NUMERICAL SIMULATIONS OF LAMINAR BURNING SPEEDS OF α-PINENE INVOLVED IN ACCELERATING FOREST FIRES

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Abstract
This paper is dedicated to a first approach for the study of the so called accelerating forest fires. It is a preliminary work to test the hypothesis of VOCs accumulation as the cause of such phenomenon. In this work we explore the ability of the numerical code Fire Dynamics Simulator (FDSv5) to simulate premixed flame spread. In a first part, the laminar burning velocities of propane/air and n-decane/air mixtures are calculated for different initial temperatures and equivalence ratio (0.7 to 1.3) at atmospheric pressure using a cylindrical combustion chamber. The preheat temperatures range for propane and n-decane fuels are respectively 300 to 423 K and 360 to 470 K. In a second part, the laminar burning speeds of the α-pinene, which is the main VOC emitted by several vegetal species, is simulated for the same equivalence ratios and initial temperatures 373 to 453 K. The obtained results of these three fuels are compared to the experimental and computed results of the literature. These comparisons demonstrate the ability of FDS to deliver reliable predictions on laminar burning velocities of premixed flames.

***Keywords*:** Accelerating forest fire, VOC, CFD, FDS code, laminar burning speed.

Introduction
Several works in literature have reported that during wildland fires spread, violent and dangerous phenomena known as eruptive fires [1,2] or accelerating forest fires [3] can appear. This phenomenon is different from usual propagation by a much faster fire front spread and a much higher heat release. Usually, wildland fires flames are assimilated to diffusion flames and the rates of spread may reach some tens centimeters per second. Accelerating forest fires considered here seem to be similar to "gas explosions" or "dust explosions" initiated by the ignition of a Volatile Organic Compounds (VOCs) cloud. So that, the flames in this paper, are not considered as diffusion flames but as premixed flames. This hypothesis has been introduced in the early work of Arnold and Buck [4] where the fire is described as a "fire ball". More recently, in a review of the Palasca accident, Dold et al. [5] have written "*the apparent quenching of the head fire in the Palasca incident does suggest that the fire might not have developed as a continuous fireline but as a form of premixed flame spread or flashover*".

Due to their lower values of Lower Flammability Limits (LFLs) than the unburned products [6], it is more likely that the "gas or dust explosion" encountered in accelerating

forest fires are initiated by the combustion of VOCs/CO/air mixture. Indeed, several vegetal species (e.g. *Rosmarinus officinalis*, *Quercus ilex*…) when heated produce and emit volatile compounds [7,8]. The composition of these VOCs is highly flammable and depends on several factors such as temperature and light [9], phenological state [10] and intraspecific and interspecific competition [11]. It is clear that the VOCs distribution in field is unsteady and heterogeneous. The measurement of premixed flame speeds of these gases is not sufficient to characterize the accelerating forest fires phenomenon. The spatial and temporal evolution of this phenomenon should be simulated by an adequate computational fluid dynamics (CFD) code like Fire Dynamics Simulator (FDS) taking into account the unsteadiness and heterogeneity aspects of the VOCs/air mixture. To reach this goal, the ability of this computational code to predict the laminar burning velocities for a homogeneous VOCs/air mixture should firstly be verified.

In present study we compute the laminar burning speeds of three fuels: propane, n-decane and VOC, namely α-pinene, emitted by several Mediterranean vegetal species. The temperature and equivalence ratio effects on the laminar burning speeds of these three fuels are studied as well. The next section is devoted to the presentation of the numerical modeling and procedure. The description of the FDS code is given. The computational domain and the grid sensitivity are detailed in this section. The third section is dedicated to the results and discussions where the computed values of the laminar burning speeds of the three fuels are compared to the experimental and numerical ones given in the literature.

Numerical modelling and Procedure

Governing equations and models

The computational framework used for the present paper is FDSv5.5 code which is one of the most commonly employed fire CFD codes [12,13,14]]. The FDSv5.5 is a Large Eddy Simulation code developed by National Institute of Standards and Technology (NIST) in the United States [15,16]. This computational code solves numerically the Navier-Stokes equations for low Mach number flows. The combustion model used in this work is based on a mixture fraction concept, which is a quantity representing the fuel and the combustion products, with a single-step reaction chemistry. The radiation transfer equation for a gray gas is solved to assess the thermal radiation contribution in the energy balance equation.

