SIMULATION OF WOOD GAS PREMIXED FLAME COMBUSTION IN A CONFINED HIGH PRESSURE REACTOR

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Abstract. *The objective of the present research is a simulation tool validation for determining wood gas - air premixed flame combustion properties. The same simulation tool is then utilized for sewage and landfill gas - air premixed flame combustion properties determination. The wood gas, obtained by wood gasification using different processes, leading to different gas compositions, may be used for future applications in internal combustion engines and electric energy production in stationary stations. The simulation is held by using the Flame Speed Calculator CHEMKIN-PRO™ software module which simulates 1-dimensional freely propagating flame for determining premixed laminar flame-speeds. The GRI-Mech™ 3 mechanism provides the mixture chemical composition and its thermodynamic and transport properties. The equivalence ratio is varied in a range between 0.6 to 1.4, the initial gas mixture temperature is varied in a range between 298 K and 400 K and the initial gas mixture pressure is varied in a range between 1 atm to 10 atm. The simulations results are compared with those few available in the literature providing quite good agreement especially close to stoichiometry. In the future, the simulations results will be compared with those obtained by an experimental combustion chamber already being designed.*

Keywords: *wood gas, Chemkin, premixed flames*

1. INTRODUCTION

The continuous increasing world consumption of energy and the fast reduction of cheap fossil fuels available, joined with increasing attention to pollutant emissions has driven increasing interest in renewable sources of energy, including biofuels research and applications.

In the Brazilian contest, most of the electric energy is produced by renewable sources, especially hydroelectric power plants, while in the transport field most of the vehicle manufacturers produce flex-fuel vehicles (FFVs), able to run either on pure gasoline, pure ethanol or blends of gasoline and ethanol. Some manufacturers produces vehicles powered with internal combustion engines (ICEs) running on gaseous fuels, either of fossil or biological origin.

Biogas is particularly significant because of possibility of application in ICEs, which are the main power source for transport vehicles and also commonly used for powering generators of electrical energy. The availability of a great number of biofuels in the present context imposes a strict determination of the characteristics required for their application in ICEs.

A major challenge for combustion scientists and engine-development engineers is to optimize engine combustion to improve fuel economy, lower pollutant emissions, and provide alternative-fuels capabilities while maintaining outstanding performance, durability, and reliability at an affordable price (Drake and Haworth, 2007).

Biogas, also referred to syngas in the following, is the product of fermentation of man and animals biological activity waste products when bacteria degrade biological material in the absence of oxygen, in a process known as anaerobic digestion. The composition of biogas may vary depending on the original biologic material and the fermentation process.

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Wood gas produced by gasification is a suitable fuel for ICEs when the presence of particle and tar are below a certain quantity. According to Hasler and Nussbaumer (1999) small scale atmospheric downdraft fixed bed gasifier produces the synthesis gas with the lower content of particulate matters and tar. Nevertheless, a cleaning process is required before the biogas can be used in ICEs. In the present work three wood gas compositions are considered, one of which is obtained with this kind of gasifier. The studied compositions are selected by Bridgwater (1995) and were object of an experimental research by Monteiro *et al.* (2009) whose results are used for the simulation program validation. The simulation program provides large combinations of compositions, initial temperature, pressure and equivalence ratios, serving as a base for the following experimental step of the work.

The laminar flame speed, S_u^0, is one of the most important parameters of a combustible mixture. On a practical level, it affects the fuel burning rate in ICEs and the engine's performance and emissions. On a fundamental level, the flame speed is an important target for kinetic mechanism development and validation. Accurate determination of laminar flame speed is extremely important for the development and validation of kinetic mechanisms for gasoline, diesel surrogate fuels and alternative fuels (Chen, *et al.* 2009).

Many important flame properties such as stability, extinction and flashback are all related to the flame speed. Flame stability is one of the major problems when using syngas fuels, due to their low calorific values (Chomiak *et al.* 1989; He *et al.* 2012). Few combustion studies are available in the literature for typical syngas compositions, and a gap exists in the fundamental understanding of syngas combustion characteristics, especially at elevated pressures that are relevant to practical combustors.

