Numerical Study Of The Effect Of Hydrogen Addition On The Laminar Flame Speed And Premixed Flame Structure Of Biogas

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Abstract- In this work, the laminar flame speed and flame structure of biogas/H2 fuel mixtures were studied numerically from pure biogas to biogas with an addition of 15% H2 in volume by using the CHEMKIN software with the GRIMECH 2.11 kinetic mechanism. The effect of hydrogen addition to biogas on laminar flame speed and flame structure has been studied as well as the variation of the aeration rate from stoichiometric conditions to lean conditions. The trends in laminar flame speed results obtained are explained by means of numerical results on temperature profile and heat release rate. CO, CO2 and NO profiles are also observed for the different mixtures studied. Hydrogen addition in biogas flames shows an important effect, especially in zones near stoichiometric flames, decreasing its effects in lean mixtures combustion.

Keywords Biogas-hydrogen, laminar flame speed, flame structure, numerical study.

1. Introduction

The necessary use of combustion technologies to reduce the dependence on fossil fuels [1] and additionally, the emission of greenhouse gases to meet the goals of climate change mitigation [2,3], have generated a continuous growth in the study[4] of the possible applications of alternative fuels such as biogas generated by anaerobic decomposition of organic substances, synthesis gas produced in the gasification of coal or biomass, liquid biofuels as fuel alcohol obtained different crops such as corn or sugar cane and biodiesel obtained from vegetable oils.

Biogas generated by the anaerobic decomposition of organic substances is a great source of energy, especially in regions or countries where economic growth causes an increasing in the generation of municipal solid waste or organic waste product of industrial or agricultural activities where its decomposition could generate this alternative fuel [3,5-7]. This biogas, composed mainly of methane (CH_4), carbon dioxide (CO_2) and other small amounts of oxygen, nitrogen, volatile compounds and even hydrogen sulphide, is generally cleaned of some of these minor compounds [8] to reduce their harmful effect on combustion systems.

The clean biogas (CH_4 and CO_2) is a fuel whose combustion properties such as calorific value, flame temperature and deflagration velocity are poor compared to conventional gaseous fuels such as natural gas or LPG [9-12]. This produces that the use of the biogas in combustion systems requires a study to that avoid the problems of flame instability associated to the lower flame speed and the change in the limits of flammability [13-16]. However, in [17], it is concluded that the use of biogas in burners for natural gas does not require significant modifications in the burners based on the profile of flame temperatures and pollutant emissions, but not on flame stability parameters. One of the ways to improve these combustion properties in to convert biogas to biomethane using different treatments that reduce the CO_2 content and its effects [18,19] as well as other minor compounds such as H_2S [8,20,21]. However, this treatment process is expensive in terms of equipment and absorbing substances such as amines. The improvement of the combustion properties of the biogas can be achieved by mixing it with another combustible gas whose combustion properties, mainly the flame speed, is greater so that the resulting mixture has combustion properties that can be compared with those of the gas Natural or LPG, reducing the problems of biogas interchangeability with these fuels [9, 22]. Hydrogen is the combustible gas that has the greatest value of flame speed at standard conditions, in addition to a higher calorific value, a higher flammability range and a higher flame temperature, and therefore, its addition to the biogas will result in an improvement of the combustion properties of this last one. Different studies have concluded that mixing the biogas with other fuels such as H_2, LPG or natural gas increases the flame speed of the resulting mixture and therefore the range of flame stability [23-27]. Hydrogen has been selected as the biogas additive to improve its combustion properties since it is a renewable fuel, with a zero greenhouse potential and which could additionally be obtained from fossil fuels through reforming processes [28] or even from the same biogas [29,30].

By means of the realization of a numerical study, it has been studied the effect of hydrogen addition on the flame structure of biogas [31,32], biogas/H_2 mixtures in diffusion flames [33], methane with CO_2 dilution [34] and syngas [35]. In this work, it is tried to determine the effect of the addition of different proportions of H_2 to a simulated biogas in the flame speed and flame structure of premixed flames. The results are intended to guide the H_2 produced from reforming other fossil fuels as an alternative to improve the combustion properties of biogas, especially in atmospheric premix burners.

2. Methodology

Different numerical simulations of biogas combustion reactions were performed in the CHEMKIN Software. Simulations of the combustion reactions of different mixtures have been performed for different aeration factors, starting with a stoichiometric mixture and increasing these aeration factors as shown in Table 1.