The combustion model of FDSv5.5 is based on the assumption that the combustion is mixing-controlled. The different species are defined as a function of mixture fraction Z that is a conserved scalar satisfying the following conservation equation:

$$\frac{\partial}{\partial t}\left(\rho Z\right)+\nabla\cdot\left(\rho\mathbf{u}Z\right)=\nabla\cdot\left(\rho D\nabla Z\right) \tag{1}$$

with

$$Z=\frac{1}{Y_{\mathrm{F}}^{I}}\left(Y_{\mathrm{F}}+\frac{W_{\mathrm{F}}}{xW_{\mathrm{CO_2}}}Y_{\mathrm{CO_2}}+\frac{W_{\mathrm{F}}}{xW_{\mathrm{CO}}}Y_{\mathrm{CO}}+\frac{W_{\mathrm{F}}}{xW_{\mathrm{S}}}Y_{\mathrm{S}}\right) \tag{2}$$

where Y_{F}, $Y_{\mathrm{CO_2}}$, Y_{CO}, Y_{S} are respectively the mass fractions of fuel, carbon dioxide, carbon monoxide and soot and W_{F}, $W_{\mathrm{CO_2}}$, W_{CO}, W_{S} are their molecular weights. Y_{F}^{I} is the fuel mass fraction in fuel stream and x is the carbon atoms number in the fuel molecule.

The temporal and spatial derivatives of the governing equations are approximated by finite differences. A scheme of second order central differencing is used to approximate the thermal and material diffusion terms. The convective terms and temporal ones are approximated respectively by predictor-corrector and explicit schemes. The radiation transfer equation is computed by means of the finite volume method.

Computational domain and conditions

The computational domain considered for this study reproduces in details the combustion chamber presented by Halter et al. [17] and Tahtouh et al. [18]. It consists in a cylindrical combustion chamber of an internal volume of 24.13 L. The inner dimensions of the steel vessel are 0.16 m radius and 0.3 m height. Figure 1 shows an overview of the computational domain. It illustrates the cylindrical combustion chamber displayed by SmokeView visualization package [19] as well as a top and a side view of this domain.

The ignition source is insured by a fixed value of heat release rate per unit area (HRRPUA) released at the center of the combustion chamber during few milliseconds. Considering that there is no loss of heat toward outside, the external wall of the combustion vessel is assumed to be adiabatic. Four thermocouples (TC1, TC2, TC3 and TC4) detect the premixed flame positions; they are placed vertically at 7 mm from the ignition source in order to avoid the effect of the initial energy deposit. During the initial phase of flame growth, the total pressure of the combustion chamber is constant, so flame radii larger than 30 mm are not taken into account in the laminar burning velocities calculation. Three initial preheat temperatures are selected for propane/air and n-decane/air mixtures. The temperature values are 300, 360, 423 K and 370, 400, 470 K respectively considered for the first and second mixtures. For α-pinene/air mixtures, the values of 373, 398, 423 and 453 K are used as initial distribution of temperatures. For all fuels, numerical simulations are carried out at atmospheric pressure and for a range of equivalence ratio varied from 0.7 to 1.3 by a 0.1 step.