In the present work, the Flame-speed Calculator *CHEMKIN-PRO* software module is applied to simulate wood gas, sewage gas and landfill gas combustion. This module simulates 1-dimensional freely propagating flame for determining premixed laminar flame-speeds. The complete *GRI-Mech* 3 reaction mechanism, in conjunction with its thermodynamic data and transport properties, has been employed for the syngas mixtures combustion simulation. The laminar flame speeds are determined for a range of equivalence ratios between 0.6 to 1.4, initial temperature between 293 K to 400 K and initial pressure between 1 atm to 10 atm. The simulations results of wood gas mixtures are compared with experimental results obtained by Monteiro *et al.* (2009).

The main motivation of the present work is determining whether and within which limits the Flame-speed Calculator *CHEMKIN-PRO* software module in conjunction with the complete *GRI-Mech* 3 reaction mechanism is a reliable simulation tool for the study of fundamental syngas combustion characteristics. For this purpose the simulation tool has been validated with available wood gas experimental data and the ranges were the simulation tool can be used to predict syngas combustion characteristics with reasonable accuracy have been determined.

2. SIMULATION DESCRIPTION

The Flame-speed Calculator model of *CHEMKIN-PRO* simulates a 1-dimensional freely propagating flame, in which the point of reference is a fixed position on the flame. The laminar flame speed by definition is the relative speed between the unburned gas mixture and the flame front. In this coordinate system, the flame speed is defined as the inlet velocity (velocity of unburned gas moving towards the flame) that allows the flame to stay in a fixed location, which is an eigenvalue of the solution method. This configuration is used to determine the characteristic flame speed of the gas mixture at specified pressure and inlet temperature. In this case there are no heat losses (by definition) and thus the temperatures should be computed from the energy equation. Flame speed depends, in part, on the transport of heat, and predicting the temperature distribution is an integral part of the flame speed calculation.

To set up the flame-speed calculation the initial temperature, initial pressure and mixtures composition are specified as entrance parameters of the Flame-speed Calculator model. The grid parameters "maximum number of grid points allowed" and "ending axial point" have been varied in the range of 50 to 800 and 0.5 cm to 30 cm, respectively, obtaining the best agreement with experimental data for the values of 100 and 20 cm, respectively. Moreover the inlet stream property of "inlet velocity" was set as default, 40 cm/s. The equivalence ratios were varied between 0.6 and 1.4. The default air composition is left as oxidizer. The default products of the complete combustion are set, i.e. CO_2, H_2O and N_2.

The thermodynamic data and transport properties for all the simulated syngas mixtures are provided by the complete *GRI-Mech* 3 reaction mechanism.

3. SYNGAS MIXTURES

As mentioned in the introduction, wood gas produced by gasification is a suitable fuel for ICEs when the presence of particle and tar are below a certain quantity. The particulate matters such as char and ash may damage moving parts, while the tar condensable phase is responsible of fouling in the piping system and heat exchangers and it is a potential problem if the synthesis gas has to be compressed (Laurence, 2012). Table 1 shows the three wood gas compositions obtained in three different gasification processes, i.e. downdraft, updraft and fluidized bed gasifiers, considered in the present work. According to Hasler and Nussbaumer (1999) small scale atmospheric downdraft fixed bed gasifier

produces the synthesis gas with the lower content of particulate matters and tar. Nevertheless, a cleaning process is required before the syngas can be used in ICEs.

Table 1. Wood gas compositions used in this work.

Species	Gasifier		
	Updraft (%)	Downdraft (%)	Fluidized bed (%)
H_2	11	17	9
CO	24	21	14
CO_2	9	13	20
CH_4	3	1	7
N_2	53	48	50

In addition to the wood gas mixtures other two kinds of syngas are considered in the present work: row landfill gas and raw sewage gas whose compositions are presented in Tab. 2.

Table 2. Landfill and sewage gases compositions used in this work.

