Ignition delay time measurements behind reflected shock-waves for a representative coal-derived syngas with and without NH_3 and H_2S impurities

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Abstract

The composition of a representative coal-derived syngas was determined by averaging 40 practical coal syngas compositions from the literature and corresponds to a departure from many recent studies which only focus on syngas blends containing just CO and H₂. Ignition delay times have been measured behind reflected shock waves for this averaged mixture with an equivalence ratio of 0.5 (0.4554% CO / 0.3297% H₂ / 0.1032% CO₂ / 0.0172% CH₄ / 0.2407% H₂O / 0.8538% O₂ in 98% Ar (mol. %)) at around 1.7, 13, and 32 atm. The same mixture was also investigated with impurities (200 ppm of NH₃ and 50 ppm of H₂S). Care was taken when working with the blends containing H₂O and NH₃ to avoid errors in the shock-tube composition; direct measurement of the water vapor mole fractions were performed using a tunable diode laser absorption diagnostic near 1.38 μm . The effect of the various constituents on the ignition delay time was also investigated by comparing to results from a baseline mixture (H₂/CO/O₂/Ar) and results with this baseline mixture with only one of the other constituents of the syngas (*i.e.* CO₂, CH₄, H₂S). Experimental data were compared with recent detailed kinetics mechanisms from the literature. Results showed that, under the conditions of this study, extending the mixture composition to include realistic concentrations of species beyond just the CO and H₂ does not have a very large effect on the ignition delay time for a coal-derived syngas. However, a comparison of this coal-derived syngas with a syngas derived from biomass, tested in an earlier study by the authors, exhibited large differences due to the larger CH₄ concentration in the bio-derived syngas. Two chemical kinetic models from the literature were found suitable to reproduce these data over most of the range of mixtures, temperatures, and pressures investigated, namely the mechanisms associated with Galway and with Princeton.

Keywords: Syngas, coal, ignition delay time, shock-tube, high pressure

1 Introduction

Coal has been used as a source of energy for several centuries but has long been criticized because of the release of toxic products (sulphur-containing compounds and oxides of nitrogen, or NO_x) during its combustion, in addition to the production of CO₂. With natural coal reserves being larger than oil and gas, it is however anticipated that energy production from coal will continue for many years to come. Hence, because of environmental concerns, methods have been developed to use coal as a cleaner energy source. One method is to convert coal into synthetic gas (syngas), a process that allows for the removal of most of the particulates, along with sulphur and NO_x compounds.

Ideally, syngas is mostly composed of H₂ and CO, in various proportions, but real syngas can also contain small hydrocarbons, H₂O, N₂, and CO₂ in reasonable amounts as well as traces of undesirable impurities such as NH₃ and H₂S [1]. These variations in syngas composition are due primarily to the large variety of feedstock and production processes. The compositional variation leads to a large deviation in combustion properties, which, in turn, makes the optimization of stable, high-efficiency gas turbines challenging [2]. To better optimize gas turbines, well-validated chemical kinetics models for realistic mixtures are therefore desirable. Unfortunately, there are very few data on complex, realistic syngas compositions to help in validating these models.

While H₂/CO mixtures have been studied in numerous conditions (see Mathieu et al. [1] and references therein), more-realistic mixtures have hardly been investigated. Indeed, aside from the addition of CO₂ [3-5], N₂ [6], H₂O [7], CH₄ [8], or NH₃ [8] to CO/H₂, only a syngas derived from a wood gasification process [9] and a bio-syngas averaged from real compositions [8] were studied, both in shock tubes. The comparison between a binary CO/H₂ fuel blend and realistic practical bio-syngas mixture with the same CO/H₂ ratio and under the same conditions in the previous study by

the authors [8] showed important differences in terms of ignition delay time (τ_{ign}) and stressed the importance of studying complex, realistic mixtures to validate models. The aim of the present study was therefore to extend the earlier work by the authors toward ignition delay time measurements for a realistic, coal-derived syngas. A practical coal syngas was derived by averaging the compositions of 40 real coal-syngases (see Mathieu et al. [1]), leading to a 40/60 ratio between H_2 and CO and the presence of CH_4 , CO_2 , and H_2O in the fuel blend. The effect of these components was investigated by adding them individually to the baseline H_2/CO mixture. Finally, the effect of the addition of impurities such as NH_3 and H_2S was studied, on both the baseline CO/H_2 and the realistic, averaged, fuel blend. Note that mixtures of H_2/CO with H_2O or NH_3 have already been investigated in Mathieu et al. [8], at identical conditions. Since the results from that study did not show any appreciable effect of these two species on τ_{ign} , the individual effects of H_2O and NH_3 addition on the binary baseline mixture were not investigated in the present study.

