



An assessment of chemical kinetics for bio-syngas combustion



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HIGHLIGHTS

- A kinetic modelling of bio-syngas combustion was performed with three detailed reaction mechanisms.
- Ignition delay times for various blends containing CH₄, CO, CO₂, H₂ and H₂O were computed.
- The agreement for low temperatures and high pressures as well as high temperatures and low pressures is satisfying.
- The poorer match reached otherwise is apparently related to five reactions influential under those conditions.
- The effect of bio-syngas composition on combustion correlated well with experimental observations.

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ABSTRACT

The present work was devoted to assess the chemical kinetic modelling of bio-syngas combustion. Three reaction mechanisms (the Gas Research Institute-mechanism GRI 3.0, its skeletal version DRM22 and Heghes' C₁–C₄ mechanism) were considered for that purpose along with series of ignition delay measurements relevant to the burning of bio-syngas. For experiments involving methane with and without considerably smaller quantities of added hydrogen, the measurements are generally overpredicted by Heghes' mechanism but underpredicted by the GRI and DRM mechanisms. Experiments involving various blends of the bio-syngas constituents were also simulated. The strong discrepancies present for high pressures and temperatures and low pressures and temperatures could be correlated to five reactions which are only influential under those conditions, four of which involving HO₂. The effects of variations in the bio-syngas composition on combustion were numerically investigated by using the GRI-mechanism. Globally it was found that an increase in any of the constituents goes hand in hand with higher amount of CO released. The ignition delay is either shortened or left unchanged as the initial concentration is increased except in the case of methane where it is raised. The results were in good agreement with experimental observations made elsewhere.

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1. Introduction

The profound environmental challenges faced by mankind at the dawn of the new millennium have made it abundantly clear that far-reaching changes in our management of energy are required. The use of renewable resources appears to be a necessary condition for achieving and upholding sustainability [1]. Among these, biofuels have to be considered and investigated with a meticulous care since they hold the promise of ensuring a transition from fossil fuels to sustainable ones [2]. Gaseous fuels from biological sources (such as biogas) are particularly promising since they can be produced from various wastes [3,4]. Biological syngas (generated from the gasification of biomass) is interesting owing to

its thermal efficiency [5] and the cleaner character of its burning in comparison to other fuels [6].

One hurdle hindering its more widespread use consists of its uncertain combustion behaviour due to the presence and interaction of multiple compounds within it. To solve this problem, an economical way would be modelling the complex underlying physical and chemical processes taking place during its combustion in industrial systems. Such a strategy allows to greatly reduce the experimental costs while tremendously increasing (or even enabling in the first place) the reliability of predictions [7]. Given the considerable computational costs involved, computational fluid dynamics (CFD) simulations of real industrial systems necessitates the utilisation of simplified chemical kinetic models [8] which themselves are obtained from the systematic reduction of detailed reaction mechanisms [9–12]. The accuracy and reliability of a reduced model are always inferior to those of the detailed

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parent mechanism. Therefore it goes without saying that the determination of trustworthy and robust detailed reaction mechanisms is a vital step of the whole undertaking. While many such models have been developed for separately accounting for the detailed chemistry of hydrogen, carbon monoxide and methane combustion, few have been determined and evaluated with respect to mixtures of such compounds as they are typically present in bio-syngas. Consequently, the present study was devoted to the evaluation and comparison of three detailed reaction mechanisms when employed for simulating experiments relevant to the combustion of this renewable fuel. In Section 2, bio-syngas and its kinetic modelling are introduced along with the three reaction mechanisms used henceforth. In Section 3 the results of the simulations are shown and discussed. In Section 4 the effects of variations in the bio-syngas composition were numerically investigated with the GRI-mechanism [13]. The conclusion and outlooks of the present work are reported in Section 5.

2. Capturing bio-syngas combustion and its kinetics

2.1. Background

Biogas is produced through the anaerobic degradation of organic material [14] and mainly contains methane and carbon dioxide. Syngas (synthesis gas) is essentially a mixture of carbon monoxide and hydrogen which is used for the synthesis of various products [15]. It is produced to a considerable extent from the gasification of coal. Bio-syngas is a synthetic gas obtained from the thermal gasification of biomass. It contains CO, CO₂, CH₄ and H₂ and is thought to be a cleaner fuel than biogas owing to its higher hydrogen content [6]. Table 1 sums up the typical composition one can find for biogas and bio-syngas [16].