Table 1. Composition of biogas and biogas/H_2 mixtures simulated

Mixture	Composition	Aeration factor n				
Pure biogas	$0.6CH_4 + 0.4CO_2$	1	1.1	1.2	1.3	1.4
Biogas + 5% H_2	$0.57CH_4 +$ $0.38CO_2 +$ $0.05H_2$	1	1.1	1.2	1.3	1.4
Biogas + 15% H_2	$0.51CH_4 +$ $0.34CO_2 +$ $0.15H_2$	1	1.1	1.2	1.3	1.4

The composition for the simulated biogas was selected as shown in Table 1 for pure biogas. This is a mean composition for a biogas typically generated in landfills or wastewater treatment plants or bio digesters of organics waste, taking into account the difficulty of finding typical biogas generation data in the literature [36]. Similar mean compositions are presents in [33-35,37,38].

The aeration factor n for combustion is introduced into the stoichiometric equation of each reaction as given below:

$$ACH_4+BCO_2+DH_2+n(a_t)(O_2+3.76N_2)\rightarrow XCO_2+YH_2O+ZN_2+WO_2 \quad (1)$$

Where n is the aeration factor and a_t is the theoretical air coefficient of the combustion reaction determined by the elementary reaction balances. The values of aeration factor was selected only for fuel lean mixtures (n >1) to support a subsequent experimental stage of the project using an atmospheric premix burner.

The CHEMKIN tool has been used to determine the laminar flame speed of the specified combustible gas mixtures. The chemical kinetics and transport equations for gas phase are solved following the free-propagation flame model to obtain the chemical species concentration profiles, the heat release rate and the temperature profile developed for adiabatic flame starting from the molar compositions of each of the selected mixtures described above and with initial values of the pressure at which the flame is developed and an approximate temperature profile. For these simulations, site conditions of pressure and temperature of 0.91 atm and 298 K were stablished and the chemical kinetics mechanisms Grimech 2.11 was used, mechanism that have been validated for the simulation of biogas flames [39-41].

3. Results and Discussion

The results of the simulations obtained in the estimation of the laminar deflagration velocity of the studied mixtures and its temperature profile, heat release rate and species profiles are presented and discussed.

3.1 Laminar Flame Speed

Numerical results of laminar flame speed obtained according with the methodology presented, for the mixtures before mentioned are shown in Figure 1. This laminar flame speed has been obtained for the different aeration factors presented in Table 1.

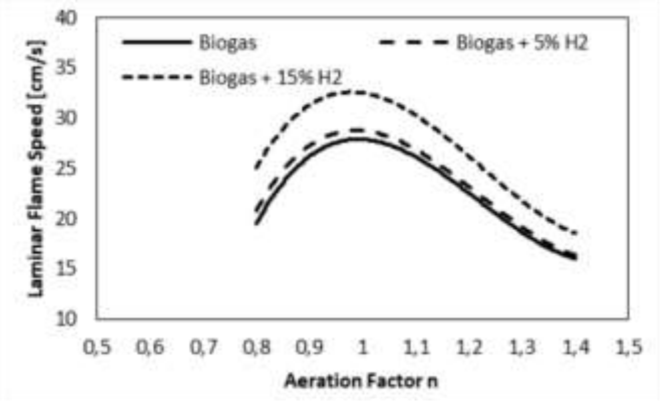

Fig. 1. Laminar flame speed of pure Biogas and Biogas/H_2 mixtures with variation of aeration factor.

The values obtained in this work for pure biogas (continuous line); shown in Figure 1, agree with reported values for biogas flames [22, 24] between 27 and 28 cm/s respectively for stoichiometric flames and similar pressure and temperature conditions. The maximum value of the laminar flame speed for the biogas/H_2 mixtures is reached, with values ranging from 27.4 m/s for pure biogas and 28.47 and 32.17 m/s for biogas with 5% H_2 and biogas with 15% H_2

respectively. For lean mixtures (n=1.4), the effect of hydrogen addition on laminar flame speed decreases, from values of 15.8 cm/s for pure biogas to 18.41 cm/s for biogas with 15% H_2. The effect of 5% of hydrogen addition in the laminar flame speed of biogas represents a small change from the pure biogas; therefore, according to results obtained, a significant improvement on laminar flame speed of biogas requires a hydrogen addition near 15% or more in volume.

