

Numerical Analysis of the Combustible Properties of Sewage Sludge Gasification Gas

Sebastian Werle

Institute of Thermal Technology, Silesian University of Technology, Gliwice, 44-100, Konarskiego 22, Poland.

Sebastian.werle@polsl.pl

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, its use may pose some difficulties. For example, it may be the design of burners and combustion chambers to ensure environmentally and energy efficient disposal. For this reason it is extremely important to know the basic properties of the 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.

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 (Tolis et al., 2010). An appropriate approach should minimize the amount of waste and maximize its recovery to useful utilization (Cuchiella et al., 2012). 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 (Sommer and Ragossing, 2011). The thermo-chemical conversion of waste biomass consists of four main processes: combustion, co-combustion, pyrolysis and gasification (Bibrzycki et al., 2014). 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 (Werle, 2011). 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 (Lee et al., 2014). 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. 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 (Smith et al., 2007) and USC-Mech (Wang et al., 2007) were used.

2. Laminar flame speed simulation

The detailed mole fraction of the analysed syngas compositions is shown in Table 1. Kinetic simulations were conducted using the one – dimensional freely propagating flame model in Cosilab 3[®] software. 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. 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 (Halter et al., 2005) and H₂/CO/air (Natarajan et al., 2007) 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 (Davis et al., 2005). 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.

Table 1: Composition of the analysed syngas (Werle, 2012)

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

3. Results and discussion

3.1 Laminar flame speeds kinetic analysis of different equivalence ratio values

Figures 1 to 5 show 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. Results for four gases, which composition was presented in Table 1 was included: (1) Sgas1 with the molar fraction of hydrogen equal to 9.0, (2) Sgas2 with the molar fraction of hydrogen equal to 11.0, (3) Sgas3 with the molar fraction of hydrogen equal to 17.0 and 4) Sgas4 with the molar fraction of hydrogen equal to 5.0. That figure also shows the laminar flame speed simulation of pure methane (5) employing GRI-Mech 3.0 and USC-Mech II. The laminar flame speed of analysed syngases [(1) to (5)] 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 92 cm/s and in the case of Sgas4 (molar fraction of hydrogen equal to 5 %) – 45 cm/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.

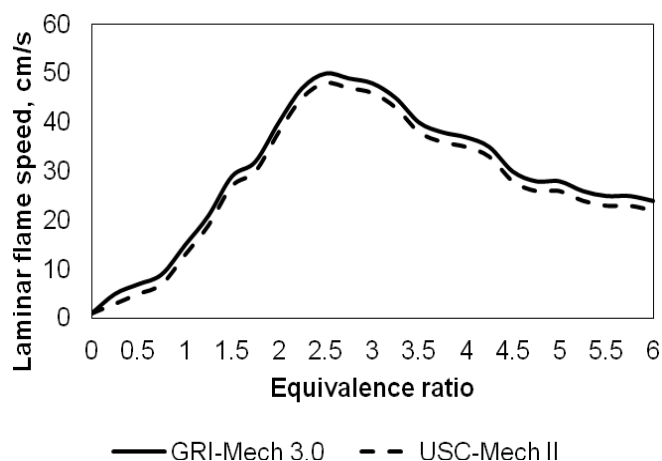
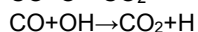
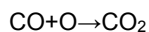


Figure 1: Laminar flame speed as a function of equivalence ratio - Sgas1

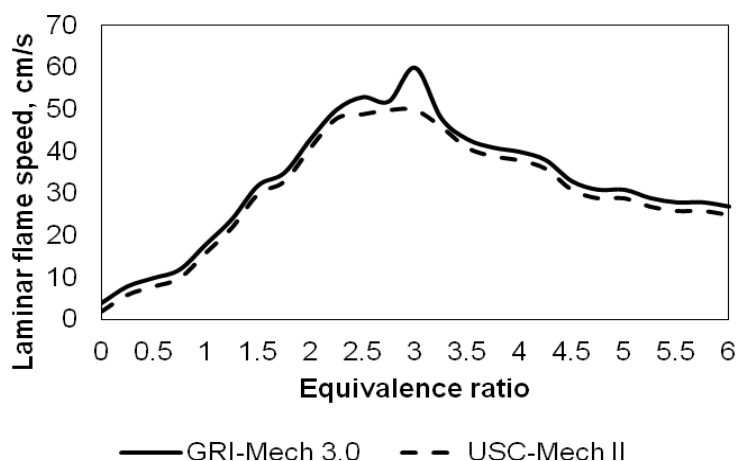


Figure 2: Laminar flame speed as a function of equivalence ratio - Sgas2

It should be also mentioned that hydrogen pose a very unique combustion characteristics which differs significantly from hydrocarbon fuels. Recent studies (Lee et al., 2014) 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.