Syngas is viewed as interesting for power generation [17] and to a lesser extent for spark ignition engines due to the increased thermal efficiency it allows [5]. As mentioned, the high hydrogen content of bio-syngas is assumed to imply a cleaner combustion than that achieved with pure methane [6]. Several promising techniques are being developed for ensuring an economically viable production of biogas and bio-syngas [18] which could greatly contribute to sustainability since they are hoped to be CO₂-neutral. The major difference between bio-syngas and syngas is that the former contains a varying amount of CH₄, which is normally absent or negligible in syngas generated out of industrial sources such as coal.

One problem hindering the utilisation of bio-syngas is the huge uncertainties related to the simultaneous presence of the different species in significantly varying amounts [6]. Before the three-dimensional simulation of complex industrial systems might be contemplated, a detailed kinetic understanding of the mixture combustion should be present. Since most reaction mechanisms describing the combustion of methane and other small hydrocarbons found in the literature have been developed and validated for separate fuels following a step-by-step progressive approach, there is (a priori) no warrant that they will be able to deliver reasonable predictions of reactant mixtures as in the case of syngas, let alone bio-syngas [19,20].

Table 1
Typical compositions of biogas and bio-syngas from biomass gasification.

Constituent (volume%)	Biogas	Bio-syngas
CH ₄	50–75	8–11
CO ₂	25–50	21–30
CO	–	28–36
H ₂	0–1	22–32
N ₂	0–10	–

This concern has led several authors to develop and experimentally validate detailed reaction mechanisms specially tailored for capturing the complex interactions taking place between carbon monoxide and hydrogen [21–23]. Such mechanisms can then be reduced to obtain models sufficiently simple for their use in CFD methodologies including direct and large-eddy simulations [24]. The current literature about the kinetics of bio-syngas combustion (the composition being reported in Table 1) is still very scarce. Gersen et al. [25] simulated the combustion of mixtures containing H₂, CH₄, CH₄–CO, CH₄–H₂ and CH₄–CO–H₂ in the absence of CO₂ for the temperature range 900–1100 K and pressure range between 20 and 80 bar. Mathieu et al. [26] carried out shock tube experiments concerning the ignition of syngas and bio-syngas of various compositions in the presence and absence of ammonia impurities. They further simulated a small part of their measurements with detailed kinetic models. The present work is part of this endeavour aiming at ensuring trustworthy predictions of the combustion behaviour of bio-syngas in practical industrial systems by first capturing the underlying detailed kinetics in an optimal manner. Its main goal is to assess the bio-syngas related performance of three reaction mechanisms mainly validated for the combustion of methane and higher hydrocarbons.

2.2. Employed reaction mechanisms

Reaction mechanisms suitable for the task at hand need to capture reasonably well the combustion of methane, carbon monoxide and hydrogen. Still, the fact that a given model is successful at describing their separate kinetics and that of syngas combustion does not necessarily entail that it will provide a decent description of that of bio-syngas since the simultaneous presence of all its compounds changes the chemical behaviour of the whole system in a non-linear way. With that complication in mind, three such reaction mechanisms were selected for the present study.

The Gas Research Institute (GRI) mechanism [13] is a model for the simulation of methane combustion which was developed through the systematic optimisation of the kinetic and thermochemical parameters with the surface mapping method (allowing the use of a great number of measurements for the parameter estimation [27,20]). Its performances with respect to the combustion of carbon monoxide and hydrogen are also satisfying. It consists of 325 elementary reactions and encompasses 53 species which accounts for the combustion of H₂, CO, CH₄, N₂ (NO_x formation) as well as reactions between the nitrogen and the hydrocarbons.

The Developed Reduced Mechanism (DRM) 22 [28] is a reduced skeletal mechanism of GRI 3.0 developed using a flux analysis and the conditions

$$R(i) < e(r)|R(\text{ref})| \quad \text{and} \quad |R(i)\delta H(i)| < e(q)Q$$

where $R(i)$ is the rate of reaction i , $R(\text{ref})$ is the rate of a reference reaction (e.g., the maximum rate), $\delta H(i)$ is the enthalpy change of reaction i , Q is the maximum value among all the terms $|R(i)\delta H(i)|$, and $e(R)$ and $e(q)$ are the chosen parameters considerably smaller than unity. The reference rates were produced using the detailed GRI-mechanism. It seemed strongly interesting to compare the performance of the GRI-mechanism with its reduced skeletal

Table 2
Experimental conditions of the hydrogen-enriched methane combustion.

Experiment	X _{H₂}	Temperature range (K)
1		1532–1882
2	7.3E–04	1631–1810
3	5.2E–03	1604–1739

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