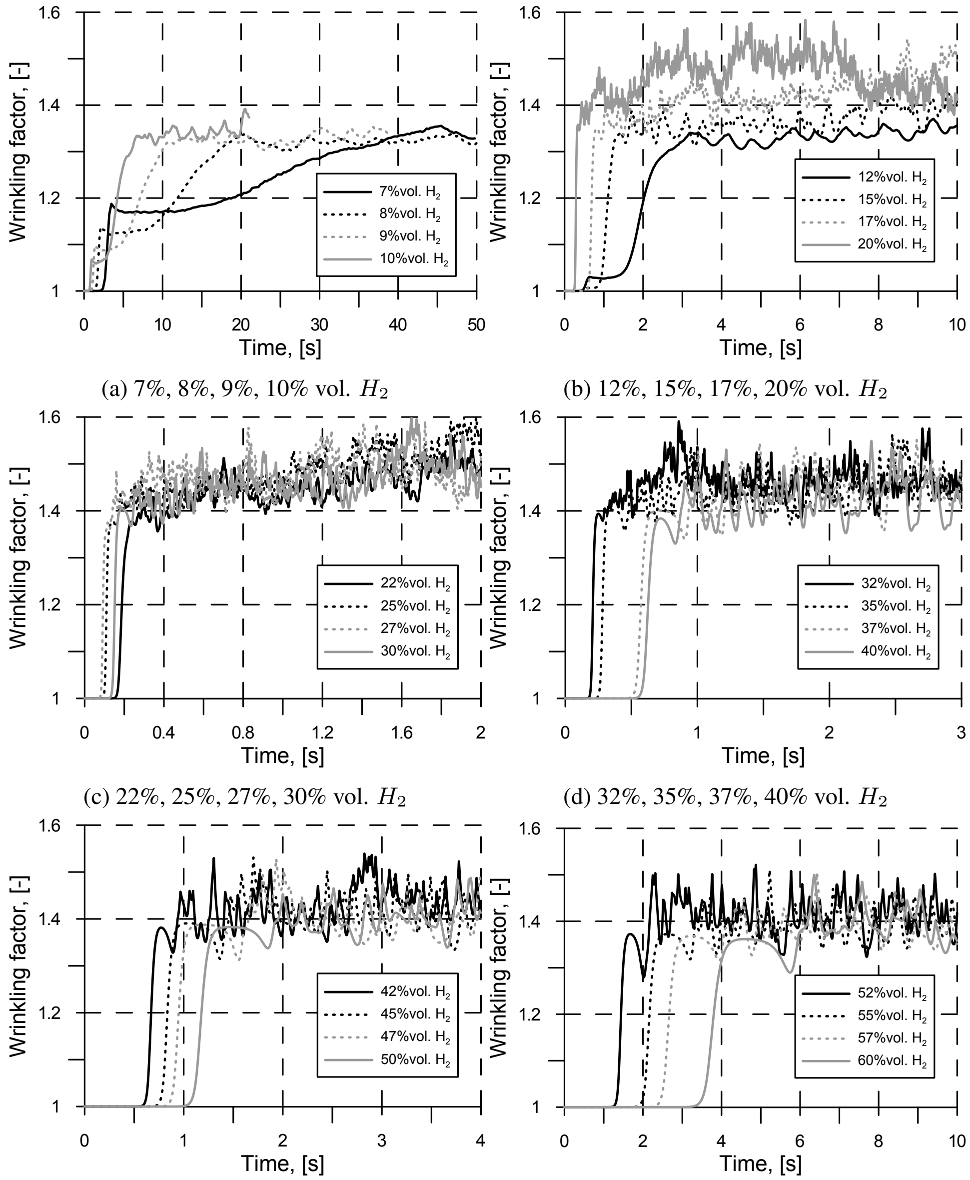
Figure 1: Results of the integration of the one dimensional Sivashinsky equation. Gray scale is the relative position of the flame relative to the average position. The positions of the cusps are represented in white.

1200 and 1300 dimensionless units of time (corresponding respectively to 16, 7.5 4.3 and 2.3 s for 7, 8, 9 and 10 vol. % H_2). Another interesting fact is the similar value that the surface wrinkling factor finally reaches for all the concentrations of H_2 (around 1.4, see Table 1). This fact, and also the quite small value that the surface wrinkling factor reaches, is attributed by G.I. Sivashinsky [17], to the asymptotic and weakly nonlinear character of the equation (1). Following this reasoning, high accuracy cannot be expected for increased amplitudes of corrugated fronts. The variation around the expected value is certainly normal, as can be concluded from the application of the Shapiro-Wilk statistical test, that delivers an uncertainty of $10^{-5}\%$. This means that with a probability of 99.7% the oscillation of the Ξ variable lies between the $\pm 3\sigma(\Xi)$. Thus, the factor $\pm 3\sigma(\Xi)$ characterizes completely the width of the channel of oscillation of the Ξ.

Table 1: Mathematical expected value and standard deviation of the parameter Ξ. Laminar burning velocity enhancement due to the Darrieus-Landau and Thermo-Diffusive instability.

