

Numerical calculation of the laminar flame speed of low calorific gases

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Abstract:

Laminar flame speed is an important parameter of the combustion process. It plays a crucial role in issues connected with the flame stability. There are many experimental methods of determination laminar flame speed of gaseous fuels, nevertheless they are very often quite complex. This is an especially big disadvantage when there is a necessity of laminar flame speed determination of not typical gases. Low calorific gases (i.e. from biomass waste gasification process) are an example of such fuel. Such gases may be characterized by high variability in composition depending on the process conditions and fuel composition before process. For this reason it is extremely important to know the basic properties of such gas. Numerical methods of the laminar flame speed calculations are quite good alternative in comparison to experimental methods. They give the opportunity to change many parameters of the process at the same time. It is especially important when general characterization of the new low calorific gaseous fuel is the most important aspect of the research. The aim of the work was numerical analysis of the laminar flame speed of the waste biomass gasification gas. Cosilab 3[®] software and following two mechanisms, namely GRI-Mech 3.0 and USC-Mech were used.

Results show that the laminar flame speed value increases as the molar fraction of hydrogen in the fuel goes up. Interestingly, the laminar flame speed increases rapidly as the amount of hydrogen increases from 5 to 17%. The laminar flame speed calculated using GRI-Mech 3.0 were slightly larger than the simulation results calculated using USC-Mech II during the entire duration of this study.

Keywords:

Numerical analysis, low calorific gas, CosiLab 3[®], kinetic mechanism, laminar flame speed.

1. Introduction

Significant increase amount of waste has become a common environmental problem globally. Thus, proper strategy for waste management is inevitable as it is a vital part of sustainability and environmental protection [1]. An appropriate approach should minimize the amount of waste and maximize its recovery to useful utilization [2]. On an international level, proper waste management – as one means for mitigating carbon emission – is well recognized in the Kyoto Protocol. In terms of climate change policy, the Kyoto Protocol is considered to be the most crucial driver for the utilization and diffusion of waste-to-energy (WTE) technology [3]. The thermo-chemical conversion of waste biomass consists of four main processes: combustion, co-combustion, pyrolysis and gasification. One of the promising thermo-chemical conversion technologies that can be used to convert sewage sludge to useful energy forms suited for small to medium size, throughput is gasification. Gasification is a unique process that transforms any carbon-based material into energy without burning it. Instead, gasification converts the materials into a gas by creating a chemical reaction. This reaction combines those carbon-based materials (known as feedstock) with small amounts of air or oxygen, breaking them down into simple molecules, primarily a mixture of carbon monoxide and hydrogen, and removing pollutants and impurities. What's left is a clean "synthesis gas" (syngas) that can be converted into electricity and valuable products. Nevertheless, such gas is characterized by high variability in composition depending on the process conditions and feedstock composition. For that reason, its use may pose some difficulties so it is extremely important to know the basic properties of such gases. An example of such properties is laminar flame speed, which plays a crucial role in issues connected with the flame stability, extinction and flashback [4].

Flame stability is one of the major problems encountered in the combustion of syngas fuels, given their low calorific values. In the combustion community, laminar flame speed is also one of the fundamental parameters that helps validate chemical kinetic models and aids the design of the combustor.