Species	Landfill (%)	Sewage (%)
CO_2	41	5.6
CH_4	53	68.5
N_2	6	25.9

The general composition of raw landfill gas is the following: methane (from 40% to 60%), carbon dioxide (from 35% to 50%), nitrogen (from 0% to 20%), oxygen (from 0% to 1%) and hydrogen sulphide (from 50 to 200 ppm) (Bove and Lunghi, 2006). The landfill gas composition that is considered in this work is the raw composition provided by Rasi *et al*. (2008) whose structure and laminar burning velocity was investigated by using detailed chemical kinetic simulations by Liu *et al*., (2010).

Finally it is considered a sewage biogas composition generated from domestic waste-water using upflow anaerobic sludge blanket (UASB) reactors. The biogas composition, shown in Tab. 2, has been determined by Lobato (2011), after the UASB reactors gas passed through a H_2S filter. The arithmetic mean of the statistical chromatography gas measurements is considered where the unspecified components are lumped into N_2 and the H_2S fraction is not taken into account. The 100% in sewage gas composition is reached increasing CH_4 percentage as it seems suggested by the work of Lobato (2011).

4. VALIDATION OF SIMULATION TOOL

In this section the simulation results of wood gas compositions are compared with the available experimental data for the simulation tool validation.

The employed Flame-speed Calculator model simulates a freely propagating flame, in which the point of reference is a fixed position on the flame. In this coordinate system, the flame-speed is defined as the velocity of unburned gas moving towards the flame that allows it to stay in a fixed location. The experimental study of Monteiro *et al*. (2009), employed as reference for this simulation validation, is obtained in a closed vessel where the velocity of the unburned gas is zero. Therefore, in this case, the laminar flame speed obtained by the simulation can be compared with the laminar burning velocity of the experimental study. Figure 1 shows this comparison for the three wood gas compositions. The best agreement between simulation and experimental results occurs close to stoichiometric and slightly rich mixture conditions. In the considered range the maximum disagreement, in the order of 20 %, occurs for the downdraft case with $\phi = 1.0$ whilst for the updraft case with $\phi = 1.2$ the disagreement is in the order of 1 %. For lean mixtures the simulation tool gives larger errors in the order of 30 %. While the experimental data are obtained in the range of ϕ between 0.6 and 1.2, the simulation provides results for ϕ between 0.6 and 1.4, showing tendency lines in agreement with experimental data. In the downdraft case the simulation doesn't converge for $\phi = 0.6$ while increasing the equivalence ratio the simulation gets closer to experimental data. In the fluidized bed case Monteiro *et al*. (2009) have got experimental data only for $\phi = 0.8$ and $\phi = 1.0$, while the simulation tool has been able to provide an additional reasonable result for $\phi = 1.2$.

The smaller laminar flame speed, S_L, value of fluidized bed mixture, compared with downdraft and updraft fixed bed S_L, may be caused by a combination of factors: the amount of H_2 in the mixture, the smaller heat value and the amount of dilution by N_2 and CO_2 in the fuel gases. The amount of H_2 in the mixture, due to its high reactivity, strongly influences the S_L. In fluidized bed mixture it is only 9 % in volume, i.e. approximately half its content in downdraft mixtures with a content of 17%. The heat value of fluidized bed mixture is 5.4 MJ/m^3 while updraft and downdraft mixture heat values are 5.5 MJ/m^3 and 5.7 MJ/m^3, respectively (Bridgwater, 1995). The amount of dilution by N_2 and