Mixtures were studied in dilute conditions, to avoid non-ideal ignition behaviour observed with real fuel-air mixtures [5], and at an equivalence ratio (ϕ) set to 0.5 to be representative of lean conditions in gas **turbines**. In addition, the authors have shown in previous studies that the ignition behaviour of hydrogen-based fuel blends is not very dependent on the stoichiometry for equivalence ratios between about 0.3 and 2.0 [10-11]. Three pressure conditions were investigated: around 1.7, 13, and 32 atm. The details of the mixture composition are provided in Table 1.

The setup used during this study is presented in the next section, followed by the experimental results. These data are then compared to recent detailed kinetics models from the literature. Results are then discussed in terms of a chemical analysis derived from the detailed kinetics modeling.

2 Experimental setup

2.1. Shock tube

Ignition delay times were measured behind reflected shock waves (RSW) in a single-diaphragm, stainless steel shock tube (15.24-cm i.d., 4.72-m long and 7.62-cm i.d., 2.46-m long for the driven and driver sections, respectively). The wave speed, extrapolated to the endwall, was measured using five PCB-P113A pressure transducers to determine post reflected-shock conditions in conjunction with the one-dimensional shock relations. The uncertainty in the temperature behind the RSW (T_5) was proven to be maintained below 10 K using this method [12]. A Kistler 603-B1 transducer, located in the same plane as the sapphire observation window (16 mm from the endwall), and a PCB-134A transducer, located at the endwall, were used to monitor the test pressure. Polycarbonate and pre-scored aluminum diaphragms were used for experiments up to 13 atm and 32 atm, respectively. Further details on the shock tube are available in Aul et al. [13].

Test mixtures were prepared manometrically in a stainless steel mixing tank. The gases were passed through a perforated tube traversing the mixing tank to allow for rapid, turbulent mixing. The test section was evacuated to 2×10^{-5} Torr or better before each experiment. The possible formation of FeCO_5 from the CO cylinder was minimized using a gas cylinder made of aluminium and a gas supply tubing of Teflon from the bottle to the experiment. Since NH_3 adsorbs on stainless steel [14], the mixing tank and shock-tube surfaces were passivated before each mixture preparation and experiment. The passivation method was as follows: introduction of around 100 torr of NH_3 for at least 5 minutes and then vacuuming for 5 minutes with the rough pump (until around 30-40 mtorr, typically) before filling the driven tube with the mixture (or the mixing tank with the mixture components). Care was also taken for the mixtures containing water vapour to ensure that there was no condensation or other losses in water between the mixing tank and the shock tube; details on the

water monitoring diagnostic are presented later in this paper. Conditions investigated during this study are summarized in Table 2, and typical ignition delay time measurements along with corresponding conditions behind RSW are provided as supplementary material.

2.2 Ignition delay time setup

The ignition delay time was defined as the time between the passage of the RSW and the intersection of lines drawn along the steepest rate-of-change of OH* de-excitation and a horizontal which defines the zero-concentration level, as documented in Mathieu et al. [15]. The OH* chemiluminescence was followed at the sidewall location using an interference filter centered at 307 ± 10 nm with a Hamamatsu 1P21 photomultiplier tube.

Uncertainties in τ_{ign} are predominantly due to the uncertainty in T_5 determination. This leads to uncertainty on τ_{ign} between around 10% below 15 atm and 20% at around 30 atm. The uncertainty associated with the determination of the steepest slope from the OH* time history profile is negligible compared to the T_5 determination. Note that the reported uncertainty takes into account the non-ideal boundary layer effects measured by the change in pressure (dp/dt) behind the RSW (less than 2%/ms during this study and in other hydrogen-based studies from our group with similar dilution levels [10-11]). Due to the dilution level used, these non-ideal effects are mainly due to the facility and not to any heat release from chemical reaction. Some representative OH* and pressure profiles are provided as supplementary material.