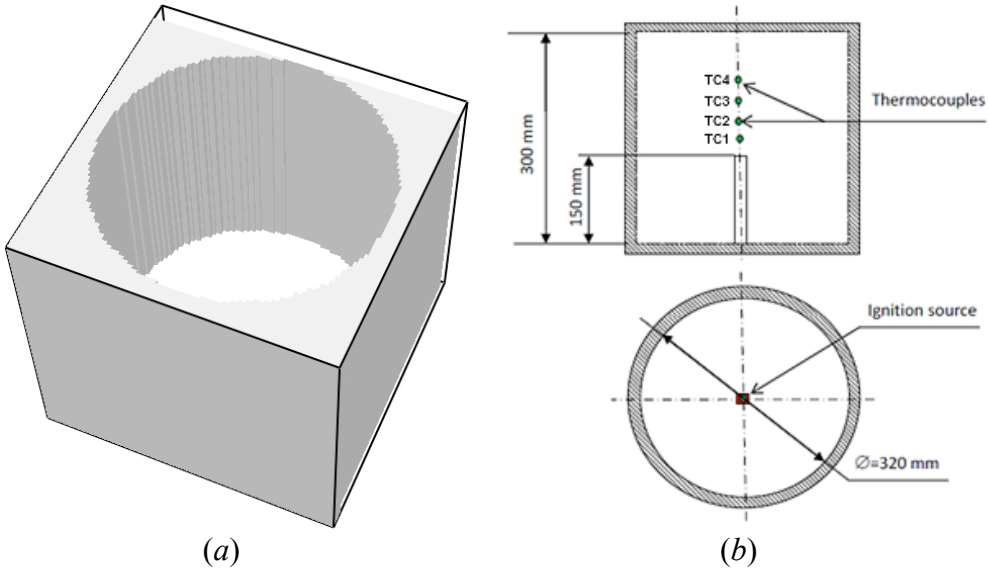


Figure 1. Overview of the computational domain: (a) Combustion chamber, (b) Top and side view.

Laminar burning velocity determination and grid sensitivity

As indicated previously, four thermocouples are placed vertically above the ignition source at the cell centers in order to track the premixed flame expansion. The distance between two thermocouples i and $i+1$ $(i=1,2,3)$ is $\Delta z_{i,i+1}\left[\mathrm{m}\right]$ so that the laminar burning speed in each zone can be written as:

$$S_L^{0,i}\ [\mathrm{m/s}]=\frac{\Delta z_{i,i+1}}{\Delta t_{i,i+1}} \tag{3}$$

where $\Delta t_{i,i+1}[\mathrm{s}]$ is the time separating two successive peaks of temperature. The laminar burning speed, for a given fuel at each equivalence ratio and initial temperature, is therefore assumed as the mean value of the different $S_L^{0,i}$ computed by relation (3). Figure 2 exhibits thermocouples temperatures profiles for stoichiometric propane/air, n-decane/air and α-pinene mixtures at two initial preheat temperatures.