3.2 Flame Structure

Observing the flame structure obtained in the different simulations, we can relate the observed increase in the flame speed with the effect of hydrogen on the kinetics of the reaction. Figures 2-4 show the temperature profiles for stoichiometric mixtures (n = 1) and lean mixtures (n = 1.2 and n = 1.4).

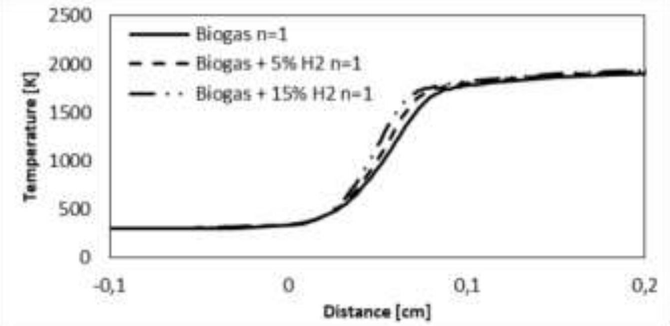

Fig. 2. Temperature profile of the reaction zone for biogas/H_2 mixtures with n = 1

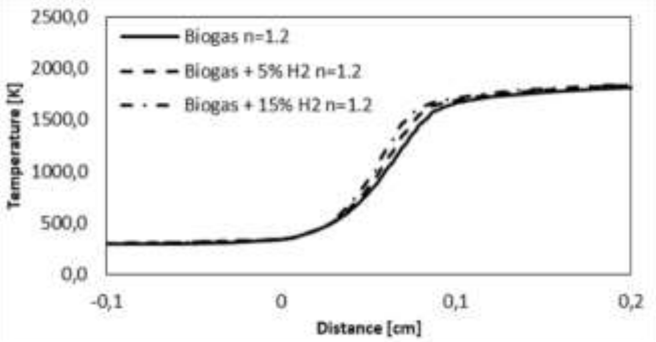

Fig. 3. Temperature profile of the reaction zone for biogas/H_2 mixtures with n = 1.2

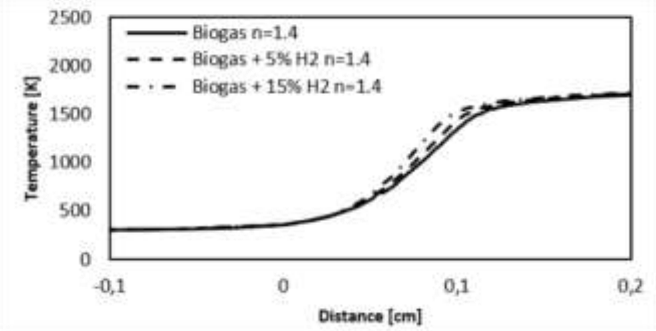

Fig. 4. Temperature profile of the reaction zone for biogas/H_2 mixtures with n = 1.4

As can be seen, the hydrogen addition to the biogas generates an acceleration of the combustion reaction. This being reflected in higher temperature gradients in the reaction zone and resulting in higher rates of heat release, which ultimately cause less thickness of the reaction zone, which is indicative of the increase in the flame speed [42,43]. The temperature profile for pure biogas of this work agree with results shown in [34]. In Figs. 5-7, it can be observed the effect of hydrogen addition in heat release rate of combustion reactions.

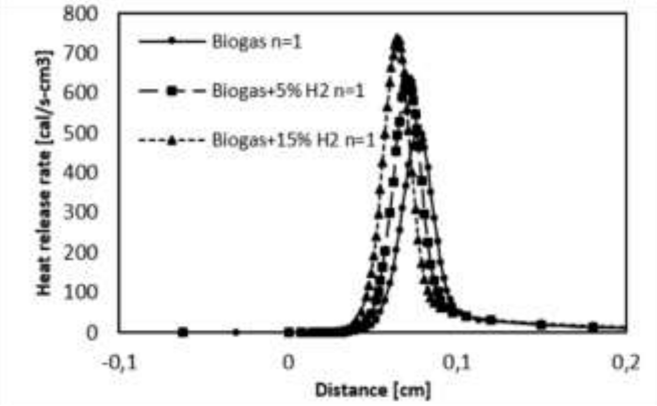

Fig. 5. Heat release rate for biogas/H_2 mixtures with n = 1

For stoichiometric mixtures, pure biogas presents a value of this maximum heat release rate of 508 cal/s-cm^3. Addition of 5% of hydrogen causes a maximum rate of heat release of 634 cal/s-cm^3 and an addition of 15% of hydrogen generates a maximum rate of heat release of 738 cal/s-cm^3. This increase in this parameter is reflected in the flame speed.