2.3 Measurements with the H₂O absorption diagnostic

To ensure that the mixture being shock heated is really the mixture that was made in the mixing tank, the amount of water vapour in the shock tube needed to be measured. There are at least 3 possible mechanisms for creating uncertainty in the final water partial pressure in the tube: 1) adsorption onto the shock-tube walls; 2) local, transient condensation within the tube while filling (if gas compression makes the local water partial pressure above the vapor pressure); and, 3) expansion of the mixture when moving from the higher-pressure mixing tank to the shock tube under vacuum, causing local condensation due to low temperatures. The best way to measure the amount of water vapor in the tube is to measure it directly, **prior to run the experiment**, using laser-light absorption at frequency ν governed by the Beer-Lambert relation, $I_T/I_0 = \exp(-k_\nu P X_i L)$, which describes the relation between the ratio of the transmitted (I_T) and incident intensity (I_0); the spectral absorption coefficient k_ν ($\text{atm}^{-1} \text{ cm}^{-1}$); pressure, P (atm); mole fraction of the absorbing species i , X_i ; and path length, L (cm). The light source was a Toptica Photonics DL100L tunable diode laser (TDL) with a DC 110 laser controller, operated near $1.38 \mu\text{m}$ and used to measure water absorption in the $\nu_1 + \nu_3$ transition band of H_2O near 1387.877 nm .

The spectral parameter k_ν was calculated for H_2O using HITRAN 2004 and a Voigt fit for the spectral line to account for Doppler and collision broadening. The argon broadening coefficients were not obtainable by HITRAN but were estimated for the selected transitions by using an argon-to-air broadening ratio described by Negali et al. [16] near 1405 nm . A schematic of the optical diagnostic setup is visible in the supplementary material. The incident laser beam was split three ways: into a Burleigh WA-1000 wavemeter with an uncertainty of $\pm 1.0 \text{ ppm}$, into a Newport 2317 Large-Area Balanced Photoreceiver with bandpass filters centered at $1384 \pm 5 \text{ nm}$ (I_0), and through the shock tube and onto another Newport 2317 Photoreceiver (I_T). An adjustable polarizer on the incident side was used to balance the incident and transmitted signals prior to filling the tube with a mixture containing water. A DI-158U DAQ system monitored the output from the photoreceivers.

Two separate, custom-made boxes isolated the incident and transmitted sides, and nitrogen was purged into the boxes to prevent ambient water vapor from interfering with the measurement. In addition to the WA-1000 wavemeter, the selected transition line was validated by analyzing the absorption using pure water vapor as described by Barrett [17].

Measurements of the water partial pressure in the shock tube were performed over the range of fill pressures utilized during experiments. The Csyn mixture was used to fill the tube, and the results are shown in Fig.1, which compares the TDL-measured water partial pressure with the mixture partial pressure (from the tank). As shown, the slope of the line fit in Fig.1 produces the measured mole fraction of 0.0023, which compares well, within 5%, with the target value of 0.0024 and is within the uncertainty of the TDL measurement. It can therefore be concluded that there is no appreciable uncertainty in the water content of the mixtures studied herein.

3 Results

3.1 Coal syngas composition effect on the ignition delay time

The effects of syngas composition on τ_{ign} at the lowest pressure investigated are visible in Fig.2. As can be seen, the ignition delay times for the baseline 60 CO/40 H₂ mixture are slightly longer, between 10 and 50% (for high and low temperatures, respectively), than for the neat H₂ mixture. An addition of CO₂ to the BS mixture does not change the ignition delay time, whereas the addition of a small concentration of methane seems to bring τ_{ign} closer to the neat hydrogen data. Although H₂S was introduced at a very small concentration (Table 1), it has a noticeable effect on τ_{ign} . Indeed, τ_{ign} is increased by nearly 2 at 1050 K and by around 35% at 1785 K, compared to the BS mixture. The results for the realistic coal syngas mixture are between those of the neat H₂ and BS mixtures, indicating only a small influence of the CO₂, CH₄, and H₂O addition under these

conditions. Noticeable changes are observed for the Csyn blend in the presence of both impurities (NH_3 and H_2S) via the Csyn-imp mixture in Fig. 2; τ_{ign} is increased by 50% at the lowest temperature investigated and decreased by around 25% at 1740K.