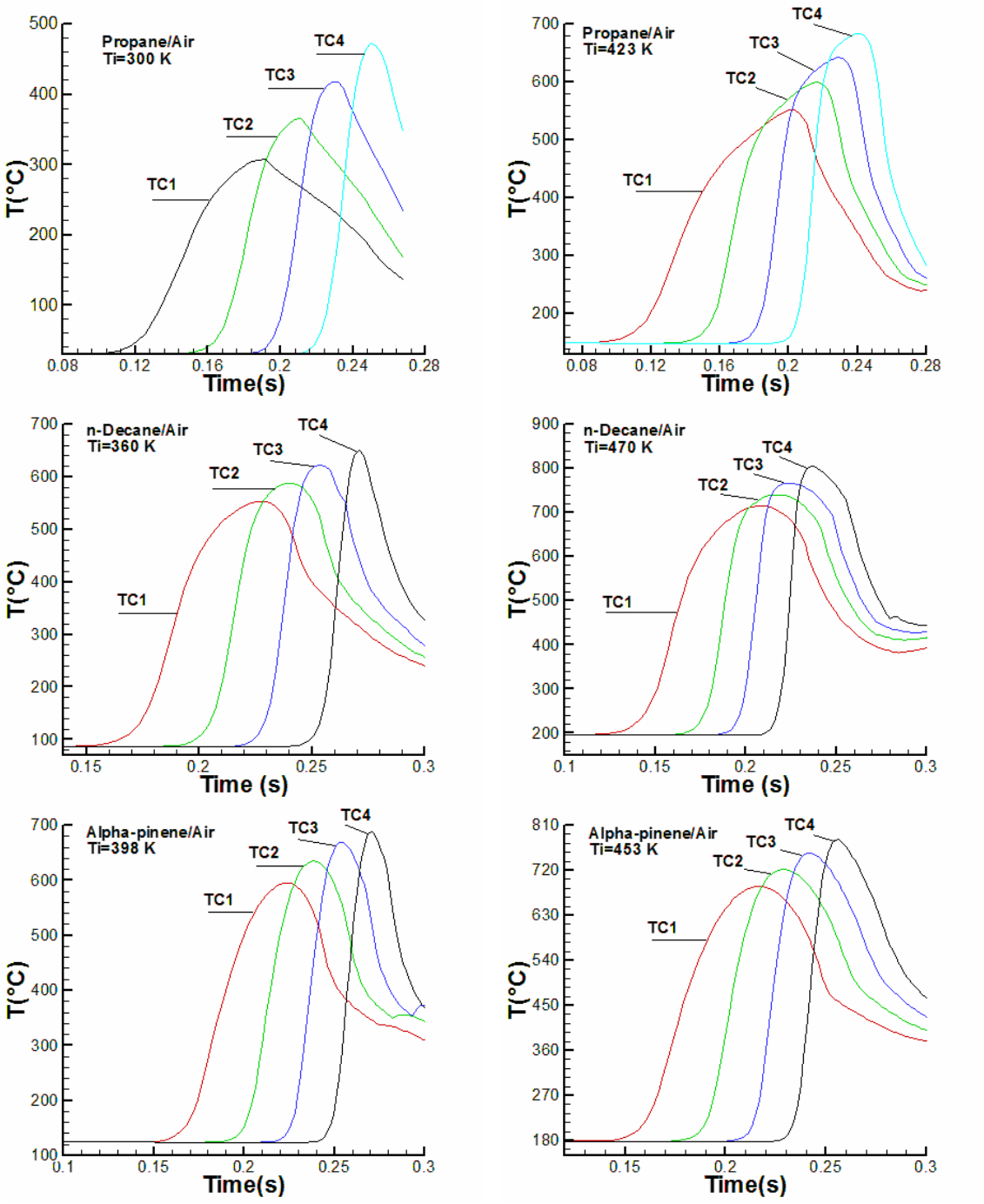
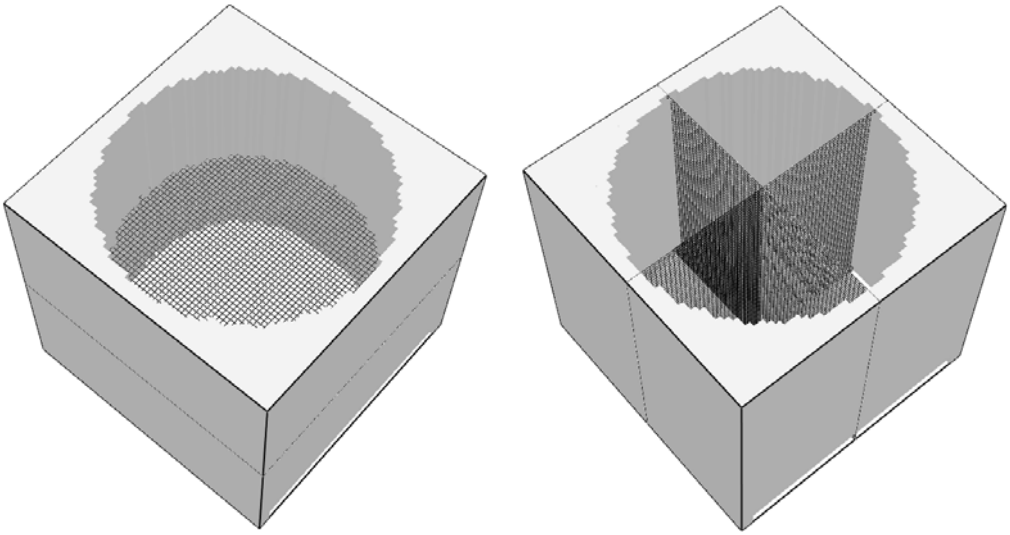


Figure 2. Thermocouples temperatures profiles for propane, n-decane and α-pinene fuels at the stoichiometry for their lowest and highest initial preheat temperatures.

The thermocouples temperatures profiles in theses Figures show that the time separating two successive temperature peaks decreases when the initial preheat temperature increases.

This decreasing in separation times is accompanied by an increase in the laminar burning speeds of the different fuels studied here. The initial preheat temperature has the same effect on the flame temperatures as on the laminar burning speeds. Indeed, the flame temperature measured by each thermocouple increases when the initial preheat temperature increases.

The grid resolution is one of the most crucial parameters in numerical simulations. In this work, an optimum grid size is selected trough a grid cell sensitivity analysis. The dimensions of the cell are taken to be $3.33\ \text{mm} \times 3.33\ \text{mm} \times 2\ \text{mm}$, giving a total meshes number of the cylindrical combustion chamber of about 1,980,000. An illustration of the grid in horizontal and vertical planes is presented in Figure 3. The simulations are performed up to 400 ms and the computing time is about 30 min using an Intel(R) Core i5 CPU 2.27 GHz with 4 GB RAM.