In previous studies, investigations of the laminar flame speed of syngas were focused on the binary H₂/CO mixture [5-10]. Nevertheless, typically syngas, aside from H₂ and CO, usually contains other substances, such as CH₄, N₂ and CO₂. In recent years, an increasing interest has been shown in the study of actual syngas compositions. For example, Monteiro et al. [11], Liu et al. [12], and Ouimette et al. [13] investigated the laminar flame speed of typical biomass-derived syngas that was composed of H₂, CO, CH₄, N₂ and CO₂ and other hydrocarbons by either experiments or simulations. Dam et al. measured the laminar flame speed of typical coal-derived syngas composed of H₂, CO, CH₄, N₂ and CO₂ at a series of equivalence ratios [14]. However, a systematic investigation of the effects of composition variations on laminar flame speed of actual syngas has been seldom reported. In previous research, authors experimentally and numerically studied the effects of H₂ content on the laminar burning velocity of typical syngas [15]. Aside from H₂, CO is also a major combustible species in syngas fuel. Moreover, the combustion characteristics of CO are quite different from those of H₂. According to the study by Rightley et al., the reaction rate of CO with hydrogen-containing species can be several times faster than that of CO with O₂ [16]. Therefore, when CO content changes, the content of the hydrogen-containing species also changes, resulting in a significant variation of the laminar flame speed. To evaluate the effects of CO, Wu et al. employed an opposed-jet burner to measure the laminar flame speed of CH₄ with different amounts of additional CO [17]. The experimental results were also compared with numerical simulations. The laminar flame speed of CH₄/CO/air mixture was found to change substantially with the addition of CO, which was considered by Wu et al. to be related to the transition of the dominant chemical kinetic steps. In a subsequent work, Cheng et al. employed the same experimental setup and numerical simulation method to investigate the laminar flame speed of H₂/CO/CH₄/air mixture with different CO contents [18].

Nevertheless, the new specific syngas like syngas from sewage sludge gasification gas have not been analysed detailed enough. Experimental methods of the determination laminar flame speed of lean gases are quite complex. Numerical methods of the laminar flame speed calculations are a good alternative in comparison to them. They give the opportunity to change many parameters of the gasification process at the same time. It is especially important, when general characterization of the new low calorific gaseous fuel is the main focus of the research.

The aim of the work was kinetic simulations of the laminar flame speed of the waste biomass gasification gases. The effects of combustion parameters on the laminar flame speed of the syngases were analyzed. Cosilab 3[©] software and following two mechanisms, namely GRI-Mech 3.0 [19] and USC-Mech [20] were used.

2. Laminar flame speed simulation

The detailed mole fraction of the analyzed syngas compositions is shown in Table 1. Kinetic simulations were conducted using the one – dimensional freely propagating flame model in Cosilab 3[©] software.

Table 1. Composition of the analysed syngas

Symbol	Syngas	Ref.	syngas composition, % vol.					LHV, MJ/m ³ _n
			CO	CO ₂	H ₂	CH ₄	N ₂	
Sgas1	Waste wood (fluidized bed)	[21]	14.0	20.0	9.0	7.0	50.0	5.24
Sgas2	Waste wood (fixed bed updraft)	[21]	24.0	9.0	11.0	3.0	53.0	5.29
Sgas3	Waste wood (fixed bed downdraft)	[21]	21.0	13.0	17.0	1.0	48.0	4.84
Sgas4	Sewage sludge (fixed bed)	[22]	28.5	15.0	5.0	1.0	50.5	4.49

The computational domain was set from 2 cm do 10 cm to ensure the boundaries sufficiently far from the flame itself so that there was a negligible diffusion of heat and mass through the boundary. For the simulations, the pressure was 1 atm and the temperature of the unburned gas mixtures was 298 K. The Freely Propagating 1D Laminar Premixed Flames (FP1DLPF) model was used. FP1DFPLF module is based on the four equations: the continuity equation, the equation of conservation of mass, energy equation and the equation of state of an ideal gas.

According to the thermal theory, a mathematical model of the laminar premixed flame contains a few assumptions:

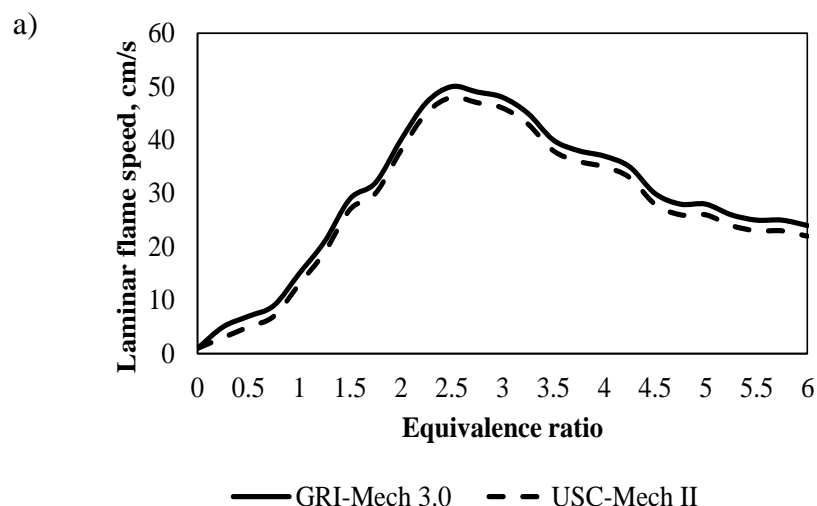
- Heat, which is ensured due to an exothermic oxidation reaction, is transported thanks to conduction (no Dufour effect).
- Mass and heat transfer does not appear between particular stream layers.
- The laminar flame thickness is relatively thin in comparison to the mean free path of a species.

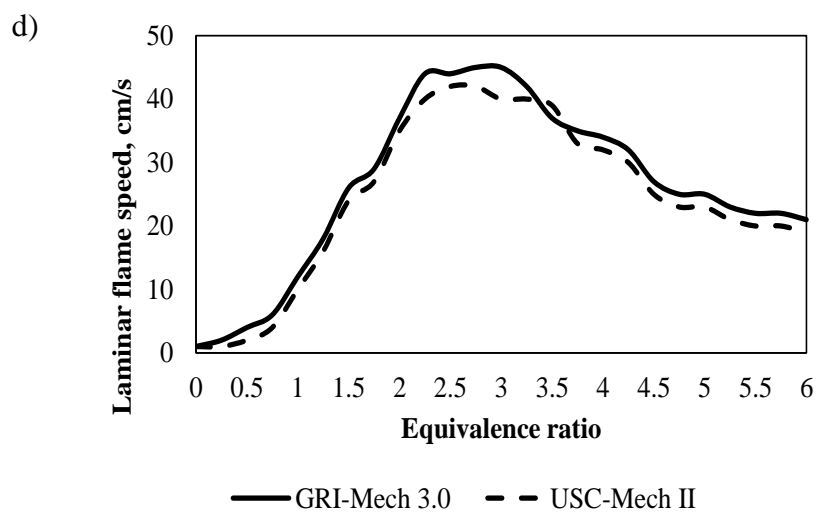
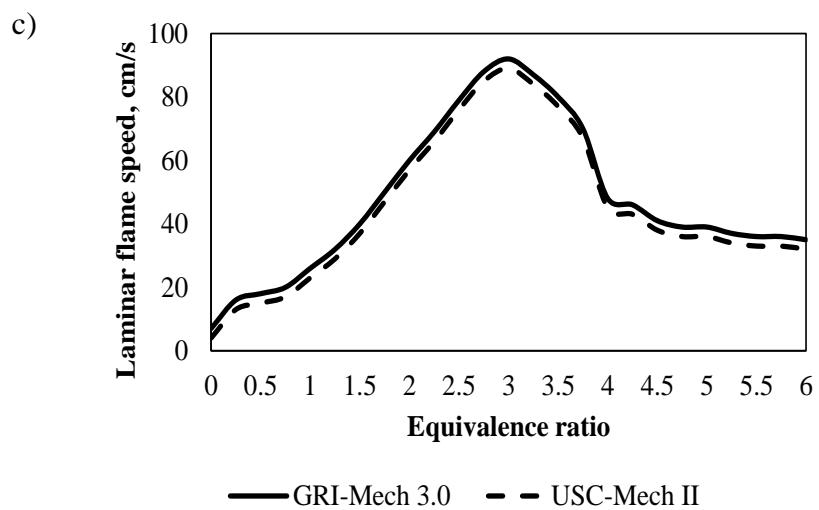
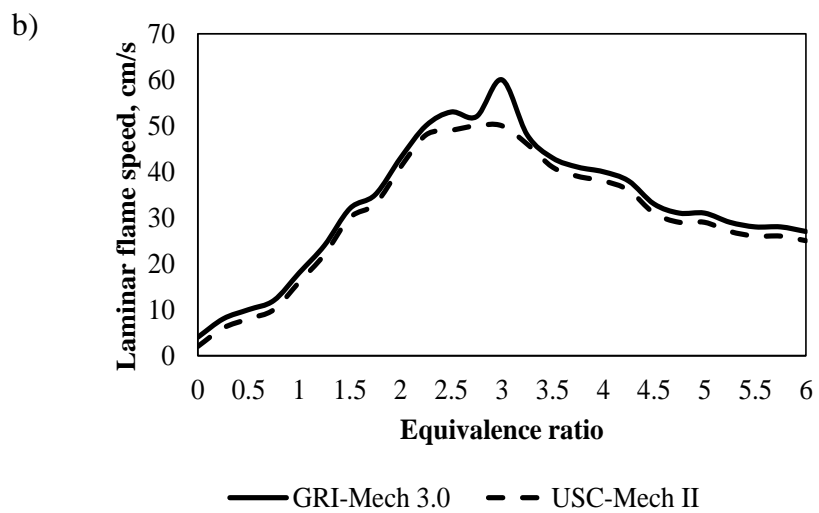
For the kinetic simulation, two mechanisms were employed: GRI-Mech 3.0 and USC-Mech II. The GRI-Mech 3.0, originally developed for methane combustion, consists of 53 species and 325 reactions. Moreover, this mechanism includes reactions that are involved in the combustion of other hydrocarbon fuels, such as ethane and propane. In recent years, this mechanism has also been employed for CH₄/H₂/air [23] and H₂/CO/air [24] flame simulations. However, the performance of GRI-Mech 3.0 in simulating the flame of actual syngas compositions remains unclear. The second mechanism, USC-Mech II, which is specially developed for H₂/CO/C₁-C₄ hydrocarbon combustion, consists of 111 species and 784 reactions. This mechanism incorporates the recent thermodynamic, kinetic, and species transport updates relevant to high-temperature oxidation of hydrogen, carbon monoxide and C₁-C₄ hydrocarbons. The USC-Mech II was developed by a series of studies over the last decades [25]. However, besides the combustible compositions hydrogen, carbon monoxide and methane, the actual syngas contain incombustible species like nitrogen and carbon dioxide, which may make a different combustion process of the syngas. Therefore, the capability of this mechanism in modeling actual syngas combustion likewise still needs further validation.