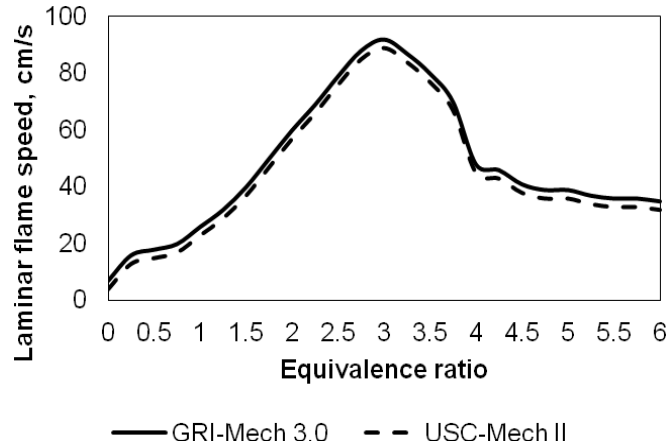


Figure 3: Laminar flame speed as a function of equivalence ratio - Sgas3

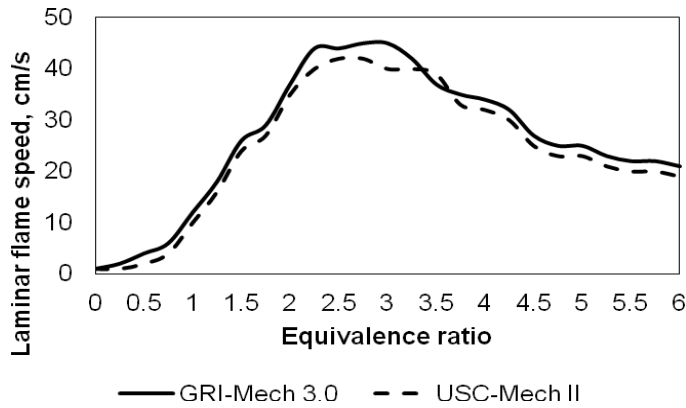


Figure 4: Laminar flame speed as a function of equivalence ratio - Sgas4

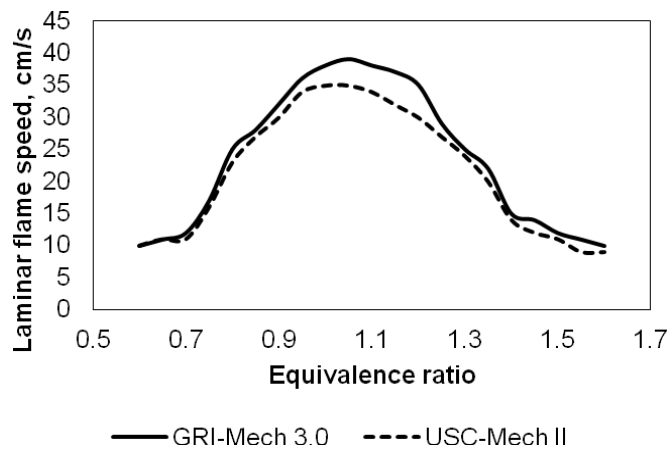


Figure 5: Laminar flame speed as a function of equivalence ratio - pure methane

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 CH₄ 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)..

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

Table 2. Maximum values of laminar flame speeds for different fuels (Kordylewski, 2008)

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

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 (Kordylewski, 2008). The calculation results are shown in Table 3.

Table 3. Maximum values of laminar flame speeds calculated from Eq. (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 eq. (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 (Wang et al., 2015). Generally, the present experimental data shows (Wang et al., 2015) 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

Use of the gasified biomass for energy final energy generation is foreseen as a very promising application. 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 %-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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