At around 13 atm, Fig.3, the difference between the neat H_2 and the BS mixture is more important than at 1.7 atm. Indeed, if τ_{ign} remains the same or nearly so at the lowest temperature investigated, the addition of CO nearly doubles τ_{ign} at 1245 K. However, it is interesting to note that the CO_2 , CH_4 , and H_2S additions did not affect τ_{ign} at 13 atm. On the other hand, the realistic mixture (Csyn) shows some noticeable differences above 1200 K, where the ignition delay time is shorter than for the baseline mixture with just CO and H_2 (up to a factor around 2). In the presence of impurities (i.e., Csyn-imp), the reduction in τ_{ign} is still observed but seems to be slightly reduced compared to what was seen at 1.7 atm.

At the highest pressure investigated, Fig.4, results are mostly the same for the neat H_2 , the BS, and the BS- H_2O , BS- CH_4 and BS- H_2S mixtures below 1200 K. Above this temperature, ignition delay times tend to be longer than for the neat H_2 mixture (up to around 30% at the highest temperature investigated). For the Csyn mixture, τ_{ign} are similar to the baseline mixture below 1200 K. Above this temperature, ignition delay times seem to be longer by about 35 to 50%. It is worth noting that the addition of H_2S alone to the H_2/CO baseline fuel blend decreases τ_{ign} below 1250 K. This effect is however almost not observed at all for the full mixture with impurities (Csyn-imp).

3.2 Pressure and syngas composition effects on the ignition delay time

Since results for the coal syngas investigated in the present study have been obtained under similar conditions (same ϕ , pressure range, and dilution level) to the bio-syngas investigated in Mathieu et al. [8], results were compared in Fig.5 to determine the relative importance of the syngas composition on τ_{ign} . As can be seen, the difference is relatively large between these two types of syngases. At the lowest pressure investigated, τ_{ign} for the bio-syngas are indeed between 50% (high temperatures) and 75% (low temperatures) longer than for the coal-syngas blend. This difference is even larger at around 13 atm where a factor between 3 (high temperatures) and 5 (low temperatures) was observed. For the highest pressure investigated, however, there is no appreciable difference between the two fuel blends. Since the ignition delay times are very close between a 50/50 and a 60/40 CO/H₂ ratio (baseline bio- and coal-syngas, respectively) [11], and since both H₂O and CO₂ addition did not exhibit any significant effect on τ_{ign} (this study and Mathieu et al. [8]), one can conclude that the differences in τ_{ign} between the bio- and coal-syngas are primarily due to the CH₄ concentration, which is around 5.2 times higher in the bio-syngas mixture. For reference, the composition of the bio-syngas mixture was 0.0029659 CO / 0.0029659 H₂ / 0.0015748 CO₂ / 0.0008924 CH₄ / 0.0020997 H₂O / 0.0095013 O₂ / 0.98 Ar (mol.) [8].

Fig.5 also allows visualizing the effect of pressure on τ_{ign} for the Csyn mixture. As can be seen, the increase in pressure has a significant and distinctive effect on τ_{ign} . When compared to typical hydrocarbon fuels, where an increase in pressure typically decreases τ_{ign} for a given temperature [18], the behavior observed from an increase in pressure for these syngas mixtures corresponds to what is commonly observed with H₂ mixtures [10]. That is, significant changes of slope on an Arrhenius plot are observed depending on the pressure condition. For example, below 1150 K, τ_{ign} are notably longer for the 13-atm case than for the 1.7-atm condition, while τ_{ign} are higher for the 32-atm data than for the 13-atm data. This pressure dependence is similar for baseline,

realistic, and pure-H₂ fuels (Figs.2-4), indicating that the H₂ chemistry dominates under these conditions, even in the presence of the small amount of CH₄ in the Csyn fuel blend.

3.3 Comparison with detailed kinetics models from the literature

The data herein were compared to predictions from detailed chemical kinetics mechanisms from the literature: the C0–C4 mechanism from Wang et al. [19] (USCII), the C1 model from Li et al. [20] (PRCT), the mechanism from Konnov [21], and the C0–C3 mechanism from Metcalfe et al. [22] (NUIG). When necessary, the OH* sub-mechanism from Hall and Petersen [23] was merged with each model since OH* was used in the experiments to determine τ_{ign} . Results are visible in Fig.6 for the baseline CO/H₂ (BS) ((a)-(c)) and for the neat coal syngas (Csyn) ((d)-(e)) mixtures. The comparisons amongst the models and the other data are visible in the supplementary material section. Note that none of the models used herein contain a H₂S or a NH₃ sub-mechanism (except Konnov [21] for NH₃). Since a H₂/H₂S mechanism has been recently validated in similar conditions by Mathieu et al. [15] with the same H₂ chemistry as used in the NUIG model, these two mechanisms were merged together along with the OCS mechanism from Glarborg and Marshall [24], to account for possible CO/H₂S interactions. However, since adding and validating the NH₃ sub-mechanism to the models is beyond the scope of this study, no model comparison was made for the Csyn-imp mixture containing NH₃.

