



# An investigation of the chemical kinetics of biogas combustion



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## HIGHLIGHTS

- Five reaction mechanisms were used for simulating ignition delay times of biogas.
- Three of the models reproduce reasonably well the ignition delay times of biogas blends.
- The formation of NO and CO has been predicted numerically under numerous conditions.
- The pollutant N<sub>2</sub>O is produced for high pressures and high CO<sub>2</sub> content in lean mixtures.

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## ABSTRACT

Chemical kinetic aspects of the combustion of biogas (containing CH<sub>4</sub>, CO<sub>2</sub> and possibly H<sub>2</sub>) have been investigated. Five reaction mechanisms were considered and tested with respect to the ignition delay times of H<sub>2</sub>–CO<sub>2</sub>–O<sub>2</sub> and CH<sub>4</sub>–CO<sub>2</sub>–O<sub>2</sub> mixtures measured in shock tubes. While the GRI (Gas Research Institute) mechanism 3.0 could not reproduce the first set of measurements, it brought up the best match for the second one directly relevant to biogas. Consequently it was employed for predicting the amounts of CO and NO produced under the same conditions. It was found that for stoichiometric and lean mixtures an increase in the initial CO<sub>2</sub> concentration lowers the production of NO and raises that of CO at higher temperatures. For rich mixtures, the production of NO is far smaller and does not follow this simple pattern. Kinetically, the reaction  $H + CO_2 \rightarrow OH + CO$  plays a greater role in the presence of CO<sub>2</sub> and must hence be accurately known. For some conditions, the environmentally problematic N<sub>2</sub>O is produced. The effects of hydrogen addition on biogas have also been predicted using GRI 3.0. The addition of 2% of H<sub>2</sub> always raises the concentration of produced CO when compared to the mixture without hydrogen. The formation of NO is increased for higher H<sub>2</sub> amounts at  $p = 1$  bar but decreased at  $p = 10$  bar. Overall, the present study supports the viability of the GRI-mechanism for the simulation of biogas combustion.

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## 1. Introduction

In the search for ways to handle global environmental problems, biofuels are hoped to represent a sustainable and environment-friendly alternative to fossil fuels [1,2]. Mainly constituted of 40–75% of methane, 25–55% of carbon dioxide (and possibly 0–10% of hydrogen), biogas is produced out of the fermentation of biomass by anaerobic bacteria. It has been deemed efficient for meeting the rural energy need of developing countries such as Nigeria [3]. Biogas can be produced from organic wastes (including manures), various by-products, and energetic plants. It can be used for the combined generation of heat and electricity, liquid or gaseous fuels as well as hydrogen which can in turn be utilised in fuel cells [4]. Investigations determined that fuel cycle emissions

related to the production and use of biogas can vary by a factor of 3–4 between two biogas systems delivering the same amount of energy [5]. In that context, optimising the combustion of biogas with respect to the amount of produced heat as well as the emission of carbon monoxide can be greatly beneficial. One obstacle hampering its more widespread use is its uncertain combustion behaviour stemming from the interaction of methane, carbon-dioxide and to a lesser extent hydrogen within it. The modelling of its combustion in industrial systems can provide accurate predictions and greatly reduce the experimental costs [6]. Computational fluid dynamics (CFD) simulations of complex industrial systems require reduced reaction mechanisms [7] which can be produced through different techniques such as the Intrinsic Low Dimensional Manifold (ILDM) [8] and Computational Singular Perturbation (CSP) [9] methods. The precision and reliability of such a simplified model are always poorer than those of the detailed parent mechanism. This shows the importance of

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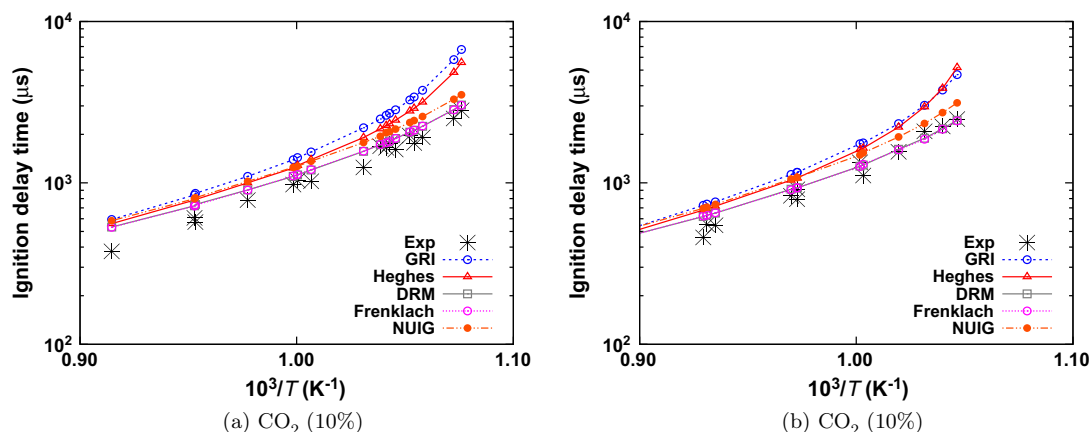


Fig. 1. Ignition delay times for the combustion of hydrogen with and without CO<sub>2</sub> [25].