3. Results and discussion

3.1. Laminar flame speeds kinetic analysis of different equivalence ratio values

Figure 1 shows laminar flame speed values as a function of equivalence ratio ϕ . Kinetic simulation was conducted for a wide range of equivalence ratio equal to $\phi = 0.0 - 6.0$. As shown in the figure the laminar flame speed increased with the equivalence ratio from the fuel-lean side and decreased with the equivalence ratio after its peak value.





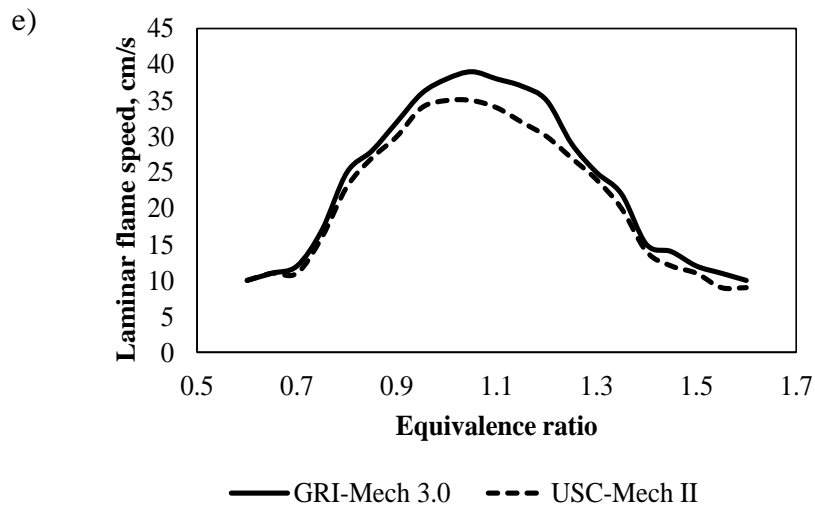
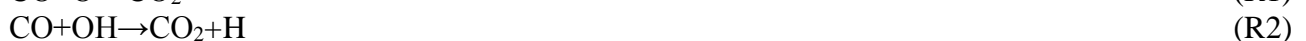


Fig.1. Laminar flame speed as a function of equivalence ratio; a) Sgas1; b) Sgas2; c) Sgas3; d) Sgas4; e) pure methane

Results for four gases, which composition was presented in Table 1 was included: (a) Sgas1 with the molar fraction of hydrogen equal to 9.0, (b) Sgas2 with the molar fraction of hydrogen equal to 11.0, (c) Sgas3 with the molar fraction of hydrogen equal to 17.0 and (d) Sgas4 with the molar fraction of hydrogen equal to 5.0. That figure also shows the laminar flame speed simulation of pure methane (e) employing GRI-Mech 3.0 and USC-Mech II. The laminar flame speed of analysed syngases [(a) to (d)] reaches its maximum at rich condition. It can be also observed, that the laminar flame speed value increases as the molar fraction of hydrogen in the fuel goes up. In the case of the Sgas3 (molar fraction of hydrogen equal to 17%) the laminar flame speed is equal to 92cm/s and in the case of Sgas4 (molar fraction of hydrogen equal to 5%) – 45cm/s. This behavior is explained by the facts that the overall reactivity of the fuel mixture increases with the amount of hydrogen and the low molecular weight of hydrogen acts to increase the diffusivity of the reactant mixture. Interestingly, the laminar flame speed increases rapidly as the amount of hydrogen increases from 5 to 17%. This is mainly due to the well known sensitivity of the carbon monoxide oxidation rate to the presence of small amounts of hydrogen containing species. The main carbon monoxide oxidation shifts from slower reaction (R1) to relatively faster (R2) as the amount of hydrogen increases, causing an increase in laminar flame speed.



It should be also mentioned that hydrogen pose a very unique combustion characteristics which differs significantly from hydrocarbon fuels. Recent studies [26] showed that variation of hydrogen composition in syngas introduces substantial adverse effects on the flame shape, emissions, blow – off and flashback limits, and most importantly combustion instability. Above the value of the equivalence ratio in which laminar flame speed reaches its maximum, there is visible slightly decrement of this parameter. It can be explained by the presence of unwanted carbonyl compounds in the hydrogen/carbon monoxide blend. These compounds tended to have strong inhibition effects on flames and were essentially effective on the rich side of the laminar flame speed curve.

The laminar flame speed of methane [(e)] increased with the equivalence ratio in the fuel-lean side, and reached its maximum value around $\phi = 1.05$. After that, the laminar flame speed decreased significantly with the further increase of equivalence ratio. Due to the different thermal diffusivity of syngas fuel mixtures from that CH_4 the equivalence ratio corresponding to the maximum laminar flame speed shifted obviously to the fuel-rich side.

Analyzing results presented on this figure, it should be also concluded that the laminar flame speed calculated using GRI-Mech 3.0 were slightly larger than the simulation results calculated using

USC-Mech II during the entire duration of this study. For the prediction of the peak laminar flame speed, the maximal difference between results achieved using both models is equal to 2.2%.