CO_2 in the fuel gases H_2-CO-CH_4 that compose the typical syngas mixtures affects its S_L value. Again, fluidized bed syngas is the highest diluted syngas (70% by volume), whilst updraft and downdraft syngas are less diluted with 61% and 62% by volume, respectively.
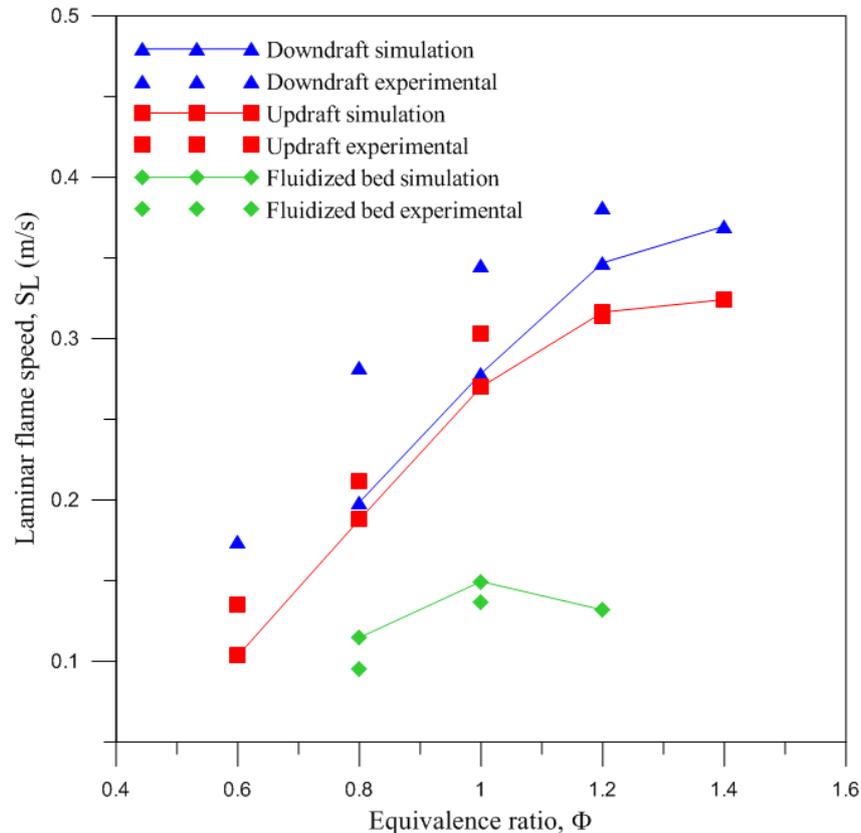

Figure 1. Simulation and experimental (Monteiro *et al*, 2009) comparison of laminar flame speed for three wood gas compositions at atmospheric pressure and unburned gas temperature of 293 K.

The complete *GRI-Mech* 3 reaction mechanism is optimized for natural gas - air combustion. Nevertheless, by comparison of simulation and experimental data it follows that the simulation tool composed by the Flame-speed Calculator *CHEMKIN-PRO* software module, in conjunction with the complete *GRI-Mech* 3 reaction mechanism, is able to simulate characteristics of combustion of wood gas mixtures with a reasonable agreement with experimental data, in a range of equivalence ratios close to stoichiometry.

5. RESULTS AND ANALYSIS

The simulation tool validated in the previous section for wood gas mixtures at atmospheric pressure and unburned gas temperature of 293 K is used in this section to determine the influence of two parameters, i.e. initial temperature and initial pressure of the unburned gas, on the laminar flame speed of raw landfill gas and raw sewage gas.

Figure 2 shows the influence of unburned gas initial temperature, T_i, on the laminar flame speed, of the three wood gas mixtures. Increasing T_i leads to a non linear increase of the laminar flame speed of all wood gas mixtures for all the equivalence ratios under consideration, according to literature (Glassman, 2008; Li *et al*., 2013). The laminar flame speed increases with increasing thermal diffusivity and volumetric chemical reaction rate. The increase of temperature promotes both the increase of thermal diffusivity and volumetric chemical reaction rate, thus explaining the results of Fig. 2.