(*a*) (*b*)

Figure 3. Illustration of computational domain grid: (a) horizontal plane, (b) Two vertical planes.

Results and discussions

Let us present firstly the obtained results of the propane and n-decane fuels with a comparison with the literature values. After that, the computed laminar burning speeds of α-pinene/Air mixtures are given and compared to the recent experimental values of Courty et al. [20].

Propane/air and n-decane/air premixed flames

As mentioned above, three initial preheat temperatures are selected for propane/air and n-decane/air premixed flames simulations. Six sets of experimental data from Duger [21], Desoky et al. [22] and Tang et al. [23] as well as a set of numerical data from Zhao et al. [24] are used for the validation of the predicted laminar burning speeds of propane fuel at these initial temperatures. Figure 4 shows the laminar burning velocities of propane/air mixtures computed by FDSv5.5 code as functions of equivalence ratio at 300, 370 and 423 K and those of literature. At room temperature, Figure 4 clearly exhibits that for all equivalence ratios, our predicted results are in good agreement with the measured values of Dugger [21] and Tang et al. [23] using two different experimental setup. Our data are also very close to the numerical ones of Zhao et al. [24] obtained via the detailed kinetic mechanism of Qin et al. [25]. For higher initial preheat temperatures, the predicted laminar burning velocities are in good agreement with those of Dugger [21] near the stoichiometry as well as with the results of

Desoky et al. [22] and Tang et al. [23] for lean mixtures. For rich mixtures, a reasonable agreement is observed with their data.

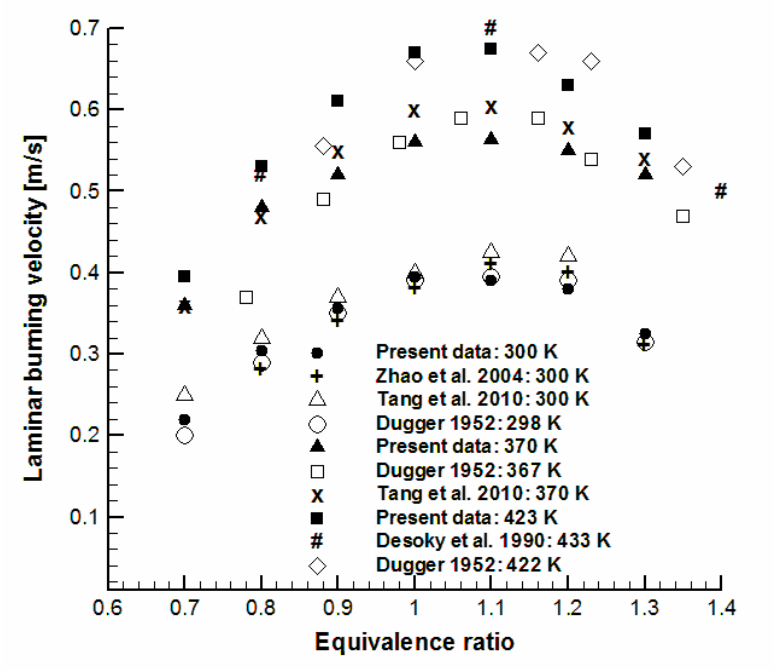


Figure 4. Comparison of the propane laminar burning speeds between the present study and those in the literature for different equivalence ratios and initial preheat temperatures.

Concerning the n-decane fuel, in Figure 5 we compare the present laminar burning speeds data with the counterflow flames measurements of Kumar and Sung [26] and numerical values of You et al. [27] obtained via a detailed kinetic mechanism at 360, 400 and 470 K.