3.2. Maximum values of the laminar flame speed calculated by the theoretical formula

Laminar flame speed results achieved using kinetic models were compared with laminar flame speed values calculated using formula (1) [27].

$$S_L^{\max} = \frac{\sum_{i=1}^n r_i \cdot S_{Li}^{\max}}{\sum_{i=1}^n r_i} \quad (1)$$

S_L^{\max} is the maximum value of laminar flame speed, cm/s; r_i is a volumetric fraction of i-th mixture component, % vol.; S_{Li}^{\max} is the maximum value of laminar flame speed for i-th mixture component, cm/s.

Data for this calculation was based on Table 2 [27].

Table 2. Maximum values of laminar flame speeds for different fuels [27]

Fuel	Equivalence ratio ϕ	S_{Li}^{\max} , cm/s
Hydrogen	1.78	325.0
Carbon monoxide	2.04	52.0
Methane	1.07	44.8
Ethane	1.14	47.6
Ethylene	1.14	73.5

The calculation results are shown in Table 3.

Table 3. Maximum values of laminar flame speeds calculated from a formula (1)

Symbol	Gas	S_L^{\max} , cm/s Calculated using eq.(1)	S_L^{\max} , cm/s Calculated using kinetic models	
			GRI-Mech 3.0	USC-Mech II
Sgas1	Waste wood (fluidized bed)	39.7	50.0	48.0
Sgas2	Waste wood (fixed bed updraft)	49.6	60.0	50.0
Sgas3	Waste wood (fixed bed downdraft)	104.0	92.0	89.0
Sgas4	Sewage sludge (fixed bed)	31.5	45.0	40.0

Analyzing results presented in table 3 it can be concluded that there are visible small differences between laminar flame speed results achieved using theoretical formula and kinetic models. Nevertheless, it should be emphasized that data presented in table 2 and used in the formula (1) are based on the different experimental methods such as flat flame, Bunsen flame, stagnation flame, spherically propagating flame, counter-flow flame and heat flux method [28]. Generally, the present experimental data shows [28] that measurement methods can give slightly different results for specific conditions. For example, comparison of the heat flux method and Bunsen flame method shows that the results based on the Bunsen method appear to be a little higher under super fuel-rich conditions due to the involvement of environmental air. Although the laminar flame speed based Bunsen method wasn't adiabatic, the results showed to be very close to the adiabatic laminar flame speed measured by the heat flux method when the equivalence ratio was smaller than 3.5.

4. Conclusions

For the power and heat sector, gasified biomass can be used as a fuel in combustion devices such as gas engines, gas turbines, boilers or industrial burners. Particularly, use of the gasified biomass for energy final energy generation is foreseen as a very promising application, possessing great potential for research and development. The combustion of gasified biomass differs from that of natural gas particularly due to its different composition of heating value. Therefore, it is crucial to understand the fundamental combustion properties of syngas with components diversity. Kinetic modeling is cheap and easy method to estimate these parameters. This is especially important in the case of syngas which typically its composition varies from various gasifier processes from 4.0% to 50.4% hydrogen, 8.1%-60.5% carbon monoxide, 1.3%-29.6% carbon dioxide, 0%-20.4% water vapor and 0%-9.3% methane.

Results show that the laminar flame speed value increases as the molar fraction of hydrogen in the fuel goes up. Interestingly, the laminar flame speed increases rapidly as the amount of hydrogen increases from 5 to 17%. This is mainly due to the well known sensitivity of the carbon monoxide oxidation rate to the presence of small amounts of hydrogen containing species.

Analyzing results achieved using two different models, it should be concluded that the laminar flame speed calculated using GRI-Mech 3.0 were slightly larger than the simulation results calculated using USC-Mech II during the entire duration of this study. Nevertheless, a comparison of those results with calculation results based on the experimental based formula shows that there are visible small differences between laminar flame speed results. Taking into consideration the advantages of the kinetic studies, such difference and laminar flame speed prediction are acceptable.

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