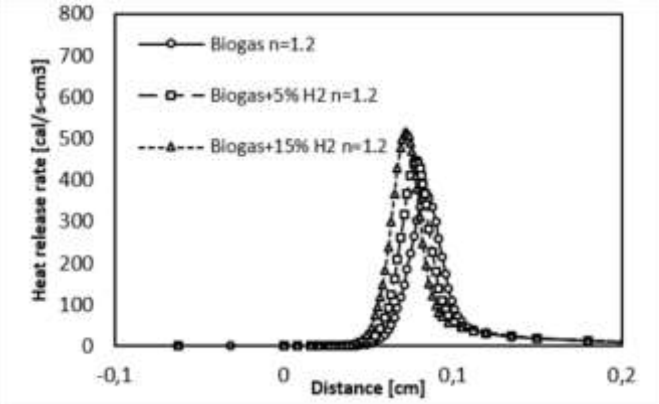

Fig. 6. Heat release rate for biogas/H_2 mixtures with n = 1.2

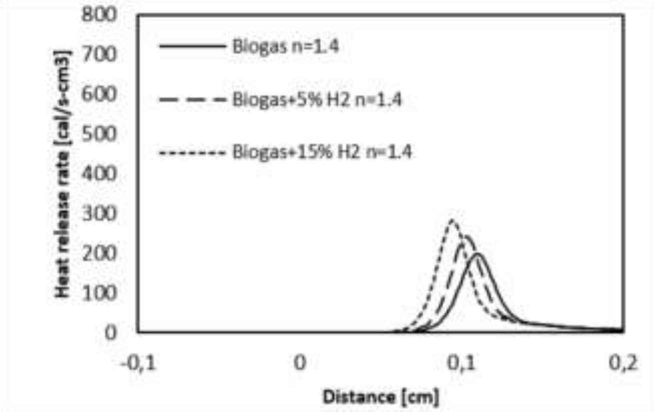

Fig. 7. Heat release rate for biogas/H_2 mixtures with n = 1.4

For the biogas/H_2 mixtures with aeration factor n = 1.2, it can be seen that the maximum value of the heat release rate for pure biogas is 366 cal/s-cm^3, increasing to 446 cal/s-cm^3 for mixing with 5% H_2 and 516 cal/s-cm^3 for mixing with 15% H_2. In this case, the increase in the rate of heat release presents a less noticeable increase than in the stoichiometric flame, as it is also observed in the flame speed. Finally, for lean flames (n = 1.4), the values of the heat release rate have values from 199 cal/s-cm^3 for pure biogas and 243 cal/s-cm^3 and 283 cal/s-cm^3 for Mixtures with 5% H_2 and 15% H_2 respectively. Reported value for heat release rate in [10], for a stoichiometric flame of biogas with 25% CO_2 is near to 800 cal/s-cm^3 and for an aeration factor of 1.25, is reported a heat release rate near of 570 cal/s-cm^3, indicating a similar trend in this results. For a similar biogas used in this work, the reported value of heat release rate in [18] agrees with the result obtained in this work, approximately 500 cal/s-cm^3.

As noted, the increase in the rate of heat release in these lean mixtures is less noticeable in absolute terms but similar in percentages (45% for stoichiometric mixture, 40% and 42% for lean mixtures). Furthermore, a little displacement in the coordinate where the reaction is developed is observed as hydrogen percentage increases, indicating the possibility of flame instability.

The relation between temperature profile and heat release rate is shown in Figure 8 and Figure 9 for stoichiometric mixtures and lean mixtures respectively.