Figure 3 shows the influence of unburned gas initial pressure, P_i, on the laminar flame speed S_L of the three wood gas mixtures. In this case, increasing P_i leads to a decrease of the laminar flame speed of all wood gas mixtures according to literature (Glassman, 2008; Li *et al*., 2013). For all mixtures the increase of P_i produces a nonlinear decrease of S_L for all the equivalence ratios under consideration. The increase of pressure promotes both the decrease of thermal diffusivity and volumetric chemical reaction rate, thus explaining the results of Fig. 3.
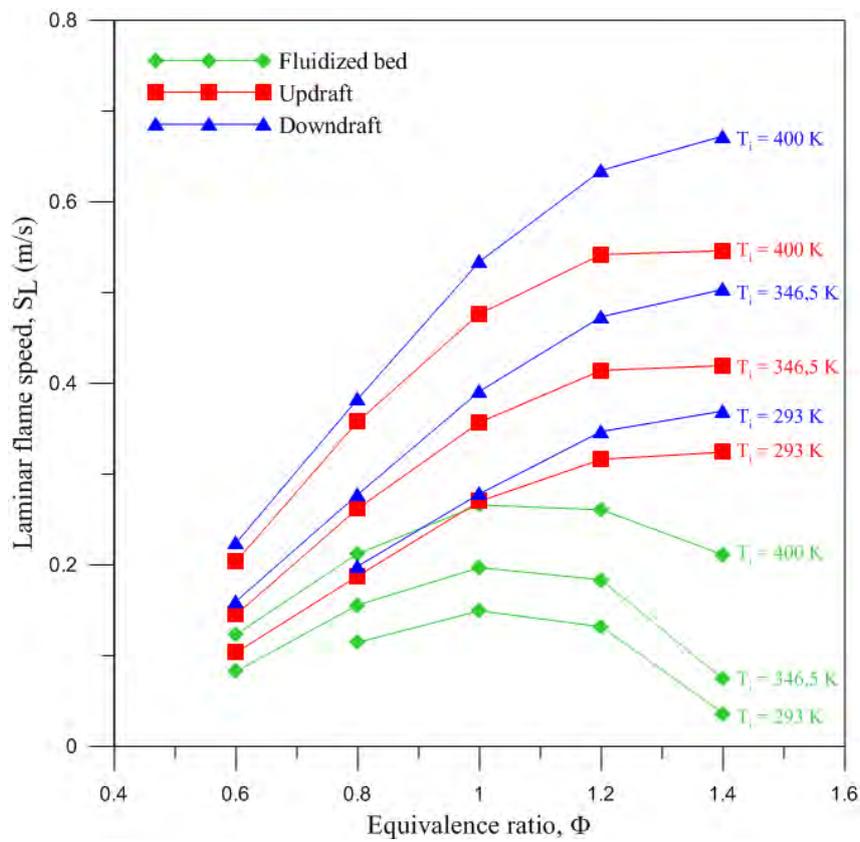
Figure 2. Unburned gas initial temperature influence on the laminar flame speed S_L of the three wood gas mixtures at atmospheric pressure.
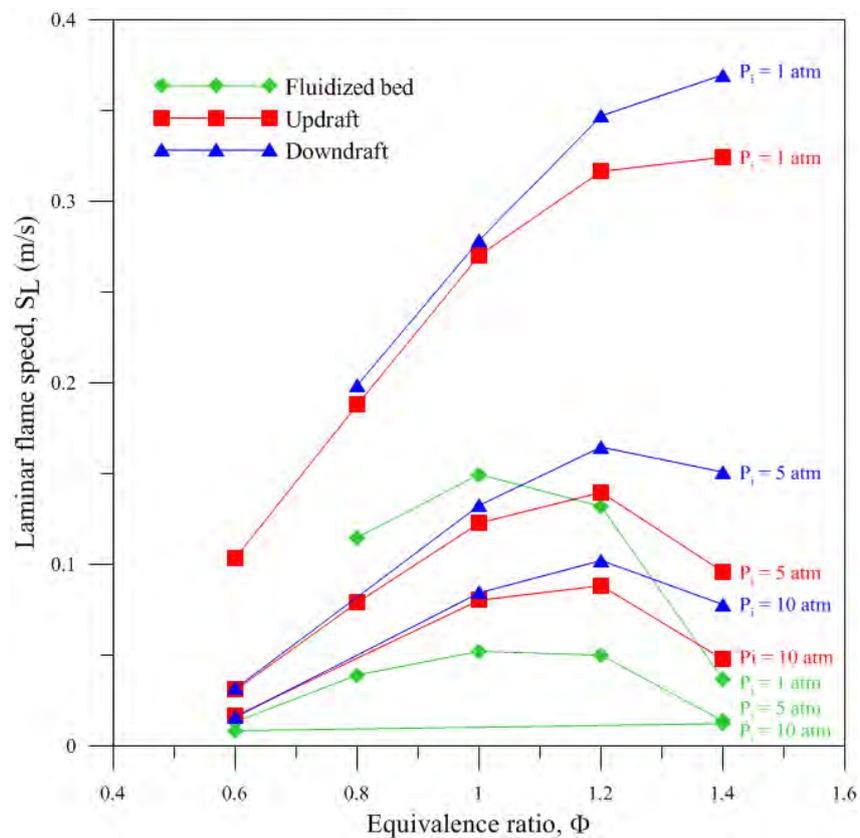