**Table 1**  
Experimental conditions of Zeng et al. [28].

Run series	Richness	$p$ (bar)	$X_{CH_4}$	$X_{O_2}$	$X_{N_2}$	$X_{CO_2}$
1	0.5	1	0.0499	0.1995	0.7506	0
2	0.5	1	0.0399	0.1596	0.6005	0.2
3	0.5	1	0.0249	0.0998	0.3753	0.5
4	0.5	10	0.0499	0.1995	0.7506	0
5	0.5	10	0.0399	0.1596	0.6005	0.2
6	0.5	10	0.0249	0.0998	0.3753	0.5
7	1	1	0.095	0.19	0.715	0
8	1	1	0.076	0.152	0.572	0.2
9	1	1	0.0475	0.095	0.3575	0.5
10	1	10	0.095	0.19	0.715	0
11	1	10	0.076	0.152	0.572	0.2
12	1	10	0.0475	0.095	0.3575	0.5
13	2	1	0.1736	0.1736	0.6528	0
14	2	1	0.1389	0.1389	0.5222	0.2
15	2	1	0.08680	0.08680	0.3264	0.5

developing or finding accurate detailed mechanisms as the first step of the modelling process. While there are good reaction mechanisms accounting for the combustion of methane and carbon monoxide, there is *a priori* no warrant that they are capable of satisfyingly describing the combustion of mixtures of CO<sub>2</sub> and CH<sub>4</sub> and to a lesser extent H<sub>2</sub>. Therefore it stands to reason that the determination of corresponding reliable and robust detailed reaction mechanisms is a crucial step of the entire enterprise.

The aim of this study is to evaluate how well existing reaction mechanisms can capture the combustion of biogas. It is closely related to a similar work by the same authors [2] concerning the combustion of bio-syngas. In Section 2, reaction mechanisms chosen for the present study are presented. In Section 3, shock tube experiments involving H<sub>2</sub>–CO<sub>2</sub> and CH<sub>4</sub>–CO<sub>2</sub> blends were simulated and the predictions of the five models were compared with experimentally determined ignition delay times. In Section 4, the formation of pollutants (NO and CO) among the above conditions was predicted using the GRI-mechanism. Further, in Section 5, the GRI-mechanism was employed to see what influence the addition of hydrogen has on pollutant formation. Finally, in Section 6 the main results of the present study are emphasized and implications for future works are described.

## 2. Evaluation of reaction mechanisms

A reaction mechanism capable of describing the combustion of biogas (containing methane, carbon dioxide and possibly hydrogen)

must be able to correctly describe the separate combustion of CH<sub>4</sub>, H<sub>2</sub> and CO. However, this is no sufficient condition since the simultaneous presence of methane and carbon dioxide can change the chemical behaviour of the whole system in an unpredictable fashion. Consequently there is a need to evaluate how well reaction mechanisms accounting for the combustion of hydrocarbons perform for the combustion of biogas. The Gas Research Institute (GRI) mechanism [10], The Developed Reduced Mechanism (DRM) 22 [11] and Heghes' mechanism [12] are three detailed reaction mechanisms accounting for the combustion of light hydrocarbons. The readers are referred to our previous publication [2] for their descriptions.

Frenklach et al. [13,14] developed a reaction mechanism accounting for the formation of Polycyclic Aromatic Hydrocarbons (PAH) under rich and pyrolytic conditions. It is based on the GRI-mechanism (version 1.2) complemented by steps describing the formation of ever growing carbonaceous species which are the precursors of the first soot particles. It could reasonably well predict diverse profiles of aromatic species and their intermediates in laminar flames. It has been considered here for investigating if it leads to better predictions for the burning of biogas under rich conditions.

The NUIG (National University of Ireland in Galway) mechanism is a C<sub>0</sub>–C<sub>5</sub> reaction mechanism resulting from a long-term endeavour aiming at determining a reaction mechanism capable of describing the combustion of various hydrocarbons under a wide range of conditions. It has a hierarchical structure and includes H<sub>2</sub>–O<sub>2</sub>, CO–CH<sub>4</sub>, C<sub>2</sub>, C<sub>3</sub>, C<sub>4</sub> and now C<sub>5</sub> submechanisms [15–18]. While the NUIG mechanism has not been specifically tailored to capture the chemistry of H<sub>2</sub>–CO–CH<sub>4</sub>–O<sub>2</sub> blends (such as bio-syngas), it gave remarkably good predictions for CH<sub>4</sub>/H<sub>2</sub>/CO experiments carried out by Gersen et al. [19] in a rapid compression machine. In the bio-syngas experiments performed by Mathieu et al. [20] in shock tubes, the NUIG predictions are often considerably closer to the measurements than those of the GRI-mechanism. Consequently, it was also deemed relevant for the simulation of biogas mixtures. Unlike that of the other four mechanisms mentioned above, its H<sub>2</sub>–O<sub>2</sub> subpart has been separately developed [21] via a thorough comparison with measurements under a greatly varied set of conditions (between 298 and 2700 K, 0.05 and 87 atm, an equivalence from 0.2 to 6 for ignition delay times in shock tube, flame speeds and concentration profiles in flames and laminar flow reactors). Furthermore, it employs the recommended rate expression for the elementary step CO + HO<sub>2</sub> = CO<sub>2</sub> + OH [22] aiming at reconciling the effect of CO in H<sub>2</sub> mixtures on the measured ignition delay times at high pressure.

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