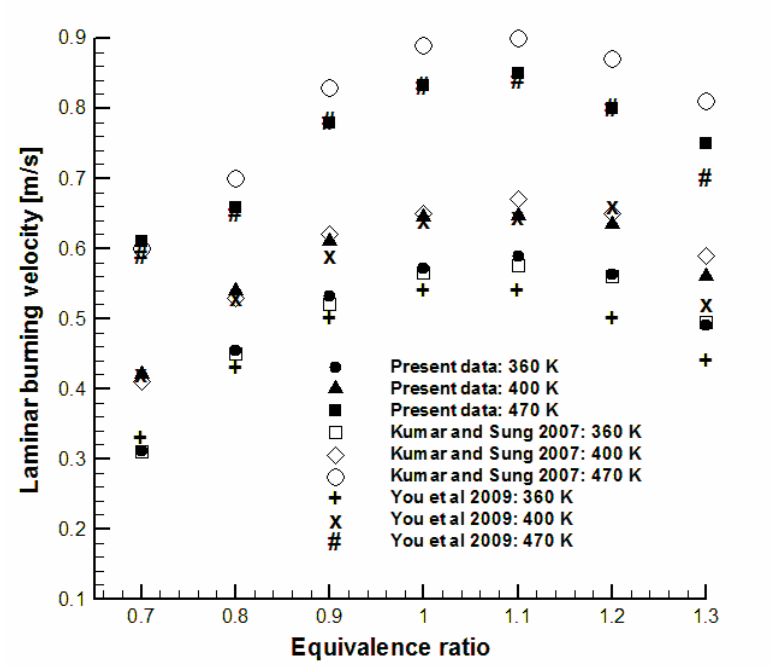


Figure 5. Predicted laminar burning velocities of n-decane/air mixtures for different equivalence ratios and initial preheat temperatures. Comparison with the literature.

As shown is this Figure, The computational predictions for n-decane fuel appear to be consistent with experimental and numerical data available in the literature at different initial preheat temperatures. We can notice that the computed values of You et al. [27] at 360 K are slightly lower than our predicted data for rich n-decane mixtures. From an equivalence ratio of 0.9, the measurements of Kumar and Sung [26] at 470 K are slightly higher than our results.

α-pinene premixed flames

Unlike the previous fuels where extensive data exist, there are very few works in the literature dealing with VOCs combustion [28]. Nevertheless, the recent contribution of Courty et al. [20] has to be highlighted. Based on the spherical expanding flames method, these authors measured the laminar burning velocities and Markstein lengths of α-pinene/air premixed flames. In previous studies [3,29] have shown that high α-pinene emissions have occurred at temperatures higher than 373 K. For that, four initial preheat temperatures are selected for the validation of the predicted laminar burning speeds of α-pinene fuel. Figure 6 summaries the computed values of α-pinene at varying equivalence ratios and initial preheat temperatures (373, 398, 423 and 453 K) as well as those measured by above cited authors at the same temperatures. We can see that for equivalence ratios of 0.7 and 0.8 at initial preheat temperatures of 373 and 398 K, FDSv5.5 computational code overestimates slightly the measured values of Courty et al. [20]. Except these two equivalence ratios at this temperature, Figure 6 shows that the predicted α-pinene flames speeds are in good agreement with the experimental data.

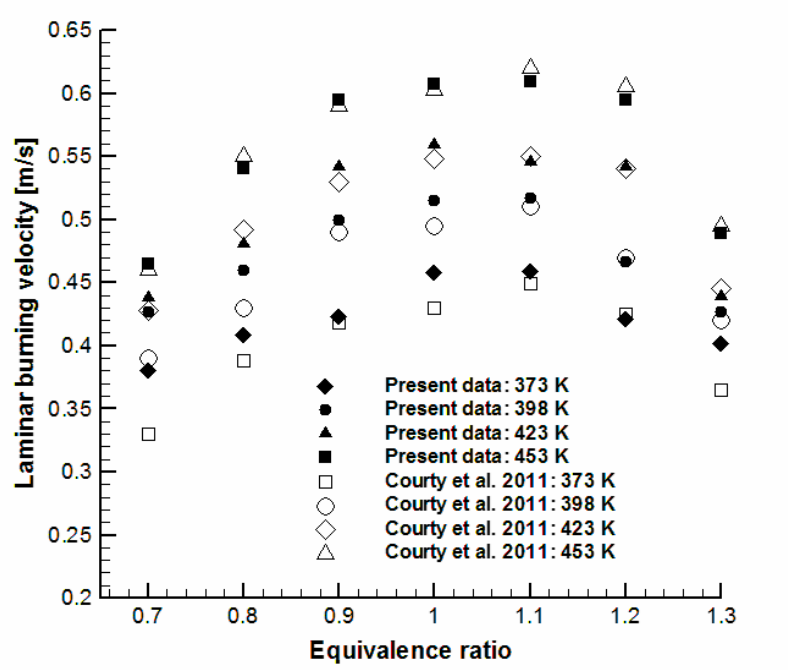


Figure 6. Computed laminar burning speeds of α-pinene/air mixtures for different equivalence ratios and initial preheat temperatures compared to experimental data.