Figure 3. Unburned gas initial pressure influence on laminar flame speed of the three wood gas mixtures, $T_i = 293$ K.

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Figure 4 shows the influence of unburned gas initial temperature, T_i, on the laminar flame speed, of landfill and sewage gases at atmospheric pressure. Figure 5 shows the influence of unburned gas initial pressure, P_i, on S_L of landfill and sewage gases at initial temperature $T_i = 293$ K. Once again the increase of temperature promotes both the increase of thermal diffusivity and volumetric chemical reaction rate, explaining Fig. 4, meanwhile the increase of pressure promotes both the decrease of thermal diffusivity and volumetric chemical reaction rate, thus explaining Fig. 5. The amount of dilution by N_2 and CO_2 in the fuel gas CH_4 is higher in sewage gas than in landfill gas, explaining the higher laminar flame speed of sewage gas presented in Figs. 4 and 5.
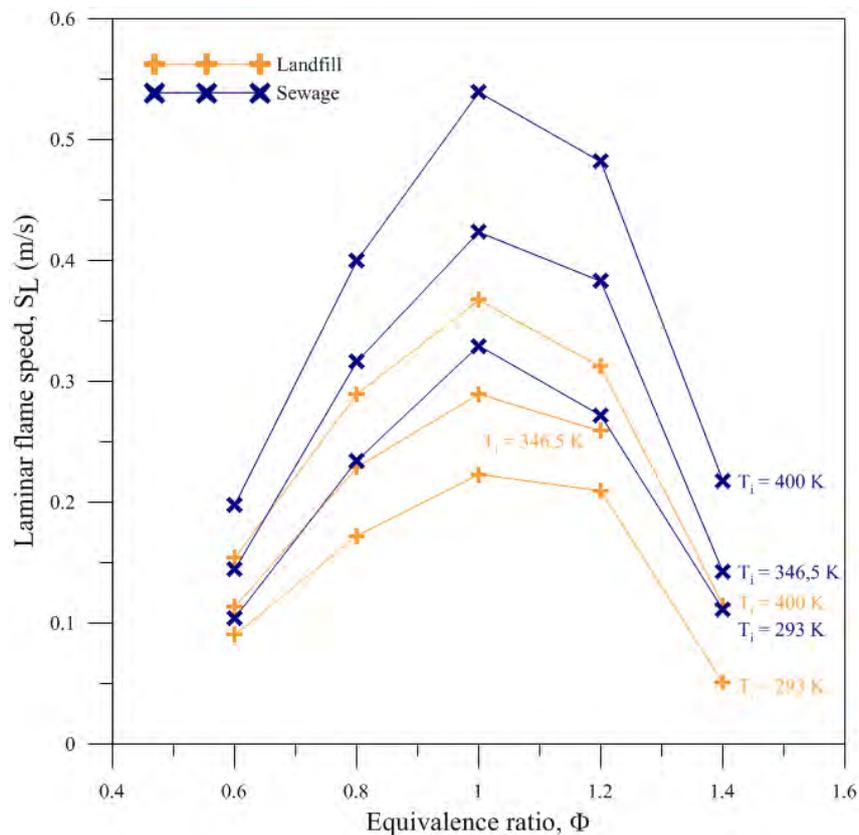