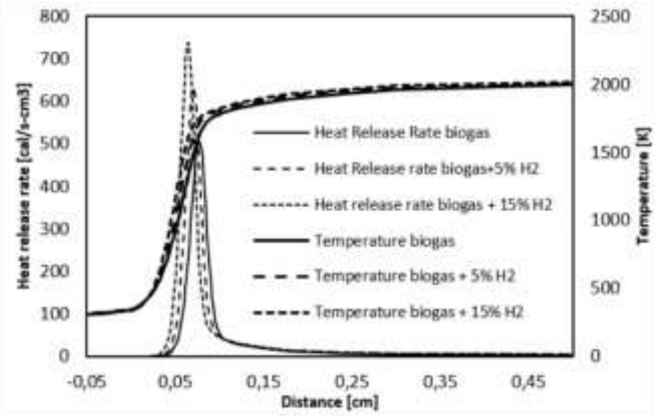

Fig. 8. Temperature profiles and heat release rate for biogas/H_2 mixtures with n = 1

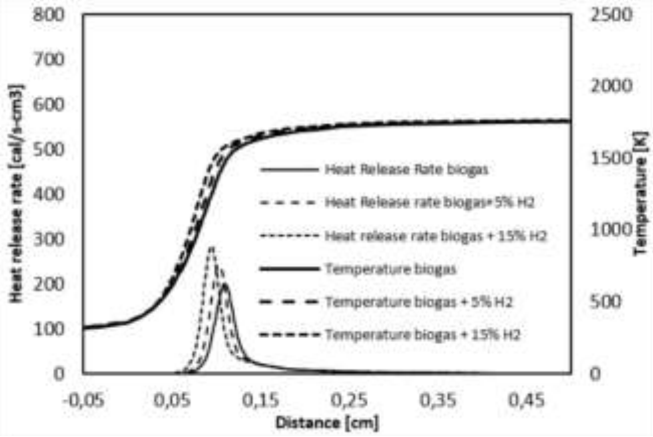

Fig. 9. Temperature profiles and heat release rate for biogas/H_2 mixtures with n = 1.4

As we can see, the hydrogen addition has a more important effect in stoichiometric mixtures but only this effect is noticeable in the heat release rate. The temperature profile remains almost unaltered for biogas/H_2 mixtures in each simulated aeration factor.

Regarding chemical species, hydrogen addition has a significant effect on the decreasing of carbon dioxide emission. In Figs. 10 and 11 it can be observed the effect in carbon dioxide emission of hydrogen addition to biogas for stoichiometric and lean mixtures respectively.