Empirical correlations of laminar burning velocities

Generally speaking, the laminar burning speeds can be fitted to a function comprising a polynomial dependence on equivalence ratio and a temperature power law [30]. This empirical correlation has the following expression:

$$S_u^0[\mathrm{m/s}] = S_u^{\mathrm{ref}} \left(1 + a_1 \left(1-\Phi\right) + a_2 \left(1-\Phi\right)^2\right) \left(\frac{T_u}{T_u^{\mathrm{ref}}}\right)^{\alpha} \qquad (4)$$

In this relationship, S_u^{ref} is the laminar burning speed at a reference point ($\Phi = 1$ and T_u^{ref}) given in m/s, $T_u\left(\text{in K}\right)$ is the initial preheat temperature and a_1, a_2 and α are constants. The values of T_u^{ref} for propane, n-decane and α-pinene are respectively 300, 360 and 373 K. The best-fitting curves have been obtained by the least squares method. This method assumes that the best-fit curves are the curves that have the minimal sum of the deviations squared from a given set of data. The results of these fitting based on a minimization simplex algorithm [31] are illustrated for propane (at 370 K), n-decane (at 360 K) and α-pinene (at 373 K) fuels on Figure 7 and the values of the different coefficients are given in Table 1.

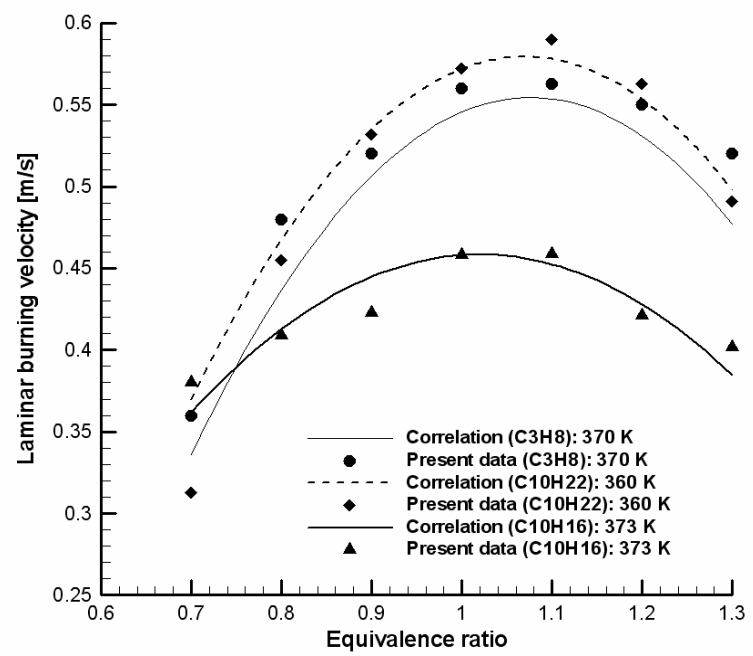


Figure 7. Best-fit curves of laminar burning velocities of propane (370 K), n-decane (360 K) and α-pinene (373 K) fuels as functions of equivalence ratio.

	a_1	a_2	α
propane	-0.4308	-2.8340	1.5399
n-decane	-0.3742	-2.6842	1.4285
α-pinene	-0.0826	-2.0581	1.4841

Table 1. Fit parameters of the empirical correlations for the laminar burning speeds of propane, n-decane and α-pinene fuels.

Conclusion

The present paper deals with the determination of the laminar burning speeds of a main VOC emitted by several vegetal species using the FDSv5.5 computational code. Although FDS has been designed to simulate diffusion flames, we have shown in this study that it can simulate the premixed flames propagation as well. To the authors' knowledge, this is the first attempt to check the code capability for predicting the laminar burning velocities of a homogeneous VOC/air mixture.

The final scope of this study is to investigate more deeply the involvement of VOCs in the phenomenon of accelerating forest fires. Indeed, as the density of VOCs is higher than the density of air when vegetation is heated by an approaching fire, these compounds could accumulate in canyons. These VOCs mixed with unburned gases and air would create a flammable atmosphere.

In a next step of the work, we will consider non-homogeneous mixture distributions of α-pinene/CO/air and will simulate the propagation of premixed flames in more complex geometrical configurations. The results of these simulations will be compared with real accidents data in order to distinguish the different hypothesis to explain accelerating forest fires.

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