Figure 4. Unburned gas initial temperature influence on the laminar flame speed
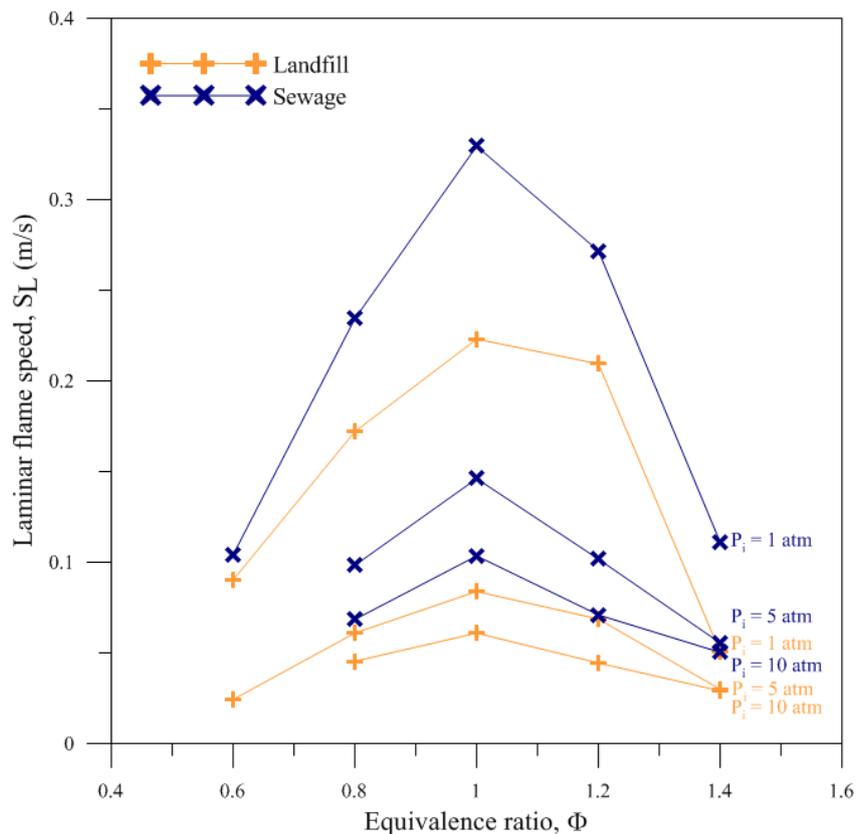
Figure 5. Unburned gas initial pressure influence on laminar flame speed of landfill and sewage gases at $T_i = 293$ K.

6. CONCLUSIONS

The capability of the simulation tool composed by the Flame-speed Calculator *CHEMKIN-PRO* software module, in conjunction with the complete *GRI-Mech* 3 reaction mechanism, for determining the laminar flame speed of syngas mixtures has been proven.

The simulation tool has been used to simulate the laminar flame speed of three wood gas mixtures, fuels with five compounds, providing reasonable agreement with experimental data especially close to stoichiometric conditions thus validating it.

The validated simulation tool has been then applied to determine the behavior of laminar flame speeds of the three wood gas mixtures and of a landfill and a sewage gas mixtures in a range of equivalence ratios between 0.6 to 1.4, varying the unburned gas initial temperature and initial pressure between 293 K to 400 K and 1 atm to 10 atm, respectively.

The simulations confirmed that an increase of unburned gas initial temperature provides an increase of laminar flame speed while an increase of unburned gas initial pressure provides a decrease of laminar flame speed for all the fuel mixtures considered in the research.

Suggestions for future works aiming to reach a better agreement between simulation and experimental data are: 1) make a simulation tool refinement creating a reduced mechanism by considering only the most relevant reactions with a sensitivity study applicable to all wood, landfill and sewage gases and 2) create a specific detailed mechanism for the five fuel compounds of the wood gas mixtures.

7. ACKNOWLEDGEMENTS

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