$\%$ $[vol.\ H_2]$	$E(\Xi)$ $[-]$	$\sigma(\Xi)$ $[-]$	U_l $[m/s]$	$U-U_l$ $[m/s]$	$(U-U_l)/U_l$ $\%$
7	1.34	0.008	0.04	0.02	52.28
8	1.34	0.014	0.06	0.03	49.23
9	1.33	0.013	0.08	0.04	50.10
10	1.34	0.015	0.11	0.06	57.61
12	1.34	0.013	0.19	0.09	47.94
15	1.38	0.024	0.34	0.20	57.51
20	1.46	0.041	0.90	0.53	59.19
25	1.52	0.032	1.60	1.35	84.32
30	1.49	0.035	2.19	1.65	75.26
40	1.42	0.043	2.88	1.99	68.94
50	1.40	0.043	2.59	1.64	63.20
60	1.38	0.037	1.86	1.05	56.28

Not less significant, especially for practical CFD simulations, is the period of time necessary for the development of the stability. Through the analysis of the Sivashinsky equation is possible to understand the scale of time, and space, for which the enhancement of the laminar burning velocity due to flame instabilities can be disregarded



(a) 7%, 8%, 9%, 10% vol. H_2

(b) 12%, 15%, 17%, 20% vol. H_2

(c) 22%, 25%, 27%, 30% vol. H_2

(d) 32%, 35%, 37%, 40% vol. H_2

(e) 42%, 45%, 47%, 50% vol. H_2

(f) 52%, 55%, 57%, 60% vol. H_2

Figure 2: Flame surface wrinkling factor Ξ vs. hydrogen concentration.

or must be accounted for. The diagrams included in the Figure 2, show the dependence on time of the wrinkling factor Ξ. Also, displays the period of time necessary for the development of the stability. Certainly, this raise the question of how sensitive are the solutions relative to the amount of initial noise. The results obtained for the reference amount of white noise has been compared with cases in which $1/10$ and $1/100$ of the amplitude of the reference case have been considered. A reduction of one order of magnitude in the amplitude of the initial perturbation represents a delay of $1s$ in the development of the instabilities.

The sensitivity of the solution to different white noises of similar amplitude was also checked. The random number generator used to create the noise was seeded at different times and numerical integrations where performed with these differentiate initial conditions. Although the solutions were different, the curves representing the evolution of Ξ seemed virtually identical. The solutions are thus statistically identical as pointed out in e.g. [3].

Although the usual way of modeling the enhancement of the flame propagation velocity due to the flames instabilities would be to trace the analogy $S_{wrinkled}/S_l \approx A_{wrinkled}/A_{planar}$, the Sivashinky equation also offers an alternative possibility. This would be to measure directly the mean burning velocity of the propagating interface. In the chosen formulation these velocity would represent $U - U_l$ and can be extracted directly from the relative flame position. The location of the flame depending on time has been depicted in the Figure 3. Clearly, after a period of formation of the coherent cusp structure in which the flame propagates mostly with the laminar burning velocity, a gradual acceleration takes place until a stationary mean velocity is reached.

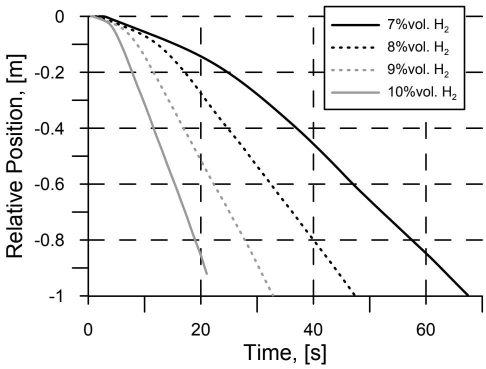


Figure 3: Mean position of the flame relative to a planar interface moving with a velocity $-U_l$ for 7, 8, 9, 10% vol. H_2.

The results obtained are included in the Table 1. To extract them, a statistical treatment of the enhancement of the mean velocity when this magnitude reaches a *stationary* value have been carried out. The standard deviations compared with the average values of the velocities remained on the order of 2%. Thus the velocities obtained can be considered really as stationary.

Although *a priori* the $(U - U_l)/U_l$ may be the preferred magnitude for the modeling, the data obtained in this variable is more disperse than the one available for $U - U_l$. The polynomial approximation $U - U_l \approx 1.01 + 2.69ln(p) - .71(ln(p))^2 - 1.38(ln(p))^3 - 0.39(ln(p))^4$ with p the percentage of H_2 in the mixture allow describing the dependence with a determination coefficient of 0.98. The total burning velocity would be them $U \approx U_l + (U - U_l)_{Siva}$ as an alternative formulation to the more classic $U \approx \Xi U_L$.

2 Conclusions

With the analysis that was carried out we have demonstrated the possibility to perform a modeling for the flame instabilities for low resolution large domain CFD calculation based in the Sivashinky equation. The advantages for the modeling of the fact that Sivashinky equation was based on first principles is somehow compensated by its asymptotic nature. Thus, the values obtained should be compared with experimental data in a second future stage of our work. Still, valuable information on the evolution, dynamics of the *Wrinkling factor* was extracted for Hydrogen-air mixtures, a fact that allow for promising results on modeling once the validation will be carried out. The somehow surprising conclusion that the Wrinkling factor reaches a common overall value for all hydrogen concentrations was extracted in our study. The dynamics driving to this value are nevertheless different, underlining the different importance and dynamics for different mixtures of the Thermo-Diffusive and Landau-Darrieus instability. The other possibility of the modeling, based on the calculation of the propagating interface is even more interesting, and should be exploited in further analysis. A model, was therefore extracted for this second possibility.

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