As can be seen in Figs.6 (a) and (d), the low-pressure data are correctly reproduced by the models. The models of NUIG, PRCT, and USCII are however slightly under-reactive. The model of Konnov is closer to (d) or even perfectly reproduces (a) the experimental results for the baseline mixture at 1.65 atm. At 11 atm, the models from NUIG and PRCT still yield nearly the same result. Data for the baseline mixture (b) are almost perfectly reproduced by these two models, while the

trend is also well captured by the models from Konnov and USCII. For the Csyn mixture (e), the trend is captured by the models but τ_{ign} is over-predicted by a factor 2 above 1200 K. Below this temperature, the USCII model is in agreement with the data, while the NUIG and Li et al. models are slightly over-predicting τ_{ign} . The ignition delay times computed with Konnov's model tend to be too short at the lowest temperature investigated for this intermediate-pressure condition.

At 32 atm, the baseline data (c) are well reproduced by the NUIG and PRCT models. The experimental trend is correctly predicted by the USCII mechanism, but τ_{ign} are too short. The model of Konnov is significantly too reactive for temperatures below 1250 K. For the Csyn mixture (f), the NUIG model reproduces the data nearly perfectly. Very good agreement was also observed with the PRCT model, for which τ_{ign} are slightly shorter than for the NUIG model. As for the baseline mixture, the USCII model reproduces the experimental trend but is too reactive, while the model from Konnov is significantly excessively reactive above 1250 K. Overall, this study shows that the models from Metcalfe et al. [22] and Li et al. [20] seem most suitable to model τ_{ign} for syngas mixtures over the entire range of conditions herein.

A comparison between the BS-H₂S mixture data and the NUIG model merged with H₂S [15] and OCS [22] sub-mechanisms is visible in Fig.7. As can be seen, experimental trends are well captured by this model, although the predicted τ_{ign} are slightly longer than the experimental ones.

Some normalized experimental OH* profiles are compared with the predictions from the models in Supplementary Material.

4 Discussion

The effect of various added species on the ignition delay times of a CO/H₂/O₂ mixture diluted in Ar was investigated in this study. Overall, the impacts of these additions were not significant, with the hydrogen chemistry still being dominant over the conditions investigated. Results were captured and well predicted by recent models from the literature, except for the high-temperature region around 13 atm for the Csyn mixture, where the models were not reactive enough. A similar observation was made by the authors at these same conditions for a biomass-derived syngas [8]. Since the τ_{ign} data are in contrast well predicted at these conditions for the baseline mixtures doped with only CO₂, CH₄, or H₂O, this result could indicate that some interactions could exist between CH₄, CO₂, and/or H₂O when all three exist in a realistic fuel blend (which relates directly or indirectly to OH formation) that are not well considered by the current models **at around 13 atm**.

Concerning the impurities, a lack of effect on τ_{ign} of NH₃ addition to syngas was previously investigated by the authors for a bio-syngas blend [8]. A chemical analysis showed that NH₃ does not react appreciably prior to the ignition event. However, computations showed that a significant proportion of NH₃ is subsequently converted to NO, which can induce important changes in the combustion properties in case of a burned-gas recirculation strategy.

Some effects were observed with H₂S addition (BS-H₂S mixture), notably at low temperature for the lowest- (increase in τ_{ign} with H₂S addition) and highest-pressure (decrease in τ_{ign}) cases. These effects were investigated using sensitivity and reaction pathway analyses. For the low-pressure case, the analysis showed that the decrease in the reactivity is mostly due to the reaction $\text{H}_2\text{S} + \text{H} \rightleftharpoons \text{SH} + \text{H}_2$, which inhibits the most-sensitive reaction $\text{H} + \text{O}_2 \rightleftharpoons \text{OH} + \text{O}$ by competing for H atoms. The complete mechanism for the increase in the reactivity at low temperature/high pressure was detailed

in Mathieu et al. [15]. Note that there is no reaction involving CO and any sulfur-containing species among the 10 most-sensitive reactions under these conditions.