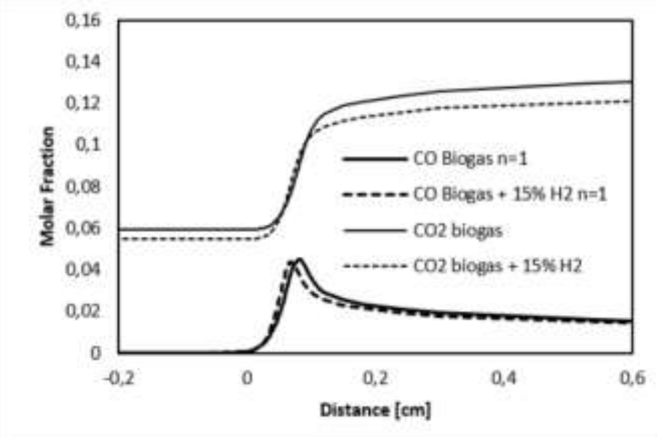

Fig. 10. CO and CO_2 profile for biogas/H_2 stoichiometric mixtures n=1

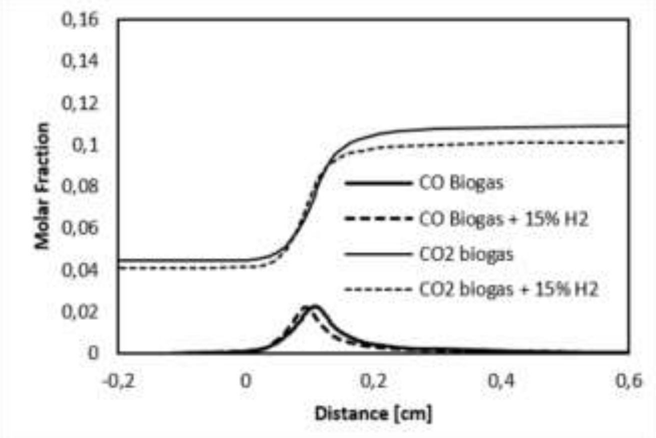

Fig. 11. CO and CO_2 profile for biogas/H_2 lean mixtures n=1.4

Hydrogen addition has not a significant effect in carbon monoxide emission under the adiabatic combustion supposition used. Similar results for CO and CO_2 concentration is presented in [10] for stoichiometric combustion of a 50% CH_4/CO_2 biogas. Finally, the effect in NO formation is shown in Figure 12. Only results for stoichiometric mixtures are shown due to for lean mixtures, NO formation is restricted by lower temperatures obtained. These conditions prevent the activation of the NOx formation zeldovich thermal mechanism, this being the main NOx formation mechanism in the combustion of gases upon the prompt mechanism and the formation mechanism due to the N_2 of the fuel due to the absence of N_2 in the biogas simulated in this work [44-47].

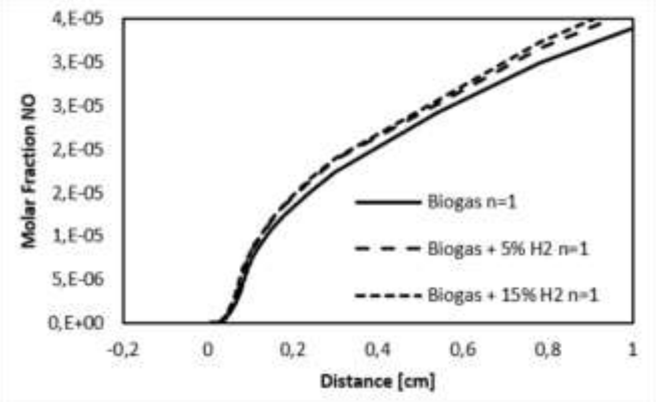

Fig. 12. NO profile for biogas/H_2 stoichiometric mixtures n=1

As can be seen, hydrogen addition to biogas may generate an increase in NO formation; however, this increase is only appreciable for stoichiometric conditions. It may be due to the higher temperature gradients and heat release rates obtained with the hydrogen addition. These conditions activate the Zeldovich thermal mechanism of NO formation how was explained before.

4. Conclusions

In this work, the laminar flame speed and flame structure of biogas and biogas/H_2 mixtures have been studied numerically under normal conditions. The results obtained shown the influence of hydrogen addition and the aeration rate on the laminar flame speed and flame structure of the mixtures studied.

The main results allow us to conclude that the laminar flame speed of the biogas under normal conditions and stoichiometric conditions reaches a value of 27.4 m/s. The addition of hydrogen allows increasing this velocity to values of 32.17 m/s with a 15% addition of H_2, implying an increase of up to 16% of this parameter. However, under lean conditions, the increase in laminar flame speed between pure biogas and the addition of 15% H_2 only reaches approximately 5% according to results presented. The increase in the laminar flame speed can be divided into two zones, one close to stoichiometric mixtures where a significant increase is observed and another one of lean mixtures where this increase is less noticeable. This indicates that the addition of hydrogen to biogas can facilitate the use of biogas/H_2 mixtures in replacement of other gases such as natural gas or LPG under conditions close to stoichiometric combustion but for conditions of high aeration of other gases, where their laminar flame speeds may be similar to those obtained for biogas/H_2 mixtures.

The addition of H_2 to the biogas generates an increase in the kinetics of the reaction. This is reflected in the higher temperature gradients in the reaction zone of mixtures with higher H_2 content and higher rates of release of heat in the reaction zone. It can be seen a different behavior to the laminar flame speed (where there is a relative increase), since in mixtures close to the stoichiometric one has an increase in this rate of up to 45% according to the results obtained and of 40% and 42% in lean mixtures.

Finally, the hydrogen addition to biogas has an effect of decreasing of carbon dioxide concentration in the flue gas, which can be seen as a beneficial effect in the reduction of emissions of greenhouse gases, however, the hydrogen addition has not and appreciable effect on carbon monoxide concentration for stoichiometric and lean conditions. The higher temperature gradients and heat release rate obtained with hydrogen addition cause a higher NO concentration in biogas flames and a displacement of the reaction zone toward reactants, which can create problems of flame instability due to the higher laminar flame speed of hydrogen.

Acknowledgements

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