5 Summary and Conclusions

To help in model validation and in designing efficient gas turbines, ignition delay times of a realistic coal-derived syngas mixture (containing CO / H₂ / CH₄ / CO₂ / H₂O and O₂) diluted in Ar were measured between 1.7 and 32 atm in a shock tube. Results showed a significant effect of pressure on τ_{ign} due to the hydrogen chemistry that dominates the ignition kinetics over these conditions. Compared to a baseline mixture with the same CO/H₂ ratio, small variations in τ_{ign} were observed with the realistic syngas mixture, but only for certain conditions. A small decrease in τ_{ign} was observed at around 1.7 atm over the range of temperature investigated. This decrease was relatively important above 1200 K at around 13 atm. For the highest pressure investigated, a small increase in τ_{ign} was observed between the Csyn and the BS mixtures above 1200 K. This increase in τ_{ign} was predicted by recent models from the literature, whereas the decrease in τ_{ign} above 1200 K at 13 atm for the Csyn mixture was not well predicted by the models. Overall, the models from Metcalfe et al. [22] and Li et al. [20] were able to predict the experimental trends and the ignition delay times with the greatest accuracy over the whole range of conditions. The comparison between the results of the present study and measurements for a biomass-derived syngas [8], which contains a higher concentration of methane, showed that ignition delay times are notably longer for the bio-derived syngas at some conditions.

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Table caption:

Table 1: Composition of the mixtures investigated in the shock tube, in % volume.

Table 2: Experimental conditions investigated behind RSW. Fuel names are as defined in Table 1.

List of tables

Table 1: Composition of the mixtures investigated in the shock tube, in % volume.

Mixture	% H ₂	% CO	% O ₂	% CH ₄	%CO ₂	% H ₂ O	%NH ₃	% H ₂ S	% Ar
Neat H ₂ [10]	1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	98.0
BS [11]	0.40	0.60	1.0	0.0	0.0	0.0	0.0	0.0	98.0
BS-CH ₄	0.385	0.578	1.022	0.015	0.0	0.0	0.0	0.0	98.0
BS-CO ₂	0.38	0.57	0.96	0.0	0.09	0.0	0.0	0.0	98.0
BS-H ₂ S	0.4	0.6	1.0	0.0	0.0	0.0	0.0	0.005	97.995
Csyn	0.3297	0.4554	0.8538	0.0172	0.1032	0.2407	0.0	0.0	98.0
Csyn-imp	0.3297	0.4554	0.8538	0.0172	0.1032	0.2407	0.02	0.005	97.975

Table 2: Experimental conditions investigated behind RSW. Fuel names are as defined in Table 1.

Mixture	T_5 (K)	P_5 (atm)	Source
Neat H_2	960-1625	1.65, 13.3, 32.8	[10]
BS	1015-1845	1.73, 12.6, 31.5	[11]
BS- CO_2	1025-1875	1.75, 12.9, 31.5	This study
BS- CH_4	1010-2010	1.71, 12.9, 31.7	This study
BS- H_2S	1050-1785	1.85, 13.0, 32.6	This study
Csyn	1050-1705	1.85, 13.2, 32.6	This study
Csyn-imp	1050-1740	1.84, 12.9, 33.0	This study

Figure captions:

Figure 1: Measured water partial pressure compared to the tank mixture value over a range of typical shock-tube fill pressures.

Figure 2: Composition effect on the ignition delay time at around 1.7 atm. Fuel mixtures are defined in Table 1.

Figure 3: Composition effect on the ignition delay time at around 13 atm. See Table 1 for fuel compositions.

Figure 4: Composition effect on the ignition delay time at around 32 atm. Fuel compositions are in Table 1.

Figure 5: Comparison between the ignition delay times of a coal- and biomass-derived syngases at around 1.7, 13 and 32 atm.

Figure 6: Comparison between experiments and models for the BS mixture at around 1.7 (a), 13 (b), and 32 atm (c) and for the Csyn mixture at around 1.7 (d), 13 (e), and 32 atm (f). Black line: NUIG [22]. Grey line: PRCT [20]. Black dashed line: USCII [19]. Grey dashed line: Konnov [21].

Figure 7: Comparison between the experiments and the model (H_2/CO from Metcalfe et al. [22], H_2S from Mathieu et al. [15] and OCS from Glarborg and Marshall [24]) for the BS- H_2S mixture.

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